



NAZARBAYEV
UNIVERSITY



NAZARBAYEV
UNIVERSITY
NATIONAL
LABORATORY ASTANA

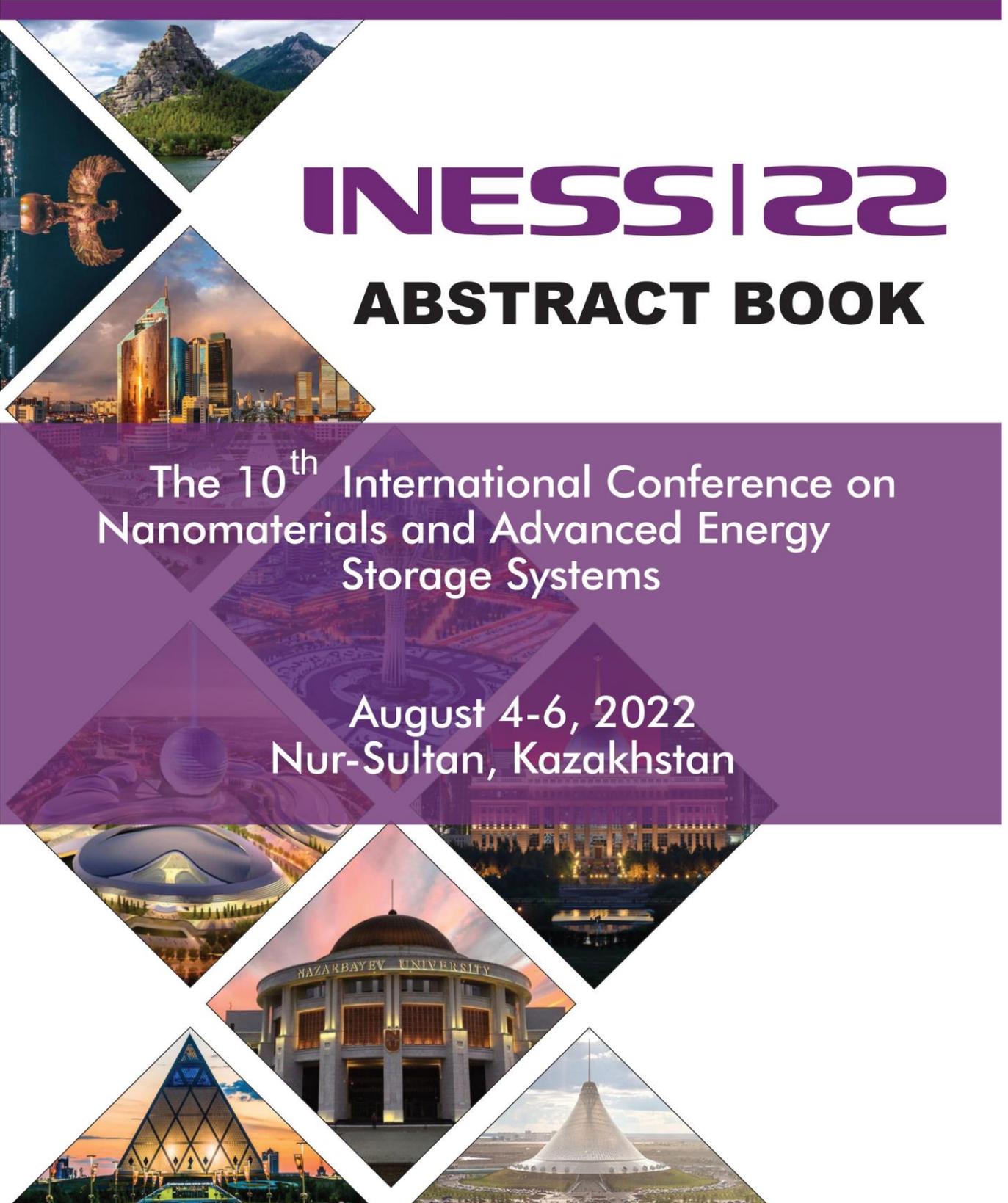


INESSI22

ABSTRACT BOOK

The 10th International Conference on
Nanomaterials and Advanced Energy
Storage Systems

August 4-6, 2022
Nur-Sultan, Kazakhstan



Dear Colleagues!

We greatly appreciate your participation and valuable contribution to our Conference. We are honored and pleased to welcome you at INESS-2022!

The Organizers will put all efforts to make this day at INESS very efficient time to exchange and discuss the ideas, establish and strengthen collaboration in various fields of research. We hope that INESS will serve as an effective platform to establish new opportunities for joint works in science and education for sustainable development and the best future.

We will be looking forward to seeing you again.

Yours sincerely,

On behalf of the Organizers,

Prof. Zhumabay Bakenov

ORGANIZERS

Nazarbayev University

Institute of Batteries LLC

National Laboratory Astana (NLA)

The conference is supported under the targeted research program

#51763/ИЦФ-МЦРОАП РК-19 “New materials and devices for defense and aerospace applications”

funded by Ministry of Digital Development, Innovations and Aerospace Industry of the Republic of Kazakhstan.



NAZARBAYEV
UNIVERSITY



NAZARBAYEV
UNIVERSITY
NATIONAL
LABORATORY ASTANA



ORGANIZING COMMITTEE

Chairman - Prof. Zhumabay Bakenov

Co-Chairman - Vassilios Tourassis

Co-Chairman - Prof. Dos Sarbassov

Scientific Committee

Prof. Sung-Soo Kim

Prof. Yanwei Wang

Prof. Desmond Adair

Prof. Zulkhair Mansurov

Prof. Seung-Taek Myung

Prof. Tayfur Öztürk

Dr. Annie Ng

Scientific Secretary

Dr. Aliya Mukanova

Technical Secretary

Dr. Yer-Targyn Tleukenov

Members

Prof. Almagul Mentbayeva

Prof. Aishuak Konarov

Dr. Arailym Nurpeissova

Dr. Berik Uzakbaiuly

Dr. Gulnur Kalimuldina

Dr. Sandugash Kalybekkyzy

Dr. Bakhtiyar Soltabayev

Dr. Nurzhan Umirov

Dr. Dauren Batyrbekuly

Dr. Ayaulym Belgibayeva

Dr. Fail Sultanov

Dr. Batukhan Tatykayev

Dr. Amanzhol Turlybekuly

Dr. Elmira Nurgaziyeva

Dr. Yerzhan Nurmakanov

Dr. Nurbol Tolganbek

Mr. Bauyrzhan Myrzakhmetov

Ms. Alfiya Kimolayeva

Organization

Institute of Batteries LLP, National Laboratory Astana,
Nazarbayev University, Kazakhstan

Nazarbayev University, Kazakhstan

National Laboratory Astana, Kazakhstan

Chungnam National University, South Korea

National Laboratory Astana, Nazarbayev University,
Kazakhstan

Nazarbayev University, Institute of Batteries LLP,
Kazakhstan

Al-Farabi Kazakh National University, Kazakhstan

Sejong University, South Korea

Middle East Technical University, Turkey

Nazarbayev University, Kazakhstan

Nazarbayev University, Institute of Batteries LLP,
National Laboratory Astana, Kazakhstan

National Laboratory Astana, Nazarbayev University,
Kazakhstan

Nazarbayev University, Kazakhstan

Nazarbayev University, Kazakhstan

NLA, Nazarbayev University, Kazakhstan

NLA, Nazarbayev University, Kazakhstan

Nazarbayev University, Kazakhstan

NLA, Nazarbayev University, Kazakhstan

NLA, Nazarbayev University, Kazakhstan

Nazarbayev University, Institute of Batteries LLP,
Kazakhstan

NLA, Nazarbayev University, Kazakhstan

NLA, Nazarbayev University, Kazakhstan

NLA, Nazarbayev University, Kazakhstan

NLA, Nazarbayev University, Kazakhstan

Nazarbayev University, Kazakhstan

NLA, Nazarbayev University, Kazakhstan

Nazarbayev University, Kazakhstan

Nazarbayev University, Kazakhstan

NLA, Nazarbayev University, Kazakhstan

Institute of Batteries LLP, Kazakhstan

Mr. Nurzhan Baikalov	NLA, Nazarbayev University, Kazakhstan
Mr. Nurbolat Issatayev	NLA, Nazarbayev University, Kazakhstan
Ms. Aizhan Rahmanova	NLA, Nazarbayev University, Kazakhstan
Ms. Assylzat Aishova	NLA, Nazarbayev University, Kazakhstan
Mr. Elnury Baltash	NLA, Nazarbayev University, Kazakhstan
Ms. Uldana Kydyrbayeva	NLA, Nazarbayev University, Kazakhstan
Ms. Aiyman Mashekova	NLA, Nazarbayev University, Kazakhstan
Mr. Arman Umirzakov	NLA, Nazarbayev University, Kazakhstan
Mr. Bagdaulet Shugay	Nazarbayev University, Kazakhstan
Ms. Assel Serikkazyeva	Nazarbayev University, Kazakhstan
Ms. Yerkezhan Yerkinbekova	NLA, Nazarbayev University, Kazakhstan
Ms. Madina Kalibek	Nazarbayev University, Kazakhstan
Ms. Aiman Bissenbay	NLA, Nazarbayev University, Kazakhstan
Ms. Akerke Kanatkyzy	NLA, Nazarbayev University, Kazakhstan
Ms. Aktilek Akhmetova	Nazarbayev University, Kazakhstan
Ms. Anar Arinova	NLA, Nazarbayev University, Kazakhstan
Mr. Islam Rakhimbek	Nazarbayev University, Kazakhstan
Ms. Madina Sarsembina	Nazarbayev University, Kazakhstan
Ms. Nardana Bazybek	Nazarbayev University, Kazakhstan

CONTENT

KEY NOTE		
1.	Rachid Yazami Innovative solutions for LIB management for electric vehicles	11
2.	Zhong Lin Wang The fundamental science and technology applications of triboelectric nanogenerators	11
3.	Kiyoshi Kanamura Research and development on Li ion battery and next generation batteries	12
4.	Seung-Taek Myung Mn-based high-capacity cathode materials for sodium-ion battery	14
5.	Sung-Soo Kim Boosting the electrochemical properties of Mg-doped SiO_x alloy by carbon coating for fabrication of high-energy lithium-ion batteries	15
PLENARY SPEAKERS		
6.	Evgeny Antipov Novel phosphates and fluoride-phosphates electrode materials for me-ion batteries	16
7.	Nae-Lih Wu Engineering artificial electrode-electrolyte interphase for advanced Li-ion batteries	16
8.	Artem Abakumov How advanced transmission electron microscopy can contribute to battery research	17
9.	Toru Wakihara Understanding and controlling zeolite synthesis	17
INVITED SPEAKERS		
10.	Hirokazu Munakata Evaluation of ionic conductivity in LiNi_{0.5}Co_{0.2}Mn_{0.3}O₂ composite electrodes of Lithium-ion batteries by DC polarization method	18
11.	Fu-Ming Wang The development of super electrically conductive Si material with polymer brush acid and emeraldine base and its auto-switch design for high-safety and high-performance lithium-ion battery	19
12.	Zulhair Mansurov Recent advances and outlook in nanotechnology	19
13.	Sergey Levchenko Novel symbolic regression and data mining approaches in energymaterials research	20
14.	Pavel Sorokin Current progress in the study of ultrathin diamond films. Achievements and challenges	21
15.	Taifur Ozturk Combinatorial development of active materials for energy storage and conversion	22
16.	Sigita Trabesinger Deciphering the mechanism of FEC-induced SEI formation in li-ion batte	23
17.	Dmitry Pelegov Limitations and capabilities of micro-Raman spectroscopy. Electrode materials for lithium battery	24
ORAL PRESENTATIONS		
18.	Desmond Adair Simulation of harvesting vibrational energy when utilizing material work functions using the modified differential transformation method	25
19.	Desmond Adair An efficient method for combining multi-criteria subjective evidence when selecting material for fuel cell bipolar plates	25
20.	Mirat Karibayev Binding, reaction, and activation energies of OH-ions interacting and reacting to some head groups of anion exchange membrane explored via the DFT method	26
21.	Saltanat Kazbek Enhancement of the porous catalyst productivity by using gaussian nonuniform activity distribution under unsteady-state regime	27
22.	Zhandos Sadirkhanov Self-powered organometal halide perovskite photodetector with embedded silver nanowires	28
23.	Sergey Tokarev Ruthenium (II) complexes of imidazo-1,10-phenanthrolines: heterogeneous electron transfer and gas sensory properties	29
24.	Alexander Ryabin Single particle approach to Raman study of LiFePO₄: spatial resolution and laser-induced decomposition	29
25.	Denis Voronin Cellulose microfibers as a versatile support for shape-stable phase-change composites for thermal energy storage	30
26.	Elena Romadina Novel organic materials for non-aqueous redox flow batteries:	31

	implementation of triarylamine and phenazine core structures	
27.	Elena Ushakova Chiral carbon dots for bioapplications	32
28.	Ainur Duisenova Model of single-electron transistor based on prismanes	33
29.	Aigerim Kabiyeva Optimal distribution of catalyst in porous pellets for a quasi-steady-state reaction with Langmuir-Hinshelwood kinetics	34
30.	Symbat Naurzkulova Ni–Ru-containing mixed oxide-based composites as precursors for ethanol steam reforming catalysts: effect of the synthesis methods on the structural and catalytic properties	35
31.	Evgeniia Stepanidenko NIR-emissive carbon dots produced from organic dyes via template-assisted method	36
32.	Aliya Zhagiparova Key factors and performance criteria in wearable strain sensors based on polymer nanocomposite	37
33.	Yuma Shimbori Kanamura Application of 3DOM PI separator to lithium metal batteries with ionic liquids-based electrolyte	38
34.	Artyom Novikov Charge-transport materials impact on the perovskite solar cells stability	38
35.	Bagdaulet Shugay Enhancement of the electrochemical performance of the cathode material $\text{NaNi}_{0.5}\text{Mn}_{0.5-x}\text{Zr}_x\text{O}_2$	39
36.	Yerkezhan Yerkinbekova Functionalized lignin-contained nanofibrous separator with high stability for safe lithium-ion batteries by UV-electrospinning	40
37.	Dmitry Kogolev Laser-assisted ablation of UiO-66 metal-organic framework on the PET surface for novel electrode materials	41
38.	Nikita Luchinin KTiPO_4F and $\alpha\text{-TiPO}_4$ as electrode materials for metal-ion batteries	42
39.	Zhuldyz Yelzhanova A morphological study of solvothermally grown SnO_2 nanostructures for application in perovskite solar cells	43
40.	Ivan Prikhno Switchable membrane materials based on electroactive polyazines	44
41.	Nikolai Vinogradov Composite aluminosilicate material based on halloysite and MCM-41 as a support for highly efficient hydrotreating catalysts	45
42.	Mikhail Petrov High-power and inexpensive organic electrolyte for redox flow battery based on anthraquinone sulfo-derivatives mixture	46
43.	Ekaterina Fedotova Effects of climate variability and climate change on wind power integration into power systems	47
44.	Anastassiya Mashentseva Composite-track etched membranes for environmental applications	48
45.	Madina Kalibek P-doped coffee ground-derived hard carbon for boosting sodium-ion batteries	48
46.	Olzhas Kaupbay Reduced form of Prussian Blue (Prussian white) cathode material for application in two electrode systems	49
47.	Fyodor Malchik Boosting MXene capacity by self-oxidation in air atmosphere for water-in-salt electrolyte-based supercapacitor	50
48.	Yerkebulan Kadyrov Ti doped ZnO films deposited by magnetron sputtering for gas sensors	51
49.	Nurzhan Baikalov Catalytic effects of different loadings of Ni nanoparticles encapsulated in few layers N-doped graphene and supported by N-doped graphitic carbon in Li-S batteries	52
50.	Lunara Rakhymbay A study of Cu-doping effects in $\text{Na}_2\text{Mn}_3\text{O}_7$ layered cathode material for Sodium-ion battery	53
51.	Ekaterina Solntseva Rosatom state atomic energy corporation capacities and technologies in hydrogen energy	54
52.	Gaukhar Smagulova Obtaining cellulose fibers from the fallen leaves	55
53.	Bayan Kaidar Obtaining compositional fibers via electrospinning method	56
54.	Nardana Bazybek Maximizing specific capacity of nutty hard carbon: Impact of treatment conditions on structural and electrochemical properties	57

POSTER SESSION

55.	Assel Zhilkashinova Structural-phase state and properties of the Cr-Al-Co-Y composite coating as a result of thermal exposure	58
56.	Aizhan Rakhmanova Synthesis of ZnO based gas sensing fiber material by electrospinning technique for detecting hazardous gases	58
57.	Nurbolat Issatayev Biomass-derived graphite as an anode material for high-performance Li-ion batteries at low temperature	59
58.	Dinara Akhmetsadyk First-principles study of Ga-N co-doped graphene nanostructures	60
59.	Haruna Abba Usman Flexible strain sensor and energy storage devices based on MXene/polymer nanocomposites: Review	60
60.	Assylan Akhanuly Perovskite solar cells with structured and planar SnO₂ electron transport layers	61
61.	Iliyas Dossayev Optimization of back-contact metal-semiconductor-metal perovskite solar cells	62
62.	Nuriya Mukhamedova Structural and mechanical properties of heat resistant titanium alloys of the Ti-24.5Al-24.5Nb (at.%) system	63
63.	Muhammad Salman Kiani Solution-processed SnO₂ quantum dots electron transport layer for flexible printed perovskite solar cells	64
64.	Hryhorii Parkhomenko Influence of mechanical stresses on recombination processes in flexible and printed perovskite solar cells	65
65.	Yerassyl Yerlanuly The effects of different electron transport layer materials on the photovoltaic properties of flexible and printed perovskite solar cells	66
66.	Rakhymzhan Zhumadilov Photodetectors made of carbon nanowalls transferred on Si and CdTe	67
67.	Arman Miniyazov Structural and phase state of carbided layer tungsten obtained in a beam-plasma discharge	68
68.	Erik Shalenov Modeling of sandwich and quasi-interdigitated back-contact perovskite solar cells	69
69.	Nuriya Mukhamedova Information and analytical system as a method for scientific information processing	70
70.	Xeniya Leontyeva Joint growth of BiOI and BiSI films in the chemical deposition process	70
71.	Igor Sokolov Effect of cyclic thermal load on beryllium	71
72.	Mayuribala Mangrulkar Influence of carbamide and thioamide additives on photostability & performance of MAPBI₃	72
73.	Pavel Bezrukov Quantum efficiency of water splitting on the surface of nanoporous layers of silver and copper iodides and copper oxide	73
74.	Yerkhat Dauletkhanov Evaluation of the strength characteristics of steel grade 35X by testing miniature samples SPT	74
75.	Kuanysh Samarkhanov On the use of lithium-containing layers to study the sputtering of lithium into noble gas via bombardment by an electron beam	75
76.	Yevgeniy Tulubayev Development of a methodology for conducting experiments with a sample of lithium capillary-porous structure at a plasma-beam installation	76
77.	Vadim Bochkov Development of a methodology for conducting experiments with a sample of tin-lithium eutectic at a plasma-beam installation	77
78.	Nursanat Parmanbek Fabrication of the Ag/DMAEMA@PET composites for efficiency removal of As(III) ions	78
79.	Dias Bekeshov Adsorption and displacement of methane in graphene-based microstructures: insight from molecular simulations	79
80.	Akmaral Utelbayeva "Electromagnetic particles" are elementary energy carriers	80
81.	Anatoly Botezatu Methoxy-substituted naphthothiophenes—single molecules' vs. condensed phase properties and prospects for organic electronics applications	81

82.	Yerkin Serik The SOH and the SOC assessment of NCR18650 PANASONIC cylindrical battery through the entropymetry	82
83.	Aigerim Aitbayeva Biomass-based biochar obtained by low-temperature pyrolysis in the presence of metal oxides: preparation, characterization and future applications	83
84.	Mariyam Mukhtarova Hydrodeoxygenation of guaicol on transition metal phosphides formed in situ	84
85.	Asset Aliyev Experimental and numerical studies of rheological behavior of non-spherical powders	85
86.	Anastassiya Khrustaleva Synthesis of 1,4-dihydropyridine derivatives in microwave flow reactor	85
87.	Azamat Yedrissov Synthesis of anti-tuberculosis drugs in a microwave flow reactor	86
88.	Maria Rubtsova Design of low-silica zeolites based on natural halloysite nanotubes	88
89.	Pavel Loktionov Calibration-free coulometric sensors for vanadium redox flow battery imbalance monitoring	89
90.	Yerzhan Mukhametkarimov Optical features of Ag/Au-WO_{3-x} plasmonic composite thin films	90
91.	Nazim Gusseinov Optoelectronic properties of layered gallium sulfide crystals	90
92.	Alina Gorbunova Is azo-coupling of p-nitrothiophenola good reaction for the evaluation of plasmon catalysis mechanism?	91
93.	Sergei Cherevkov Improvement of light harvesting in optoelectronic devices by amphiphilic carbon dots	91
94.	Zhandos Tolepov Structure and electronic properties of layered Ge-Sb-Te based alloys	92
95.	Nursultan Sapar Development of core-shell structured HCNF/Si anode material via coaxial electrospinning technique for new generation of lithium-ion batteries	93
96.	Diana Suleimenova Pt-free and efficient counter electrode with nanostructured MnCo₂S₄ for dye-sensitized solar cells	94
97.	Nursultan Jyeniskhan Analysis of RIM-driven turbines: A Literature Review	95
98.	Ademau Aliakbarova Highly efficient bio-based carbonaceous counter electrode for dye-sensitized solar cells	95
99.	Shamshiya Amerkhanova Adsorption of polyetheneglycol and propylene glycol onto themodified glass microspheres	96
100.	Gulzat Nuroidayeva The SOH and the SOC assessment of LiNi_{0.88}Co_{0.09}Al_{0.03}O₂ cathode material for lithium-ion batteries through the entropymetry	96
101.	Assel Alimkhanova Application of biogenic zinc oxide nanoparticles in the degradation of organic dyes	97
102.	Anastassiya Mashentseva Determination of optimal synthesis conditions of the Cu@PET composites using Taguchi robust experiment design	98
103.	Assyl Adylkhanova Fabrication of the free-standing Ni_xS_y microflowers for Li-ion batteries	98
104.	Saule Kokhmetova Kinetics of sodium intercalation-deintercalation processes into an Eldfellite cathode material with a MoS₂ surface layer	99
105.	Yaroslav Zhigalenok Establishing regularities of charge transfer through corrosive films on lithium	100
106.	Kaiyrgali Maldybayev Selecting a membrane for supercapacitor batteries with water-based electrolyte	100
107.	T.A. Akatay Establishment of regularities of the influence of factors that determine the electrochemical stability window of aqueous electrolytes for sodium-ion batteries	101
108.	Andrey Kurbatov Simulation of intercalation processes in poorly conductive materials	102
109.	Alena Starodubtseva On electrochemical activity of Zn₂(EDTA)(H₂O) in aqueous sodium-ion based electrolytes	103

110.	Margarita Ryabicheva Impact of substrate surface preparation method on SEI formation regularities during electrochemical deposition of lithium	104
111.	Nuray Zhalgas Application of LiFePO₄ cathode on substrate by electrophoretic deposition technique	105
112.	Assel Serikkazyeva The deposition and electrochemical study of multilayered Li_xSn alloy anode for lithium-ion microbatteries	105
113.	Fail Sultanov Graphene-like porous carbons as a sulfur host for lithium-sulfur batteries	106
114.	Yer-Targyn Tleukenov Three-dimensional modeling of all solid-state lithium-ion batteries	107
115.	Aiym Rakhmetova SnSe@porous carbon nanofibers as a free-standing anode for low-temperature lithium-ion batteries	108
116.	Ayaulym Belgibayeva Low-temperature performance of Sn_xP/C composite nanofibers as free-standing anode materials for lithium-ion batteries	109
117.	Makpal Rakhmatkyzy Enhancing the low-temperature characteristics of a Li/graphite half-cell by the comprehensive modification of electrolyte	109
118.	Batukhan Tatykayev Solid-state synthesis of nanostructured LiMPO₄ cathode materials for Li-ion batteries	110
119.	Uldana Kydyrbayeva Obtaining nanostructured red phosphorus as an anode material for Li- and Na-ion batteries	111
120.	Madina Sarsembina I-V characterization of p-n heterostructures obtained by GLAD	111
121.	Ilyas Mukushev Microwave-assisted synthesis of LISICON structured Li₃V₂(PO₄)₃/graphene composite	112
122.	Kazna Tassybay Biomass graphene derived from date seeds as an anode material for lithium-ion battery	113
123.	Assem Mubarak Layer by layer arrangement of a hybrid piezo-triboelectric nanogenerator based on a biocompatible flexible PVDF composite and Al electrode for implantable cardiac pacemaker	113
124.	Arman Umirzakov Thin-film sulfur cathode for Li-S microbatteries	114
125.	Raigul Jumanova Electrochemical behavior of an electrode based on TiO₂ as a perspective anode for magnesium-ion batteries	115
126.	Emmanuel Chisom Nnwaogu 3D printing of high-performance electrodes for all-solid-state rechargeable lithium-ion batteries	116
127.	Yerzhan Nurmakanov A Flexible and Wearable Single Electrode Triboelectric Nanogenerator	117
128.	Aisar Abdrakhmanov, Aruna Rakhimzhanova Preparation of a piezoelectric porous mat aerogel	118
129.	Elmira Nurgaziyeva Functionalized polytetrahydrofuran-based solid polymer relectrolytes for safe lithium-ion batteries by UV-cross-linking	118
130.	Yelnury Baltash Effect of doping with cations and anionic groups on the ionic conductivity properties of latp solid electrolytes for li-ion batteries	119
131.	Tayfur Öztürk Factors affecting the design of hydrogen separators based on dense metallic membranes	120
132.	Islam Rakhimbek Functional PAN carbon nanofibers decorated with nickel and nickel oxide nanoparticles for lithium-sulfur batteries	121
133.	Aigul Shongalova Ionic conductivity of LATP-based thin film solid electrolytes prepared by magnetron sputtering	122
134.	Assem Zhanabayeva Sol-gel synthesis of LiFePO₄ for LIB based on lithium carbonate from Kazakhstani spodumene feedstocks	123
135.	Arman Miniyazov Investigation of surface carbide layers of tungsten under the influence of helium plasma	124

136.	Akzhan Bekzhanov Synthesis of LiCoO₂ thin-film cathode for lithium-ion microbatteries	126
137.	Dana Kurmangaliyeva Passivation of zinc dendrites by spin coating method	125
138.	Kamila Maratova Effect of acid etching of stainless-steel foils in rechargeable lithium-ion batteries	126

Innovative solutions for LIB management for electric vehicles

Rachid Yazami

School of Materials Science and Engineering, Nanyang Technological University, Singapore

E-mail: rachid@kvi-battery.com

Lithium-ion batteries will play a central role in the energy transition from internal combustion vehicles (ICV) to electrical vehicles (EV). The major car industry will stop producing ICB and move to EV by 2030-2035. In this perspective EV should meet the current performances of ICV, including tank filling vs. battery pack charging time, driving ranges, safety, costs and lifespan.

Current LIB charging methods fall short to fully charge (0-100% SOC) an EV battery pack in a time below 60 minutes. Only partial charge (i. e. 20-80/90%) can be achieved below 30 min, providing limited driving range.

In this presentation we will introduce a new method for charging LIB based on voltage control as opposed to current control (CCCV, MSCC...) called 'non-linear voltammetry' (NLV). NLV enables fully charging most LIB below 30 minutes even in 6 min in some cases without excessive heating.

We will also discuss how thermodynamics-based methods help detect internal short circuits in a LIB cell, which enhances battery safety especially in EV application.

The fundamental science and technology applications of triboelectric nanogenerators

Zhong Lin Wang

Beijing Institute of Nanoenergy and Nanosystems, Chinese Academy of Sciences, Beijing, China.

School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, Georgia USA

E-mail: zhong.wang@mse.gatech.edu

Triboelectric nanogenerators (TENGs) was invented in 2012, which is based on coupling of triboelectrification and electrostatic induction effects, which is the most effective approach for converting mechanical energy into electric power. TENG is playing a vitally important role in the distributed energy and self-powered systems, with applications in internet of things, environmental/infrastructural monitoring, medical science, environmental science and security. In this talk, we first present the physics mechanism of triboelectrification for general materials. Our model is extended to liquid-solid contact electrification, reviving the classical understanding about the formation of electric double layers. Secondly, the fundamental theory of the TENGs is explored based on expanded Maxwell equations for a mechano-driven system. We will present the applications of the TENGs for harvesting all kind mechanical energy that is available but wasted in our daily life, such as human motion, walking, vibration, mechanical triggering, rotating tire, wind, flowing water and more. Then, we will illustrate the networks based on triboelectric TENGs for harvesting ocean water wave energy, for exploring its possibility as a sustainable large-scale blue energy. Lastly, we will show that TENGs as self-powered sensors for actively detecting the static and dynamic processes arising from mechanical agitation using the voltage and current output signals.

Research and development on Li-ion battery and next generation batteries

Kiyoshi Kanamura

*Department of Applied Chemistry for Environment, Graduate School of Urban Environmental Sciences
Tokyo Metropolitan University, 1-1 Minami-Osawa, Hachioji, 192-0397 Tokyo, Japan*

E-mail: kanamura@tmu.ac.jp

Some next generation batteries with Li metal anode have been developed to realize higher energy density of rechargeable batteries for electric vehicles (EV) and energy storage system (ESS). Especially, Li-air, Li-S, All Solid-State Battery with Li metal anode have been investigated to be utilized in EV and ESS applications. Most of researches have focused on cathode side. Recently, Li metal anode has been studied to improve its cycle performance and safety issue. Rechargeable Lithium Metal Battery (LMB) has been also extensively investigated to realize higher energy density of battery. The cathode of LMB is same with those of lithium-ion battery, so that the cathode does not have any problems. On the other hand, Li metal anode does not have adequate rechargeability due to a dendrite form deposition of Li which sometimes leads to an internal short circuit problem of cell. In addition, the dendrite of Li has very large surface area which can react with electrolyte and provides a porous structure of Li metal anode which contributes an expansion of anode. In order to solve these problems, some excellent efforts have been performed by using new electrolyte, new separator, new current collector and new cell design. Here, LMB developed in our group will be introduced. Our researches have been more focused on separator and electrolyte which can suppress the dendrite formation of Li, as below.

New separator: Three Dimensionally Ordered Macroporous (3DOM) Poly Imide (PI) Separator (3DOM-PI separator) 3DOM-PI separator consists of two types of pores, one is a macropore and another is connecting small pore between macropores. This structure provides very uniform current distribution in the cell to suppress the Li dendrite formation, leading to long cycle life of Li metal anode. The morphology of Li deposited at anode side of the cell with 3DOM-PI separator is different from the dendrite shape, resulting in minimize chemical reactions of electrolytes with Li metal anode. The pore distribution and size are optimized to suppress the current distribution in the cell which is important for suppressing the dendrite formation of Li metal. In addition, the mechanical property of 3DOM-PI separator also influences the rechargeability of Li metal anode.

New electrolyte: Dimethoxy Ethane (DEE) with 3 mol dm⁻³ LiFSI (DEE/LiFSI) The chemical reactions of electrolyte with Li metal are one of important factors for the morphology change of Li metal and cycle performance of the cell. These reactions consume the electrolyte inside the cell. The amount of electrolyte inside the cell is not so much, so that the consumption of electrolyte results in increase of the cell resistance and larger current distribution in the cell, leading to dendrite formation of Li metal. When the excess electrolyte in the cell is consumed, the cell will be dead. In this study, we have employed highly concentrated electrolyte system. Dimethoxy Ethane (DEE) with 3 mol dm⁻³ LiFSI is one of promising electrolytes to reduce the chemical reactions of electrolyte with Li metal.

By using the optimized 3DOM-PI separator and DEE/LiFSI electrolyte, LMB can be fabricated. The cathode material is LiNi_{0.5}Mn_{0.2}Co_{0.3}O₂ (NMC). Figure 1 shows the discharge and charge curves of the cell during 95 cycles. From the first cycle to the 50 th cycle, the discharge capacity does not decrease. The stable discharge and charge behavior is observed. After 50th cycle, the discharge capacity decreases gradually. At 150th cycle, the discharge capacity is 20 mA h which is 50 % of the initial discharge capacity.

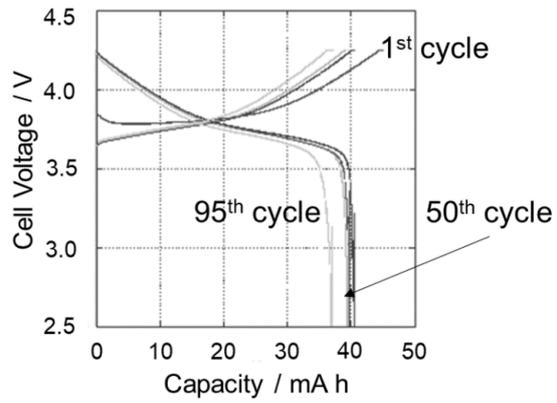


Figure 1 Discharge and charge curves of NMC/3DOM-PI with DEE/LiFSI/Li cell.

In this way, LMB has been developed by using new separator and electrolyte. The obtained cycle performance is not enough good. In future cycleability should be improved. At this moment, the target cycle number is 500. In order to realize this target, new interfacial control between Li metal surface and separator with electrolyte is strongly required.

Mn-based high-capacity cathode materials for sodium-ion battery

Seung-Taek Myung

*Hybrid Materials Research Center, Department of Nano Technology and Advanced Materials Engineering, Sejong
Battery Institute, Sejong University, Seoul, 05006, South Korea*

E-mail: smyung@sejong.ac.kr

The development of sodium-ion batteries (SIBs), which are promising alternatives to lithium-ion batteries (LIBs), offers new opportunities to address the depletion of Li and Co resources; however, their implementation is hindered by their relatively low capacities and moderate operation voltages and resulting low energy densities. To overcome these limitations, considerable attention has been focused on anionic redox reactions, which proceed at high voltages with extra capacity. This presentation covers the origin and recent development of anionic redox electrode materials for SIBs, including state-of-the-art layered oxides. We sequentially analyze the anion activity–structure–performance relationship in electrode materials. Finally, we discuss remaining challenges and suggest new strategies for future research in anion-redox cathode materials for SIBs.

Boosting the electrochemical properties of Mg-doped SiO_x alloy by carbon coating for fabrication of high-energy lithium-ion batteries

Sung-Soo Kim^{1,4*}, Orynassar Mukhan¹, Nurzhan Umirov², Byoung-Min Lee³, Ji-Su Yun¹, Jae-Hak Choi³, and Jaewoo Lee⁴

¹Graduate School of Energy Science and Technology, Chungnam National University, Daejeon, 34134, Republic of Korea

²National Laboratory of Astana, Nazarbayev University, 53 Kabanbay Batyr, Nur-Sultan, 010000, Kazakhstan

³Department of Polymer Science and Engineering, Chungnam National University, Daejeon, 34134, Republic of Korea

⁴Tera Technos Co., Ltd, Daejeon, 30011, Republic of Korea

*E-mail: kimss@cnu.ac.kr

The use of high-capacity SiO_x-containing anode materials to increase the energy density limited by the utilization of low gravimetric-specific-capacity commercial carbonaceous materials (e.g., graphite) has recently received great interest. However, a low initial Coulombic efficiency (ICE) and other inherent disadvantages of SiO_x such as huge volume changes and poor electron transportation result in complicating its widespread use.

To tackle these issues, herein, we designed a facile, cost-effective, and mass-producible phenolic resin-coated Mg-SiO_x anode composite for high-performance lithium-ion batteries (LIBs). Compare to the carbon film produced by the chemical vapor deposition (CVD) method, carbon coated Mg-SiO_x based on the phenolic resin is found to act as a direct contact protection electrolyte-electrode interface and boosts kinetics of Li⁺ transport among the electrodes, resulting in the lowest charge transfer resistance, the highest ICE, and superior stable cycleability. As a result, the phenolic resin-coated Mg-SiO_x alloy electrode delivers a stable specific capacity up to ~1700 mAh g⁻¹ after 100 cycles. When tested using an industrial protocol, a full cell pairing of the Mg-SiO_x@C/graphite blended anode and commercial LiNi_{0.8}Mn_{0.1}Co_{0.1}O₂ cathode achieve a gravimetric and volumetric energy density of 467 Wh Kg⁻¹ and 953 Wh L⁻¹, respectively, which is higher than that of the cell based on the conventional graphite.

Acknowledgment

This work was financially supported by the Korea Institute of Energy Technology Evaluation and Planning (KETEP) grant funded by the Ministry of Trade, Industry & Energy (MOTIE, Korea) (Grant No. 20016022 and 20012715).

Novel phosphates and fluoride-phosphates electrode materials for Me-ion Batteries

Evgeny Antipov

Lomonosov Moscow State University, Moscow, 119991, Russia
Skolkovo Institute of Science and Technology (Skoltech), Moscow 121205, Russia
E-mail: evgeny.antipov@gmail.com

The development of metal-ion batteries intensifies the research on electrode materials for Na/K-ion batteries as viable alternatives to the Li-ion technology. The Na/K-based oxides and polyanion materials are scrutinized as cathodes aiming to enhance the specific energy, durability and rate capability. Whereas the layered oxides display greater volumetric energy density, the polyanion materials usually exhibit better cycling and thermal stability and higher C-rate capabilities due to covalently bonded structural frameworks. The polyanion compounds reveal an extra dimension in their crystal chemistry, which significantly extends the playground for designing materials with superior electrochemical performance. Further advantages are expected from the synergistic effect of combining different anions (such as $(\text{XO}_4)^{p-}$ and F^-) in the anion sublattice.

An overview of the research on novel phosphates and fluoride-phosphates as prospective electrode materials for the Na/K-ion batteries will be presented with a special emphasis on the interrelation between composition, synthesis conditions, crystal structure and electrochemical properties of the materials intended for practical applications.

Acknowledgment

This work was supported by the Russian Science Foundation (grant No. 17-73-30006).

Engineering artificial electrode-electrolyte interphase for advanced Li-ion batteries

Nae-Lih Wu

Department of Chemical Engineering, National Taiwan University, Taipei 106, Taiwan
Email: nlw001@ntu.edu.tw

While the theoretical capacity of an electrode is determined by the bulk properties of the active materials, the various practical performance indices, such as rate capability, cycle stability and safety, of the electrode heavily depend on the conditions of the interface between the electrolyte and active material. There have typically two ways to modify the properties of the interface. For one, chemical additives are introduced into the electrolyte and they are designed to undergo redox reactions at the surfaces of the active materials upon charge/discharge of a battery to form *in-situ* a so-called solid-electrode-interphase (SEI) layer for modifying the interfacial properties. With this method, a conformal surface coating can be formed at the “active surfaces” in a precise manner. The composition and structure, and hence the eventual function-ability, of the SEI is determined by a very complex and very often unpredictable relations among the electrochemical properties of the additives and the parent electrolyte and the charge-discharge protocols. Alternatively, for the other method, a permanent artificial SEI (ASEI) with designed compositions is applied onto the surfaces of the active materials. The coating process is typically carried out onto the active materials before they are subjected to electrode manufacturing. The ASEI approach provides some advantages over the natural SEI method. First, the compositions, and sometimes the structures, of the ASEI can be pre-designed with oriented function(s) for each of its components. The pre-design concept enables selections of wide varieties of chemical compositions containing different combinations of organic and inorganic materials. We present in this talk examples of using polymeric materials for modifying various LIB active materials in the context of enhancing rate capability, cycle stability and improved safety.

How advanced transmission electron microscopy can contribute to battery research?

Artem Abakumov

*Center for Energy Science and Technology, Skolkovo Institute of Science and Technology, Nobel Street 3, 121205
Moscow, Russia*

E-mail: a.abakumov@skoltech.ru

The design and improvement of the cathode materials for Li-ion batteries requires detailed knowledge on the crystal structure at different charge/discharge states and comprehensive understanding of the processes occurring at the nanoscale or even atomic scale level, as many electrode materials demonstrate highly inhomogeneous non-equilibrium behavior. Advanced transmission electron microscopy (TEM) is by far the most suitable and direct tool to look at the materials down to atomic scale. Recent progress in the quantitative electron diffraction methods and aberration-corrected scanning TEM imaging will be illustrated here with the examples of atomic structure investigation of various cathode materials. Electron diffraction tomography provides quantitative diffraction data enabling reliable structure solution and refinement from extremely small crystallites, typically smaller than 1 nm³. Aberration-corrected scanning transmission electron microscopy (STEM) delivers local information with sub-Å resolution. Employing various STEM techniques for visualization of cation migration, metal clustering, anion-anion bonding, oxygen vacancies will be exemplified with layered oxide cathode materials. Observations are supported with local chemistry assessment with spatially-resolved energy-dispersive X-ray analysis and electron energy loss spectroscopy.

Acknowledgement

This research was supported by Russian Science Foundation (grant 20-13-00233).

Understanding and controlling zeolite synthesis

Toru Wakihara

*Institute of Engineering Innovation, The University of Tokyo
Yayoi 2-11-16, Bunkyo-ku, Tokyo 113-8656, JAPAN*

E-mail: wakihara@chemsys.t.u-tokyo.ac.jp

Zeolites are artificially synthesized from silicon sources, aluminum sources, mineralizing agents and structure-directing agents in batch systems under hydrothermal conditions. To fulfill the wide industrial demands, efficient synthesis of zeolites with controllable crystallization kinetics is considered crucially important. It is believed that the amorphous aluminosilicate obtained by mixing raw materials first undergoes an induction stage, where its structure changes to a more stable amorphous state, and then a "crystal nucleus," the smallest entity that can be recognized as a crystalline phase, is formed. Thus, if the process of initial structural evolution of zeolites can be clarified and controlled, it will be possible to design and synthesize zeolites with controlled structure and composition in a rational manner. Furthermore, it is expected to make a significant contribution to the discovery of theoretical zeolites with unknown structure and composition. However, the multifaceted formation process of zeolites cannot be simply explained by the classical nucleation theory, in which monomers aggregate to reach a critical size. Furthermore, the aperiodic structure of the aluminosilicate precursor invalidates the conventional crystallographic characterization, and this amorphous-to-crystalline transition process is still a black box. This talk will focus on the synthesis of zeolites, explaining how zeolites are formed in the hydrothermal synthesis process and how they can be controlled.

Evaluation of ionic conductivity in $\text{LiNi}_{0.5}\text{Co}_{0.2}\text{Mn}_{0.3}\text{O}_2$ composite electrodes of lithium-ion batteries by DC polarization method

Hirokazu Munakata*, Shota Ozawa, Kiyoshi Kanamura

Department of Applied Chemistry for Environment, Graduate School of Urban Environmental Science

*E-mail: munakata@tmu.ac.jp

The detailed understanding of ion transport in porous electrodes is necessary for the precise design of battery performance. So far, their ionic conductivity has been measured by AC impedance spectroscopy. However, the ionic conductivity measured by this method corresponds to a steady state value, and does not reflect the practical battery operating conditions. Based on this background, we have worked on the evaluation of ion conduction in porous electrodes under DC polarization, which is closer to the operating conditions of battery. In this study, the ionic conductivity in $\text{LiNi}_{0.5}\text{Co}_{0.2}\text{Mn}_{0.3}\text{O}_2$ (NCM523) composite electrodes was evaluated particularly focusing on how it changes during charge-discharge cycles.

Fig. 1 shows the ionic conductivity in NCM523 composite electrodes before and after 10 cycles of charge-discharge with different upper cut-off potentials. The ionic conductivity of $\sim 1 \text{ mS cm}^{-1}$ in pristine NCM523 composite electrode decreased to 0.90, 0.62 and 0.55 mS cm^{-1} after the cycle tests with upper cut-off potentials of 4.0, 4.3 and 4.5 V vs. Li/Li^+ , respectively. It has been reported that the decomposition of electrolyte species and the following their accumulation easily occur on NCM composite electrodes. In fact, those decreases in the conductivity showed good correlation with the irreversible capacity in the charge-discharge cycles: the total values of irreversible capacity increased from 0.8 to 2.2 and then 2.9 mAh by changing the upper cut-off potential from 4.0 to 4.3 and then 4.5 V vs. Li/Li^+ . This result suggests that the pathways of ions in NCM523 composite electrodes would be obstructed by the electrolyte decomposition products. It is well-known that the irreversible capacity can be reduced by addition of electrolyte additives such as fluoroethylene carbonate (FEC). The effect of FEC addition on the suppression of conductivity decrease will be also discussed for further clarification of ion transport in NCM523 composite electrodes.

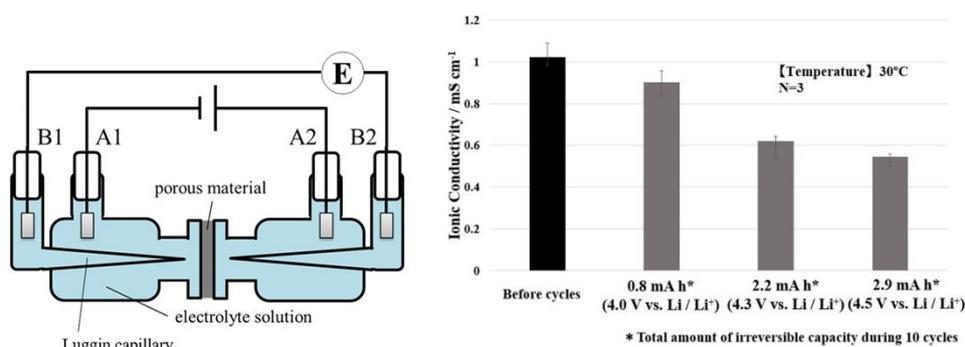


Fig. 1 (a) Schematic illustration of the cell designed for the ion conductivity measurement under DC polarization. (b) Ionic conductivity in NCM523 composite electrodes including $1.0 \text{ mol dm}^{-3} \text{ LiPF}_6 / \text{EC} : \text{DEC} = 1 : 1$ (in vol.) before and after 10 cycles of charge-discharge with different upper cut-off potentials of 4.0, 4.3 and 4.5 V vs. Li/Li^+ .

The development of super electrically conductive Si material with polymer brush acid and emeraldine base and its auto-switch design for high-safety and high-performance lithium-ion battery

Fu-Ming Wang

Graduate Institute of Applied Science and Technology, National Taiwan University of Science and Technology, Taipei, Taiwan

Email: mccabe@mail.ntust.edu.tw

Silicon is a promising anode material that can considerably increase the energy density of lithium-ion batteries (LIBs) owing to its high theoretical capacity and low cost. However, its huge volume changes and low electrical conductivity damage the structural stability of the material and reduce the reaction kinetics, thus resulting in poor electrochemical reversibility and rate performance. In this study, the super electrically conductive (SEC) Si material was developed by using a polymer brush and emeraldine base on the surface of each Si particles to improve the kinetics and maintain the stability of electrochemical properties. The results revealed that compared with the bare Si electrode, the Si-SEC electrode enhanced electrical conductivity by 10⁴ times, reduced 75% of charge transfer resistance and the direct contact of electrolytes, prevented volume changes with high mechanical properties, and supported high diffusivity of the interfacial layer. The Si-SEC electrode delivered an initial capacity of 2650.0 mAh g⁻¹ with a high columbic efficiency of 86.3%. After 300 cycles, the capacity remained at 1850.0 mAh g⁻¹ with high cycle retention. The rate performance of the SEC-Si electrode was excellent for 577 mAh g⁻¹ at 4C without requiring carbon/graphite composites and any electrolyte additives. Several techniques such as scanning electron microscopy, X-ray photoelectron spectroscopy, transmission electron microscopy, operando transmission X-ray microscopy, and operando X-ray diffraction were employed to investigate the effects of the SEC layer on Si. The SEC layer also provides auto-switch function by neutralizing the local pH of the electrode surface, which significantly increases the interfacial impedance to terminate current. This new designed Si material can be used to enhance the life, energy density, and safety issue of LIBs.

Recent advances and outlook in nanotechnology

Zulkhair Mansurov

Institute of Combustion Problems, Almaty, Kazakhstan

E-mail: ZMansurov@kaznu.kz

R. Smalley in his famous article [1] noted 10 urgent problems associated with the development of mankind. Among them are clean air, clean water, energy, health. Fundamental and applied research is carried out in these areas at the Institute of Combustion Problems. This paper presents the results of these research obtained by our scientists during the last 5 years.

- Energy intensive nanocarbon materials;
- Bio-waste-derived few-layered graphene/SrTiO₃/PAN as an efficient photocatalytic system for water splitting;
- Obtaining carbon fibers based on coal tar pitches by the method of electrospinning;
- Obtaining of Biologically Soluble Membranes Based on Polymeric Nanofibres and Hydroxyapatite of Calcium;
- Synthesis of nanocarbon sorbents for water purification from heavy metal ions;
- Synthesis of nanocarbon sorbents for sorption of toxic gases.

Novel symbolic regression and data mining approaches in energy materials research

Sergey Levchenko

Skolkovo Institute of Science and Technology, Moscow, Russia

E-mail: s.levchenko@skoltech.ru

Important properties of energy materials, such as activity and selectivity of a catalyst or a thermoelectric's figure of merit, are in general difficult to predict, in particular from first principles. The problem lies in the extreme complexity of the relation between the atomic composition of a material and its functional properties at realistic temperatures and pressures. We demonstrate how to bridge this complexity with artificial intelligence (AI) on several examples.

Single-atom metal alloy catalysts (SAACs) have recently become a very active new frontier in catalysis research. The simultaneous optimization of both facile dissociation of reactants and a balanced strength of intermediates' binding make them highly efficient and selective for many industrially important reactions. However, discovery of new SAACs is hindered by the lack of fast yet reliable prediction of the catalytic properties of the sheer number of candidate materials. We address this problem by applying a compressed-sensing approach SISSO parameterized with density-functional inputs. Besides consistently predicting high efficiency of the experimentally studied SAACs, we identify more than two hundred yet unreported candidates. Some of these candidates are predicted to exhibit even higher stability and efficiency than the reported ones. Our study demonstrates the importance of finding descriptors directly from data, as well as provides a recipe for selecting best candidate materials from hundreds of thousands of transition-metal SAACs for various applications.

Employing SISSO in an active-learning framework, we have also predicted and experimentally confirmed stable medium-temperature polycrystalline p-type thermoelectric (TE) materials with a very high figure of merit (> 2). This breakthrough became possible due to the AI-assisted exploration of the vast materials space of a known class of TE materials, which allowed us to find materials with an optimal balance between conflicting parameters.

Moreover, using subgroup discovery, an AI approach that discovers statistically exceptional subgroups in a dataset, we develop a strategy for identification of most important parameters of a catalytic material and competing mechanisms of a catalytic reaction. The approach is used to develop physical understanding of hydrogen activation at SAAC's and address the problem of converting CO₂ to fuels and other useful chemicals.

Acknowledgement

This research was supported by grants RSF 21-13-00419 and RFBR-INSF 20-53-56065

Current progress in the study of ultrathin diamond films. Achievements and challenges.

Pavel Sorokin

National University of Science and Technology MISiS, 4, Leninsky av., Moscow, 119049, Russian Federation

E-mail: PBSorokin@misis.ru

With the developments in the field of 2D materials, nowadays of growing interest is synthesis and investigation of 2D diamond or diamane, whose potential properties put it in par with the most promising nanostructures such as graphene, h-BN or MoS₂. Nevertheless, the diamane study at the early research stage, still facing a number of challenges. Below I will outline current progress in the study of this material.

What makes these films interesting and motivates the efforts in their syntheses? Primarily, diamane films inherit from their bulk ancestor a number of remarkable properties highly desirable in materials research and applications. Ultrahard coatings with broad-range optical transparency, also a host-material for single-photon emitter defect-centers for quantum computing, superconductivity, biologically active substrates, biosensors, etc. The electronic properties of diamane strongly depend on the type of surface termination (and surface orientation), therefore it has potential for applications in nanooptics and nanoelectronics and can serve as a promising platform for micro- and nanoelectromechanical systems

The diamane synthesis currently is a priority goal, which however remains rather challenging. It was proposed that such thinnest “ultimate diamond slab” can in principle be achieved by purely chemical means, without any pressure - in striking contrast to bulk graphite-diamond transformation. Thus, the approach of using chemistry instead of (or together with) pressure seems to be the most promising, if not the only possible way for obtaining the thinnest diamond films. The chemically induced phase transformation appears to be the way to produce diamane, its feasibility already confirmed in a number of experiments. Besides production of films, it can be used for transforming the structure of nanoclusters, as shown in the pressureless formation of nanodiamonds from amorphous carbon. Moreover, it seems also to allow transforming other structures, e.g., the promise of the van der Waals heterostructures suggests possible synthesis of diamond/BN heterolattices. In general, the transformation of the diamane from few-layer graphene depends on many factors, including both external conditions and features of the graphene structure, whose defects can significantly affect the final 2D diamond structure. In my talk I will discuss our latest findings on the subject.

Acknowledgement

P.B.S. gratefully acknowledges the financial support of Russian Science Foundation (Project identifier 21-12-00399).

Combinatorial Development of Active Materials for Energy Storage and Conversion

N. Özgür Darıcıoğlu¹, Yiğit Akbaş¹ and Tayfur Öztürk^{1,2,*}

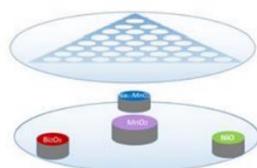
¹ENDAM, The Centre for Energy Materials and Storage Devices, METU, Ankara, Turkey

²INNOVASCOPE Materials Technologies Ltd. Sti. METUTECH, Ankara, Turkey

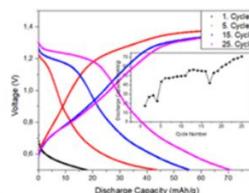
*E-mail: ozturk@metu.edu.tr

Active material development in energy storage and conversion as in similar development other fields of materials research have largely followed Edisonian approach of focusing on one material composition at a time. The approach requires a careful pre-consideration in selecting the material composition and the success depends largely on the suitability of the initial choice made for the material. Combinatorial approach is an alternative method whereby a large number of samples each with different compositions are produced simultaneously. They are then screened in a fast manner to single out the material(s) with best performance. The materials selected are then fully characterized as is customary for the conventional method. The combinatorial approach is more efficient in terms both time and effort and yield more fruitful.

In this work, we describe a sputter deposition system which we specifically designed for combinatorial material development. The system designed could incorporate up to 6 sputter targets 2 inches in diameter plus the central one in 3 inches which would provide the base composition.



Combinatorial geometry for fabrication of thick film material library for Zn-MnO₂ batteries. Three peripheral targets are in triangular geometry, substrates above mimicking the position of targets underneath.



Charge-Discharge profiles at selected cycles for Bi_{0.06}Na_{0.34}Ni_{0.17}Mn_{0.44}O_x, Insets showing the cyclic discharge capacity

In this presentation, following a brief review of the previous achievement, we concentrate on combinatorial development of cathode material for Zn-MnO₂ battery. This is a low-cost battery, with limited rechargeability, mostly used as primary battery. There is, however, considerable interest in this chemistry to make it truly rechargeable, preferably with two electron exchange, i.e. Mn⁴⁺ → Mn²⁺. We therefore modified MnO₂ in quaternary configuration, where MnO₂ was modified with other oxides, namely Bi₂O₃, Na_{0.7}MnO₂ and NiO Fig.2. A total of 36 cathodes were deposited on nickel substrate typically 2.5 mm thick each with a different composition. The results show that thick film cathodes are largely amorphous in as-deposited state but upon chargedischarge the structure rearranges into crystalline form into layered d-MnO₂ structure. Two regions were identified as potential cathodes one region was close to NiO corner. and the other regions had moderately large Na content.

Acknowledgements

The work reported is supported by TÜBİTAK with project number 118M076 which we gratefully acknowledge

Deciphering the mechanism of FEC-induced SEI formation in li-ion batteries

Sigita Trabesinger

Pazl Scherrer Institute, Forschungsstrasse 111, 5232 Villigen PSI, Switzerland

E-mail: sigita.trabesinger@psi.ch

High energy density is one of the clear trends in future battery technologies, especially in portable devices and mobility sectors. Energy density of Li-ion cells can be increased by using materials with higher capacity and by extending operating voltage window of the cell. Despite the fact that the positive electrodes have lower capacities than the negative ones, the increase of negative electrode capacity also leads to significant improvement of energy density.

There is a number of negative electrode active materials, whose capacity is many times higher than that of graphite, such as silicon, tin oxide and others. However, these materials often exhibit large volume expansion upon lithiation and therefore an SEI formed on their surface is unstable. The most popular strategy for improving their cycling stability is the use of electrolyte additives that are reduced at the potentials more positive than the electrolyte solvents. Their decomposition products are incorporated in the SEI, leading to a more stable electrode/electrolyte interface. One of the most-investigated electrolyte additives is fluoroethylene carbonate (FEC), because it has been shown to lead to a significant performance enhancement of Si- and Sn-based anodes. Many reaction pathways have been proposed but there is currently no agreement on the exact type of chemical compounds constituting the decomposition products, as well as on the mechanism of FEC decomposition.

For this reason we conducted the systematic study, tracking morphological and chemical changes during electrochemical decomposition of FEC, and found that despite FEC often being referred as “film-forming” additive, in the first stage of its decomposition, spherical particles, mainly consisting of lithium fluoride, are formed. And only later the carbonate-rich film covers the entire electrode, covering as well the LiF-rich spheres. This phenomenon has been overlooked by researchers earlier due to very simple reason (disclosed in the talk).

We have also found that the size and amount of particles strongly depend on the testing cell medium, where electrolytes with higher dielectric constant lead to larger particle size, as do the high-capacity active electrode materials, both contributing to final properties of FEC-derived SEI. The results of this study provide a deeper understanding of how fluorine additives work and enables tuning of the SEI properties by using laws of simple crystal-growth theory to fit the conditions leading to the desired morphological and chemical outcome.

Acknowledgements

This research was supported by InnoSuisse (Project number 18254.2)

Limitations and capabilities of micro-Raman spectroscopy. Electrode materials for lithium battery

Alexander Ryabin, Alexei Nikiforov, Dmitry Pelegov*

Institute of Natural Sciences and Mathematics, Ural Federal University, Yekaterinburg, Russia

*E-mail: dmitry.pelegov@urfu.ru

Raman spectroscopy is an inexpensive and convenient tool for prompt structural characterization. Most research groups have access to confocal Raman microscopes with claimed submicron spatial and subsecond temporal resolutions. Raman spectroscopy is widely used in material science, solid-state chemistry, and electrochemistry. But this unique tool is often considered to be auxiliary to other methods and is commonly used as a “black box” without proper understanding of its limitations and capabilities.

Limitations often originate from the specifics of the objects under study. The first is that electrode materials for lithium batteries are granular objects with particle sizes of micron and submicron scale. Unlike single crystals and nanoparticles, microparticles are maybe the most complicated objects for an accurate physical description since their size is close to the probing wavelength and the Raman study can be considered neither local nor intergral.

Another limitation is that Raman spectroscopy can't be considered as a “non-destrative” tool of structural characterization. Most part of popular electrode materials alter under the action of the probing laser beam and we have shown a variety of degradation products and pathways.

The issues mentioned above limit the accurate interpretation of the obtained Raman spectra, but Raman spectroscopy is still a power tool for structural characterization and detection of imperfections. Its limitations can be overcome by using either the single-particles approach, increasing spatial resolution, or the statistical approach, enabling mesoscale characterization.

Acknowledgement

The research was funded by the Russian Science Foundation (project No 22-22-00350, <https://rscf.ru/project/22-22-00350>).

Simulation of harvesting vibrational energy when utilizing material work functions using the modified differential transformation method

Desmond Adair*, Torybek Kenzhekhanov, Gulnur Kalimuldina
*Mechanical & Aerospace Engineering, Nazarbayev University, Nur-Sultan, 010000,
Republic of Kazakhstan*

*E-mail: dadair@nu.edu.kz

It is possible to scavenge energy from mechanical vibrations and subsequently use this energy to provide power, usually, for low-powered electronic devices. The current simulations investigate the charging phenomenon which occurs between bodies with different work functions, while experiencing mechanical vibrations. The work function of a given material can be defined as the minimum thermodynamic work (or energy) which can free an electron from the solid material to a point in the vacuum immediately adjacent to the material surface. In essence, a work function energy harvester has many similarities to an electrostatic energy harvester except for the fact that the work function energy harvester requires no external power supplies nor dielectric materials which have quasi-permanent electric charge or dipole polarization. This work is part of a system which can generate electrical power derived from mechanical vibrations. The method of investigation used here is modelling using the Differential Transform Method (DTM), The DTM is modified to include the non-linear terms found in the governing equation. This necessitates the inclusion of Adomian polynomials. Some validation of the method is done by comparison with previous experimental results.

An efficient method for combining multi-criteria subjective evidence when selecting material for fuel cell bipolar plates

Desmond Adair^{1*}, Kairat Ismailov², Gulnur Kalimuldina¹
¹*Mechanical & Aerospace Engineering, Nazarbayev University, Nur-Sultan, Kazakhstan*
²*NUFYP, Nazarbayev University, Nur-Sultan, Kazakhstan*

*E-mail: dadair@nu.edu.kz

The work here demonstrates a quick and efficient method for combining subjective evidence provided by several expert researchers (ERs) concerning the selection of the most suitable material for metallic bipolar plates used in polymer electrolyte fuel cells. Many materials may be suitable for such plates, but often choices have to be made concerning multiple and often conflicting material attributes. As a first iteration in the decision process, the number of alternative materials can be greatly reduced using the Fuzzy TOPSIS (Fuzzy Technique for Order Preference by Similarity to Ideal Solution) multi-criteria decision analysis algorithm for ranking the material alternatives. This may then be followed by a greatly reduced number of necessary experiments on only several of the materials to finally identify the optimum. This methodological tool can be used to speed up the material selection process considerably using a set of predefined criteria. A set of criteria and a set of alternatives based on various characteristics are developed and evaluated through expert questionnaires. The proposed method also provides weights for a given criteria so leading to the ranked list of material alternatives, and hence the optimal solution. A user-defined code has been developed using the Python computer language to facilitate the implementation of the method, and an example involving six material alternatives thought suitable for bipolar plate manufacture is given to illustrate the process.

The proposed approach of combining subjective evidence may be applied to other problems involving material selection.

Binding, reaction, and activation energies of OH⁻ ions interacting and reacting to some head groups of anion exchange membrane explored via the DFT method

Mirat Karibayev^{1*}, Bauyrzhan Myrzakhmetov², Sandugash Kalybekkyzy², Almagul Mentbayeva^{1,2}, Yanwei Wang^{1,3}**

¹*Department of Chemical and Materials Engineering, School of Engineering and Digital Sciences, Nazarbayev University, Nur-Sultan 010000, Kazakhstan.*

²*Laboratory of Advanced Materials and Systems for Energy Storage, Center for Energy and Advanced Materials Science, National Laboratory Astana, Nazarbayev University, Nur-Sultan 010000, Kazakhstan*

³*Laboratory of Computational Materials Science for Energy Applications, Center for Energy and Advanced Materials Science, National Laboratory Astana, Nazarbayev University, Nur-Sultan 010000, Kazakhstan*

*E-mail: mirat.karibayev@nu.edu.kz, **E-mail: yanwei.wang@nu.edu.kz

The main drawback of Anion Exchange Membranes is related to the chemical instability of cationic head groups and the transportation of hydroxide ions at alkaline conditions and elevated temperatures. At this stage, our research was devoted to understanding the stability and transportation mechanism of hydroxide ions in detail and aiming to reach and keep the performance of AEM for a long time. In this regard, the quantum chemical properties for binding of various hydroxide ion-quaternary ammonium (QA) head group systems were investigated by the DFT method in implicit water to get binding energy. Then, the nucleophilic substitution degradation reaction of various hydroxide ion-QA head group systems were studied by the DFT method at the different hydration levels. Finally, the results of the DFT methods were in line with experimental results on chemical stability and ion exchange capacity.

In this work, we carried out by DFT calculation to get optimized structures of our designed systems, to understand the binding energy of hydroxide ion with six different QA head groups, and degradation reaction of hydroxide ion with two different QA head groups of AEM. Results of binding energies show the following order of the binding strength of OH⁻ ion with six various QA head groups: a) > c) > f) > d) > e) > b), which suggest that the group b) has a high transportation rate of OH⁻ ion via QA head groups of AEM. Considering the comprehensive studies of the Nucleophilic Substitution (SN₂) degradation reactions for QA head groups c) and f), the chemical stability of QA f) is found to be higher than that of QA c), because the activation energy of QA c) is lower than that of QA f), while the reaction energies for QA c) and QA f) are similar at the different hydration level.

Acknowledgement

This work was supported by the research grant AP09057868 “High performance polymer-based anion exchange membranes for alkaline fuel cells” projects from MES RK, and 080420FD1906 “Development of composite anion exchange membranes with improved chemical and mechanical stability” from Nazarbayev University. The authors are also grateful to Nazarbayev University Research Computing for providing computational resources for this work.

Enhancement of the porous catalyst productivity by using gaussian nonuniform activity distribution under unsteady-state regime

Saltanat Kazbek^{1*}, Vsevolod Andreev², Piotr Skrzypacz³, Boris Golman^{1}**

¹*Department of Chemical and Materials Engineering, School of Engineering and Digital Sciences, Nazarbayev University, 53 Kabanbay Batyr Ave, Nur-Sultan 010000, Kazakhstan*

²*Department of Heat Power Setups, Faculty of Energy and Electrical Engineering, Chuvash State University, Cheboksary 428015, Russia*

³*Department of Mathematics, School of Sciences and Humanities, Nazarbayev University, 53 Kabanbay Batyr Ave, Nur-Sultan 010000, Kazakhstan*

*E-mail: saltanat.kazbek@nu.edu.kz, **E-mail: boris.golman@nu.edu.kz

The porous catalyst is used to speed up a variety of chemical processes. The active centers are usually evenly distributed throughout porous catalyst pellets. The concentration of a reactant decreases with pellet depth, and the active sites near the pellet center are not always involved in promoting the chemical reaction. The nonuniform distribution of active centers, particularly near the pellet surface, may boost productivity and lower catalyst production costs. Moreover, the unsteady-state regime with periodically changing bulk concentration and temperature can increase productivity under specific conditions. The purpose of this study is to analyze the unsteady-state reaction and diffusion in the catalyst pellets with Gaussian nonuniform activity distribution and Langmuir-Hinshelwood kinetics for maximization of catalyst productivity. The ratio of averaged productivities is determined to demonstrate the benefit of Gaussian nonuniform activity distribution over uniform one. The parametric study is carried out using the developed Matlab software. The effects of the Biot numbers for mass and heat transfer, energy generation factor, Thiele modulus, Arrhenius numbers for absorption and reaction, breadth of Gaussian distribution, and optimal position for active centers distribution are studied on catalyst performance.

The results of the numerical experiments confirm that the optimal position for active center distribution is near the pellet surface. There is productivity enhancement while increasing Biot numbers for mass and heat transfer, energy generation factor, Thiele modulus, and Arrhenius number for reaction. Changing the Arrhenius number for absorption does not show a significant effect on the productivity ratio, but it shifts the optimal position of active centers. The ratio of averaged productivities increases as the dispersion of active centers narrows. The optimal control is studied to maximize the productivity ratio by changing the Gaussian distribution, bulk concentration, and temperature simultaneously.

Acknowledgment

This research was supported by the research grant 021220FD0351 from Nazarbayev University.

Self-powered organometal halide perovskite photodetector with embedded silver nanowires

Zhandos Sadirkhanov^{1*}, Almaz Beisenbayev², Yerassyl Yerlanuly², Marat Kaikanov² and Askhat Jumabekov^{2**}

¹*Department of Physics, Nazarbayev University, 010000 Nur-Sultan, Kazakhstan*

²*Department of Chemical Engineering, Nazarbayev University, Nur-Sultan 010000, Kazakhstan*

*E-mail: zhandos.sadirkhanov@nu.edu.kz

**E-mail: askhat.jumabekov@nu.edu.kz

Metal-semiconductor-metal (MSM) configuration of perovskite photodetectors (PPDs) suggests easy and low-cost manufacturing. However, the basic structures of MSM PPDs include vertical and lateral configurations, which require the use of expensive materials such as transparent conductive oxides or/and sophisticated fabrication techniques such as lithography. Integrating metallic nanowire-based electrodes into the perovskite photo-absorber layer to form one-half of the MSM PPD structure could potentially resolve the key issues of both configurations. Here, a manufacturing of solution-processed and self-powered MSM PPDs with embedded silver nanowire electrodes is demonstrated. The embedding of silver nanowire electrode into the perovskite layer is achieved by treating the silver nanowire/perovskite double layer with a methylamine gas vapor. The evaporated gold layer is used as the second electrode to form MSM PPDs. The prepared MSM PPDs show a photoresponsivity of 4×10^{-5} AW⁻¹ in the UV region and 2×10^{-5} AW⁻¹ in the visible region. On average, the devices exhibit a photocurrent of 1.1×10^{-6} A under white light (75 mW cm⁻²) illumination with an ON/OFF ratio of 83.4. PPDs device characterization is based on the main and important photodetectors measuring techniques, which illustrates all the benefits of the structure. The results presented in this work open up a new method for development and fabrication of simple, solution-processable MSM self-powered PPDs.

Acknowledgement

This research was supported by the Nazarbayev University Faculty Development Competitive Research Grant (Grant Number: 110119FD4512), Nazarbayev University Collaborative Research Grant (Grant Number: 021220CRP1922), Young Scientist Grant from the Ministry of Education and Science of the Republic of Kazakhstan (Grant Number: AP08052412).

Ruthenium (II) complexes of imidazo-1,10-phenanthrolines: heterogeneous electron transfer and gas sensory properties

Sergey Tokarev^{1*}, Anatoly Botezatu¹, Olga Fedorova¹, Abulkosim Nasriddinov², Marina Rumyantseva²

¹*INEOS RAS, Russia, Moscow, Vavilova St. 28*

²*Lomonosov Moscow State University, Faculty of Chemistry, Russia, Moscow, 1-3 Leninskiye Gory*

*E-mail: tokarev@ineos.ac.ru

In this work, a series of imidazo[4,5-f][1,10]phenanthroline-containing ligands and their monoruthenium(II) and heterobimetallic complexes were synthesized (Fig. 1 left). These complexes are capable of photo-induced electron transfer to the conduction band of some semiconductor materials (Fig. 1 right). Such photosensitization process will reduce the operating temperature of semiconductor gas sensors and thus reduce their energy consumption.

We have shown that energies of HOMO and LUMO of complexes were suitable for electron transfer from excited state to the conduction band of SnO₂ and In₂O₃. LUMOs of synthesized complexes are of triplet nature with a high lifetime sufficient for electron transfer. Modification of the surface of nanoparticles of SnO₂ and In₂O₃ with Ru(II) complexes gave hybrid organic-inorganic materials that were studied as sensitive elements for gas sensors to NH₃, NO₂ and NO. Hybrid

sensors appeared to have reproducible sensory signal in the presence of analyte gases at room temperature in air under periodic illumination with visible light LEDs. Some materials were able to determine NO₂ and NO within 0.25–2 ppm at room temperature under illumination with red LED. The MPC of the daily dose of NO is 2.6 ppm. Second cation in heterobimetallic complexes helped to control affinity of the surface towards one or another gas, which resulted in improved selectivity of gas analysis.

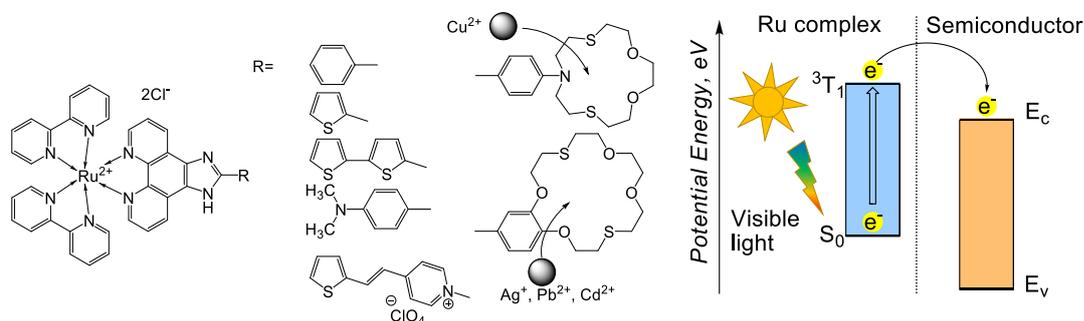


Figure 1. left: Structures of synthesized complexes; **right:** photoinduced sensitization in a hybrid semiconductor-dye material

Acknowledgements.

The reported study was funded by RSF according to the research project №17-73-30036.

Single particle approach to Raman study of LiFePO₄: spatial resolution and laser-induced decomposition

Alexander Ryabin^{*}, Dmitry Pelegov^{**}

Institute of Natural Sciences and Mathematics, Ural Federal University, Yekaterinburg, Russia

^{*}E-mail: Ryabin.Alexandr.1@yandex.ru, ^{**}E-mail: dmitry.pelegov@urfu.ru

Raman spectroscopy (RS) is one of the most promising candidates for industrial quality control tool for lithium battery industry. But there is a gap between chemical and physical aspects of materials characterization.

Despite the abundance of publications focused on solid-state chemistry and electrochemistry, there is a lack of research on physics of laser-particle interaction. To correctly interpret the experiment results, it is required to understand from what area the signal is received and what processes light can induce in the sample.

To define the RS resolution, we examined a 72 single LiFePO₄ (LFP) particles of different sizes on a Raman-active Si substrate. The ratio of intensity of Si band near 521 cm⁻¹ to one for major LFP band near 951 cm⁻¹ was used as a main characteristic parameter.

We showed that the probing depth of micro-Raman spectroscopy can greatly exceed instrumental estimation and reach several microns due to the particle morphology and variation of local optical properties conceivably caused by a variation of defect concentration. At the same time the edges of microscale particles and pores block Raman response from underneath layer more effectively than particles of transparent LFP. As a result, the μ RS measurement in a small pore can be attributed to superficial probing.

Six of 72 particles altered during RS probing and revealed a heterogeneity in pathways and products of laser-induced degradation of LFP. Some decomposed particles kept their form, while others became spherical, possibly due to melting. The disordered α -Fe₂O₃ phase was observed for all the decomposition products, but the second phase differs. For two of six particles, the second

phase is γ -Li₃Fe₂(PO₄)₃, which is typical for complete oxidation. The second phase with characteristic triplet 940-1015-1080 cm⁻¹ remained unidentified.

We hope that this work can help to organize relatively non-destructive RS measurements, properly interpret the obtained results, and take another step towards a better understanding of physicochemical processes, induced in microscale particles, regardless of the driving force origin – laser irradiation, heating, or cycling.

Acknowledgement

The research was funded by the Russian Science Foundation (project No 22-22-00350, <https://rscf.ru/project/22-22-00350>).

Cellulose microfibers as a versatile support for shape-stable phase-change composites for thermal energy storage

Denis Voronin^{1*,**}, Alexandra Pirtsul¹, Rais Mendgaziev¹, Maria Rubstova¹,
Kirill Cherednichenko¹, Dmitry Shchukin², Vladimir Vinokurov¹

¹National University of Oil and Gas “Gubkin University”, Leninsky Prospekt 65, Moscow 119991, Russia.

²Stephenson Institute for Renewable Energy, Department of Chemistry, University of Liverpool, Liverpool L69 7ZD, UK

*E-mail: denis.v.voronin@gmail.com, **E-mail: denis.v.voronin@gmail.com

Phase change materials (PCMs) offer an exciting way to facilitate the consumption of renewable and develop responsive energy management by storing and releasing thermal energy as latent heat of reversible phase transitions. Organic PCMs are attractive due to their high latent heat storage capacity and reliability of thermal properties, however, they lack shape stability. In our study, we propose a facile approach for the preparation of that shape-stable phase-change composites by simple adsorption of organic PCMs (as exemplified by fatty acids) onto the surface of the supporting cellulose microfibrils (MFC). The proposed method is simple, cheap, sustainable, and can be easily upscaled for mass production of the phase-change composites with tuneable thermal properties for energy storage applications. Cellulose is attractive due to its abundance, good mechanical properties and high specific surface area. We have demonstrated the preparation of shape-stable phase-change composite fibers containing 60, 65, and 70 wt% stearic acid with the latent heat storage capacity of 108 – 125 J/g with only 2% fluctuation in melting and freezing enthalpies during cyclic heating/cooling tests.

Additionally, the cellulose surface is rich in active hydroxyl groups. This allows for chemical modification of cellulose fibers to prepare the phase-change composites with enhanced functional properties. In particular, magnetite-modified MFC was employed for the preparation of multifunctional phase-change composites for bimodal thermal/electromagnetic energy storage. In particular, MFC was modified with magnetite nanoparticles in a tunable way via co-precipitation of Fe²⁺ and Fe³⁺ salts of various concentrations. The saturation magnetization of 23 emu/g was achieved in MFC with 31 wt% of magnetite. The phase-change composites were prepared by adsorption of lauric acid onto magnetite-modified MFC. The resulted composites demonstrated the saturation magnetization of 11.2 emu/g and latent heat storage capacity of 90 J/g corresponding to the loading efficiency of lauric acid of 49 – 51%. The IR-imaging revealed the efficient accumulation of the latent heat in the phase-change composite under the simulated sunlight and high frequency alternating magnetic field along with the excellent shape-stability of the composites during the melting of lauric acid.

Acknowledgement

This research was supported by Russian Science Foundation, project № 21-79-00176.

Novel organic materials for non-aqueous redox flow batteries: implementation of triarylamine and phenazine core structures

Elena Romadina^{1*}, Alexander V. Akkuratov², Keith J. Stevenson¹

¹Skolkovo Institute of Science and Technology, Bolshoy Boulevard 30, bld. 1, Moscow, Russia

²Institute of Problems of Chemical Physics, Russian Academy of Sciences, Semenov Prospect 1, Chernogolovka, Moscow Region, Russia

*E-mail: Elena.Romadina@skoltech.ru

The rapid growth of the role of renewable energy sources dictates new requirements for the electrochemical energy storage devices. Among them, redox flow batteries (RFBs) are regarded as a promising technology, since their advantages of excellent scalability, low cost, easy fabrication and operation, long lifetime, and safety. Today inorganic RFBs are penetrating the market, however, low specific capacity in conjunction with with low electrochemical stability window of aqueous electrolytes (≈ 1.5 V) and safety issues, hinders their wide-scale commercialization.

Herein, we studied a group of organic materials based on aromatic amines with general formulas of $NPh_3R_nBr_m$ and $N_2Ph_5R_nBr_m$ where $R = -(OCH_2CH_2)_2-OCH_3$. All the compounds demonstrated high solubility in MeCN, which potentially enables outstanding specific capacities approaching 134 Ah L⁻¹. Compounds demonstrated one or two quasi-reversible electron transition processes with redox potential up to 0.6 V vs. Ag/AgNO₃ reference electrode, what makes them perspective catholyte materials. For the RFB investigation butylviologen perchlorate (0.75V vs. Ag/AgNO₃, ~1.15 V battery voltage) was chosen as the redox pair. Firstly, the selection of the most appropriate electrolyte was performed: it was shown that the usage of the TBABF₄ and NaClO₄ produces the stable characteristics of RFB performance. Final RFB tests proved that the most promising systems are capable to exhibit 65% of maximum capacities and more than 95% Coulombic efficiency after 50 cycles.

On the next step we synthesized and investigated novel phenazine derivative with oligomeric ethylene glycol ether substituents as promising anolyte material. The designed compound undergoes a reversible and stable reduction at -1.72 V vs. Ag/AgNO₃ and demonstrates excellent (>2.5 M) solubility in MeCN. A non aqueous organic redox flow battery assembled using novel phenazine derivative as anolyte and substituted triarylamine derivative as a catholyte exhibited high specific capacity (~93% from the theoretical value on the first cycles), >95% Coulombic efficiency and good cycling stability.

To summarize, investigated materials establish themselves attractive for future research: obtained parameters open promising future directions for their usage as redox-active materials for non-aqueous RFBs.

Chiral carbon dots for bioapplications

Elena Ushakova^{1*}, Ananya Das², Evgeny Kundelev¹, Anna Vedernikova¹, Sergei Cherevko¹, Denis Danilov³, Aleksandra Koroleva³, Evgeniy Zhizhin³, Anton Tsympkin¹, Aleksandr Litvin¹, Alexander Baranov¹, Anatoly Fedorov¹, and Andrey L. Rogach^{4,5}

¹*ITMO University, Saint Petersburg, Russia.*

²*University of Rochester Medical Center, Rochester, New York, USA*

³*Research Park, Saint Petersburg State University, Saint Petersburg, Russia*

⁴*Department of Materials Science and Engineering, and Centre for Functional Photonics (CFP), City University of Hong Kong, Kowloon, Hong Kong SAR, China*

⁵*Shenzhen Research Institute, City University of Hong Kong, Shenzhen, China*

*E-mail: elena.ushakova@itmo.ru

The term carbon dots generally refers to colloidal nanoparticles (usually less than 10 nm in diameter) with inorganic cores which are composed of sp²/sp³ hybridized carbon domains, and a great variety of chemical functional moieties at the surface. Carbon dots draw a considerable attention in recent years due to their well-documented biocompatibility, high stability, and attractive optical properties, in particular strong, color-tunable photoluminescence. These merits offer promising potential for applications of carbon dots in bioimaging and biomedicine, including photoacoustic imaging, photothermal and photodynamic therapy. Another important issue in carbon dots bioapplications is the possibility to synthesize chiral nanoparticles with optical activity in 200-400 nm spectral region.

We developed two approaches to synthesize chiral carbon dots: the surface post-synthetic treatment and one-pot synthesis in the presence of chiral organic molecules. Both approaches result in formation of chiral nanoparticles with improved photoluminescence and emergence of chiral signals attributed to the optical transitions of the carbon core of the nanoparticles. It was shown that the optical activity of carbon dots originate from (i) the presence of chiral precursors attached to the carbon dot surface, which were observed in the 200-250 nm spectral region; (ii) hybridization of lower-energy levels of chiral chromophores in aggregates formed at the surfaces of or within nanoparticles, with chiral signals observed in the 250-300 nm spectral region; and (iii) interactions of chiral chromophores with polycyclic aromatic hydrocarbons and their aggregates with different configurations formed within carbon dots, which can be attributed to formation of the their chiral core.

Model of single-electron transistor based on prismanes

Ainur Duisenova^{1*}, Daulet Sergeyev²

¹*K. Zhubanov Aktobe Regional University, 34A Moldagulova avenue, 030000 Aktobe, Kazakhstan*

²*T. Begeldinov Aktobe Aviation Institute, 39 Moldagulova avenue, 030012 Aktobe, Kazakhstan*

*E-mail: ainura_duisenova@mail.ru

In recent years, the effect of correlated tunneling of single electrons has been used to solve the further reduction in the size of electronic elements. The essence of this effect is the Coulomb blockade of electron transport and orderly motion of elementary charges, arising due to their interaction by means of an electric field. This led to the birth of single-electronics, the "core" of which is electronic devices based on single molecules. In this work, within the framework of density functional theory, the transport properties of a single-electron transistor (SET) based on C₁₂H₁₂, C₁₂F₁₂, C₁₈H₁₂, C₁₈F₁₂ prismanes are model investigated. The optimization of prismane molecules was carried out using the exchange-correlation functional of the generalized gradient approximation (GGA), which allows to describe such structures most accurately. The electrostatic difference potential, molecular energy spectrum, and total energy SET are calculated on the basis of prismanes. It is shown that the area of Coulomb diamond SETs based on prismane with passivated hydrogen atoms (C₁₂H₁₂) is significantly larger than others, also significantly decreases when a hexagonal ring (C₁₈H₁₂) is added in the central part. It is revealed that the area of the Coulomb diamond SET based on the prismane passivated with fluorine atoms (C₁₂F₁₂) is smaller, but when a hexagonal ring (C₁₈F₁₂) is added in the central part, it increases noticeably. The values of gate voltage for opening prismane transistors with a minimum source-drain VSD voltage are determined. It is found that in transistors based on a – C₁₂F₁₂, b – C₁₂F₁₂ and c – C₁₂F₁₂ in the absence of gate voltage, current transport is blocked in the range of Source-Drain bias $\pm 3.73\text{V}$, $\pm 4.28\text{V}$ and $\pm 4.33\text{V}$ respectively, and in transistors based on a – C₁₂H₁₂, b – C₁₂H₁₂ and c – C₁₂H₁₂ in the absence of gate voltage, the Coulomb blockade acts within a small range of source-drain bias $\pm 0.25\text{V}$, $\pm 0.35\text{V}$ and $\pm 0.25\text{V}$ respectively. The conditions for switching transistors from the Coulomb blockade mode to the single-electron tunnelling mode are determined. The obtained results may be useful for the calculation of new types of SETs.

Acknowledgement

This research was supported by the Committee of Science of the Ministry of Education and Science of the Republic of Kazakhstan (grant № AP08052562).

Optimal distribution of catalyst in porous pellets for a quasi-steady-state reaction with Langmuir-Hinshelwood kinetics

Aigerim Kabiyeva^{1*}, Vsevolod Andreev², Piotr Skrzypacz³, Boris Golman^{4**}

¹Department of Chemical and Materials Engineering, School of Engineering and Digital Sciences, Nazarbayev University, 53 Kabanbay Batyr Ave, Nur-Sultan 010000, Kazakhstan

²Department of Heat Power Setups, Faculty of Energy and Electrical Engineering, Chuvash State University, Cheboksary 428015, Russia

³Department of Mathematics, School of Sciences and Humanities, Nazarbayev University, 53 Kabanbay Batyr Ave, Nur-Sultan 010000, Kazakhstan

⁴Department of Chemical and Materials Engineering, School of Engineering and Digital Sciences, Nazarbayev University, 53 Kabanbay Batyr Ave, Nur-Sultan 010000, Kazakhstan

The conditions for enhancing the performance of a porous catalyst granule with a controlled activity profile are investigated for a catalytic reaction with Langmuir-Hinshelwood kinetics. The nonisothermal reaction and diffusion in the pellets with spherical, cylindrical, and planar shapes are studied, considering the presence of external mass and heat transfer resistances. The objectives of this paper are to investigate the influence of kinetic parameters on the productivity of the catalyst pellet, to find the optimal distribution of active catalyst in a porous pellet in the quasi-steady-state nonisothermal reactions, and to determine the main trends and dependencies by varying the parameters, such as Biot numbers, Thiele modulus, etc .

The mathematical models for chemical reactions with diffusion and non-uniform activity distribution in porous catalyst pellets were derived and analyzed. The maximum productivity (or effectiveness factor) can be achieved by expressing the distribution of active catalyst as Dirac δ - function. Due to the fact that the δ -function activity profile can only be considered theoretically, the Gaussian activity distribution was also studied.

As a result, the optimal position of the Dirac δ - function for productivity maximization was found. Then, the range of values of step-size, Biot numbers, and Thiele modulus for which the Gaussian productivity is close to the δ - function was obtained.

The parametric study leads to the conclusion that the higher productivity of porous catalyst pellets can be reached with non-uniform activity distribution in a quasi-steady state rather than with a steady-state uniform case. In addition, extremal control analysis was performed based on Lagrange equations, and such controlled profiles give the minimum value of productivity, while all the profiles other than that will result in greater productivity.

Acknowledgment

This research was supported by the research grant 021220FD0351 from Nazarbayev University. [4] Aïtcin, P. C., & Flatt, R. J. (Eds.). (2015). Science and technology of concrete admixtures. Woodhead Publishing.

Ni–Ru-containing mixed oxide-based composites as precursors for ethanol steam reforming catalysts: effect of the synthesis methods on the structural and catalytic properties

Symbat Naurzkulova^{1*}, Marina Arapova², Bakytgul Massalimova¹, Vladislav Sadykov².

¹Taraz State University, Taraz, Kazakhstan

²Borshkov Institute of Catalysis, Novosibirsk, Russia

*E-mail: Simbat_3@mail.ru

To date, hydrogen is the most environmentally friendly fuel for various energy and heat generators (fuel cells, internal combustion engines and mobile power plants). In context of the green energy of the future, hydrogen is associated with a promising technology of electrochemical generators based on solid oxide fuel cells (SOFCs) with internal or external reformer of fuels, whose main qualities are environmental friendliness, mobility and high efficiency. Moreover, due to fuel source flexibility, such devices can successfully provide reforming of various carbon-containing fuels, including bio-renewable ones. Among others, a great attention is paid to the ethanol steam reforming process. Since the catalyst for internal fuel reforming in SOFC is a multifunctional layer supported on the anode, it must satisfy many requirements: (1) activity in the reaction of steam reforming of oxygenates (breaking C–C and C–H bonds), (2) thermochemical stability (resistance to sintering and carbonization), (3) compatibility with anode layers (stability to delamination and cracking) and (4) mixed ionic-electron conductivity. Today, it is known that some nanocomposite materials, including complex oxides of transition and rare-earth elements (RRE) with the structures of perovskite, fluorite, or spinel, have the aforementioned properties. Today, the synthesis of such composites with optimal characteristics is an urgent task of hydrogen energy. In this study, catalyst precursors based on perovskite–fluorite nanocomposites with the general formula $[\text{LaMn}_{1-x}\text{B}_x\text{O}_{3+\delta}/\text{Ln}_{1-y}\text{Zr}_y\text{O}_2]$ (1:1 by mass), B = Ni, Ru, Ln = Pr, Sm, Ce were synthesized by three different methods. Two synthesis methods — sequential polymeric method (formation of Ni- and Ru-containing perovskite from a polymer matrix in the presence of already formed fluorite oxide) and ultrasonic dispersion of as-prepared complex oxides in isopropanol with addition of surfactant — provide formation of nanocomposites with a developed interphase between phases. In the one-pot synthesis method from a polymer containing all cations, the perovskite phase is not formed due to La incorporation into the fluorite matrix, with inclusions of amorphous Mn oxides and NiO phase being present. As the result, the highest concentration of surface metal sites in reduced catalysts was revealed for nanocomposite prepared by the sequential polymeric method, while the lowest concentration was observed for samples prepared by the one-pot method. Catalytic activity of nanocomposites in ethanol steam reforming correlates with the surface density of metal sites. They are stable to coking and provide full conversion of ethanol and hydrogen yield above 70% at 650°C for 10 h.

NIR-emissive carbon dots produced from organic dyes via template-assisted method

Evgeniia Stepanidenko^{1*}, Ivan D. Skurlov¹, Pavel D. Khavlyuk², Dmitry A. Onishchuk¹, Aleksandra V. Koroleva³, Evgeniy V. Zhizhin³, Irina A. Arefina¹, Dmitry A. Kurdyukov⁴, Daniil A. Eurov⁴, Valery G. Golubev⁴, Alexander V. Baranov¹, Anatoly V. Fedorov¹, Elena V. Ushakova^{1,**} and Andrey L. Rogach^{5,6}

¹Center of Information Optical Technologies, ITMO University, Kronverksky Pr. 49, 197101 Saint Petersburg, Russia

²Chair of Physical Chemistry, TU Dresden, Zellescher Weg 19, 01069 Dresden, Germany

³Centre for Physical Methods of Surface Investigation, Saint Petersburg State University, Universitetskaya emb. 7-9, 199034 Saint Petersburg, Russia

⁴Laboratory of Amorphous Semiconductors, Ioffe Institute, 26 Politekhnicheskaya Str., 194021 Saint Petersburg, Russia

⁵Centre for Functional Photonics (CFP), Department of Materials Science and Engineering, City University of Hong Kong, Hong Kong 999077, China

⁶Shenzhen Research Institute, City University of Hong Kong, Shenzhen 518057, China

*E-mail: stepanidenko.e@mail.ru, **E-mail: elena.ushakova@itmo.ru

Luminescent carbon dots (CDs) are gaining much interest because of their advantageous properties including high photo- and chemical stability, efficient photoluminescence (PL) over a wide spectral range and low cytotoxicity. One of the current challenges is the synthesis of CDs with PL in the near infrared (NIR) spectral region, which are attractive for bio-related applications. In this work, we developed a template-assisted method for the formation of red and NIR-emissive CDs by annealing

of organic dye precursors with yellow (Rhodamine 6G - Rh) and NIR (IR1061) PL in the pores of mesoporous silica microspheres. This method allowed the formation of nanoparticles soluble in polar solvents, which is promising for bioimaging and sensing in cells and tissues. Correlation of morphology and chemical composition with optical properties of obtained CDs was revealed and two types of optical center responsible for the CDs emission were established: the carbon aromatic network and dye derivatives. By varying annealing temperature of IR-dye it was found that an increase of the temperature results in the formation and further growth of a carbon aromatic network with optical transitions in the visible spectral range, while dye-based optical centers are decomposed resulting in the decrease of optical density and emission intensity in the NIR spectral range. Finally, we were able to produce NIR emissive CDs with a PL band at 1085 nm, and photoluminescence quantum yield of 0.2%, which is the highest value reported so far for CDs with PL band longer than 1050 nm. Thus, the template-assisted method used here is a powerful tool for the controlled and tunable CDs synthesis.

Acknowledgement

This work was financially supported by the Russian Science Foundation (RSF22-13-00294).

Key factors and performance criteria in wearable strain sensors based on polymer nanocomposites

Aliya Zhagiparova^{1*}, Gulnur Kalimuldina^{1**}, Md. Hazrat Ali¹, Abdullatif Lacina Diaby², Sherif Araby^{1**}

¹Department of Mechanical and Aerospace Engineering, Nazarbayev University, Nur-Sul tan, 010000, Kazakhstan

²UniSA Online (STEM), University of South Australia, SA 5095, Australia

*E-mail: aliya.zhagiparova@nu.edu.kz

**E-mail: gkalimuldina@nu.edu.kz, Sherif.Gouda@nu.edu.kz

Recently, there has been a growing demand for wearable electronic devices/strain sensors in soft robotics body-health monitoring, human-machine interface, and human motion detection. Wearable strain sensors feature fast and multi-stimuli sensitivity, high flexibility, ultra-stretchability, and biocompatibility. Although the progress in flexible strain sensors is exponential, the production of wearable sensors undergoes several challenges, such as reliability and reproducibility. The development of flexible and stretchable strain sensors is growing within two streams: (i) engineering microstructure with high functionality to respond to various stimuli such as bending, twisting and tension/compression strains; and (ii) exploring novel materials including functional nanofiller and flexible substrates/matrixes. An in-depth understanding of the sensing mechanism of the flexible strain sensors based-polymeric nanocomposites is needed to fabricate reliable and reproducible sensors and move from the prototype phase into the industry phase. In this review, we discuss types of strain sensors and fabrication methods. Conductive polymers such as polyaniline and polypyrrole and functional fillers, including carbon-based and metal-based nanomaterials to synthesize wearable strain sensors, are systematically compared and discussed. Key parameters such as linearity, gauge factor (sensitivity) and hysteresis are explained in the context of the recently published work. Morphology measurements, structure-property relations and electromechanical properties of the flexible sensors are critically reviewed. Finally, current challenges and perspectives in relation to the wearable strain sensors are concluded.

Acknowledgement

This research was supported by research grant 240919FD3914 “Self-Charging Rechargeable Lithium-ion Battery” from Nazarbayev University

Application of 3DOM PI separator to lithium metal batteries with ionic liquids-based electrolyte

Yuma Shimbori^{*}, Hirokazu Munakata, Kiyoshi Kanamura^{**}

Department of Applied Chemistry for Environment, Graduate School of Urban Environmental Sciences, Toyko Metropolitan University, 1-1 Minamioosawa, Hachioji, Toyko, 192-0397, Japan

*E-mail: shimbori@inorg777.apchem.ues.tmu.ac.jp, **E-mail: kanamura@tmu.ac.jp

Ionic liquids have attracted attention as promising electrolyte candidates that can realize nonflammable rechargeable batteries. However, conventional polyolefin separators cannot be used due to low affinity with them, and glass filters with thicknesses of several hundred micrometers have been used as alternatives. Therefore, we have developed a three-dimensionally ordered macroporous polyimide (3DOM PI) membrane with a thickness of 30 micrometers as a separator having good affinity with ionic liquids. In this study, 3DOM PI separator was applied to Li metal batteries with [LiFSI]₁[Pyr₁₃FSI]₁ (FSI = bis(fluorosulfonyl)imide, Pyr₁₃ = N-methyl-N-propylpyrrolidinium) as an ionic liquid-based electrolyte, and its effect on the battery performance was evaluated.

Glass filter (Whatman, GF/A), surfactant-coated PP separator (Celgard, Celgard®3401) and 3DOM PI separator were used. The effect of separator on Li deposition/dissolution behavior was tested in Li (600 μm)/Li (20 μm) cells by applying a constant current of 1 mA cm^{-2} for 1 h. Fig. 1 shows the potential profiles of Li deposition/dissolution in the Li/Li cells with different separators. The cell with a glass filter showed a sudden decrease in the polarization potential during the initial Li deposition process, resulting in very small polarization in the following cycles. This behavior suggests the occurrence of internal short circuit due to inhomogeneous Li deposition. The cells with surfactant-coated PP separator and 3DOM PI separator showed the better cyclability. In Particular, the stable Li deposition/dissolution over 150 cycles was confirmed for the cell with 3DOM PI. As is well-known, large current distribution induces the inhomogeneous Li deposition/dissolution and causes internal short circuits. Therefore, the stable potential profile of the cell with 3DOM PI separator suggests that Li deposition/dissolution proceeds uniformly. In fact, the smoother deposition of Li was confirmed in the cell with 3DOM PI.

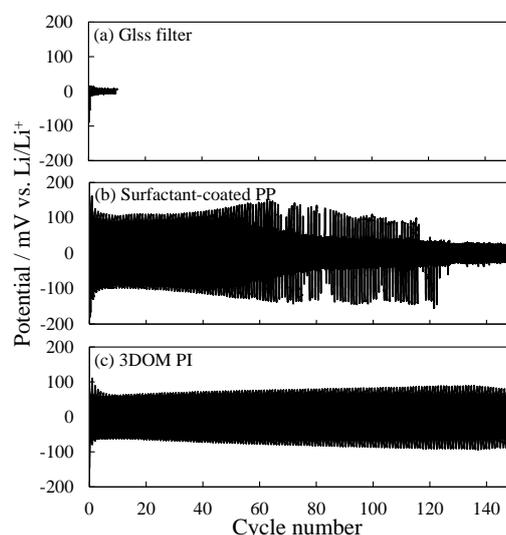


Fig. 1. Potential profiles of Li deposition/dissolution in the Li/Li cells with different separators.

Acknowledgement

This research was supported by JSPS KAKENHI Grant Number JP21J21182.

Charge-Transport Materials Impact on the Perovskite Solar Cells Stability

Artyom Novikov^{1*,**}, Marina Tepliakova¹, Olga Yamilova¹, Lyubov Frolova², Gennady Shilov², Nadezhda Dremova², Ivan Zhidkov^{3,4}, Ernst Kurmaev^{3,4}, Pavel Troshin², and Keith Stevenson¹

¹Skolkovo Institute of Science and Technology, Nobel St. 3, Moscow 121205, Russia.

²IPCP RAS, Semenov Prospect 1, Chernogolovka, 141432, Russia.

³Russia Institute of Physics and Technology, Ural Federal University, Mira 9 str., Yekaterinburg 620002, Russia

⁴M. N. Mikheev Institute of Metal Physics of Ural Branch of Russian Academy of Sciences, S. Kovalevskoi 18 str., Yekaterinburg 620108, Russia

*, ** E-mail: Artyom.Novikov@skoltech.ru

Perovskite solar cells (PSCs) represent one of the most promising photovoltaic technologies now reaching power conversion efficiency (PCE) values more than 25%. However, their commercialization is still hindered by the poor stability of complex lead halides comprising their active layer. It was shown repeatedly in previous works that charge-transport materials (CTMs) employed in PSCs can affect their operational stability significantly by reacting with the perovskite materials or, in contrast, protecting the perovskite. Yet, to date, there have been no systematic investigation of this issue.

This work presents a systematic study of the impact of both hole-transport (HTMs) and electron-transport (ETMs) materials on the photochemical stability of bulk of the perovskite films and finished perovskite solar cells. A large set of primarily inorganic and hybrid organic-inorganic bilayer charge-transport layers was investigated. An array of complementary physicochemical characterization techniques such as UV-vis absorption spectroscopy, X-Ray diffraction, X-Ray photoelectron spectroscopy, and scanning electron microscopy was employed to assess the rate of active layer degradation in contact with various CTMs under continuous illumination. Additionally, the PCE of the finished devices comprising different CTMs was tracked as function of exposure

time to estimate the solar cells lifetime under operation conditions.

The obtained results demonstrate a significant CTM influence on the perovskite stability. Among the HTMs it was shown that there is a strong correlation between the HTM's reduction potential and both bulk material and device stability, suggesting that redox reactions are the major source of HTMs adverse effect on PSCs stability.

In ETMs, however, a significant discrepancy between bulk material and device stability was observed, implying that more complex interfacial processes such as charge carrier trap formation or chemical processes in a very thin layer determine ETMs effect on the PSC stability.

Thus, in this work the crucial importance of proper CTM selection to achieve high PSC stability is demonstrated, several most promising CTMs are identified, and an important selection criterion for HTMs related to their redox properties is suggested.

Enhancement of the electrochemical performance of the cathode material $\text{NaNi}_{0.5}\text{Mn}_{0.5-x}\text{Zr}_x\text{O}_2$

Bagdaulet Shugay^{1*}, Aishuak Konarov^{1**}

¹*Department of Chemical and Materials Engineering, School of Engineering and Digital Sciences, Nazarbayev University, Nur-Sultan, 010000, Kazakhstan*

*E-mail: bagdaulet.shugay@nu.edu.kz, **E-mail: aishuak.konarov@nu.edu.kz

The development of the cathode material for beyond lithium-ion batteries plays a critical role in advancing technical progress and ensuring the long-term viability of our society. However, because of the poor performance of SIBs, many novel technical solutions are delayed or hindered. Our research work enhanced electrochemical parameters such as capacity retention and structural stability by proposing Zr ion doping because of the larger ionic radius compared to Mn and Ni ($r_{\text{Mn}^{(4+)}}=53$ pm, $r_{\text{Ni}^{(2+)}}=69$ pm, and $r_{\text{Zr}^{(4+)}}=79$ pm), which can enhance the bond of TM and oxygen atoms. The substitution of transition metals by Zr inactive metal ions leads to enlarged interlayer spacing for Na^+ and superior micro-nano level cathode structure with a high ion diffusion rate and unblocked diffusion paths for redox agents. Compared to non-substituted $\text{NaNi}_{0.5}\text{Mn}_{0.5}\text{O}_2$, the Zr substituted material exhibits more continuous phase transitions and lattice parameter changes and no substantial contraction of interslab spacing in the layered structure. Zr improves the reversibility of structural changes and structural stability, resulting in superior sodium battery performance. The highest capacity retention illustrates 3% doped material upon the charge, and discharge cycling tests 0.1C rate in the cut-off voltage of 2.0 to 4.5 V. The capacity retention of 3%-Zr doped material demonstrates a 10% improvement in capacity retention after 100 cycles.

Acknowledgement

This work was supported by the Ministry of Education and Science of the Republic of Kazakhstan Grant (AP08856179), "Boosting the electrochemical performance of the cathode material for beyond lithium-ion batteries".

Functionalized lignin-contained nanofibrous separator with high stability for safe lithium-ion batteries by UV-electrospinning

Yerkezhan Yerkinbekova^{1,2*}, Sandugash Kalybekkyzy^{1,2**}, Nurbol Tolganbek², Zhumabay Bakenov^{1,2}, Almagul Mentbayeva²

¹National Laboratory Astana, Nazarbayev University, Nur-Sultan, Kazakhstan

²Department of Chemical and Materials Engineering, School of Engineering and Digital Sciences, Nazarbayev University, Nur-Sultan, Kazakhstan

*E-mail:yerkezhan.yerkinbekova@nu.edu.kz, **E-mail: sandugash.kalybekkyzy@nu.edu.kz

As an indispensable part of lithium-ion batteries, separators play a key role in influencing the performance of lithium-ion batteries. In this study, a functionalization of lignin-contained nanofibrous separator for the LIBs by UV-electrospinning technique was presented. First, biopolymer lignin was modified to obtain a UV-active maleated lignin (ML). Further, ML was combined with UV-curable formulations (up to 30 wt%) and physical, as well as electrochemical characteristics of PAN/ML/HMEMO/PEGDA (PMHP) separators were investigated (Fig.1). The produced electrospun PMHP separators with a thickness of 25 μm enhanced their porosity, electrolyte uptake, heat resistance, and mechanical and electrochemical characteristics compared to a commercial Celgard-2400 separator due to their unique structure. The PMHP2 membrane with 20 % of ML content exhibited significantly higher ionic conductivity, $2.79 \times 10^{-3} \text{ S cm}^{-1}$ than that of the same cell with commercial Celgard-2400 ($6.5 \times 10^{-4} \text{ S cm}^{-1}$). Furthermore, Li dendrite formation was suppressed with the use of a PMHP2 membrane over lengthy 1000 cycles, which are proved by Li stripping/plating analysis.

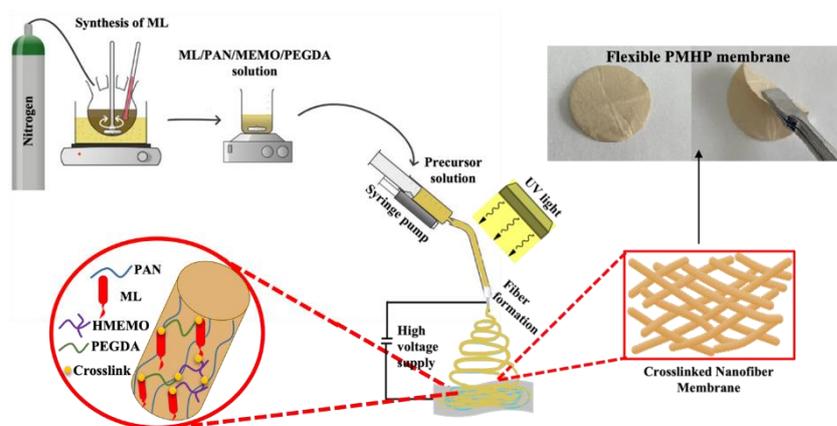


Figure 1. Schematic illustration of PMHP membrane by UV-electrospinning method

Acknowledgment

This research was supported by the research grant #AP08855889 “Development of Flexible and Safe Next-Generation Li-Ion Batteries” from the Ministry of Education and Science of the Republic of Kazakhstan

Laser-assisted ablation of UiO-66 metal-organic framework on the PET surface for novel electrode materials

Dmitry Kogolev*, Oleg Semyonov, Maksim Fatkullin, Olga Guselnikova, Pavel S. Postnikov**

Tomsk Polytechnic University, 634050 Tomsk, Russian Federation

*E-mail: kogolev@tpu.ru, **E-mail: postnikov@tpu.ru

Currently, one of the main trends in the chemistry of MOFs is their use as a raw material for the production of carbon-based nanomaterials, which have a high potential for further use as electrocatalysts. However, despite the steady progress in the development of technologies, carbonization is a complex and energy-intensive process that requires optimization and search for new solutions.

Recently, a Zhou's team of researchers from China and Singapore and co-workers has proposed a new approach towards the carbonization of thin layers of MOFs under the laser irradiation (Adv. Funct. Mater., 2021, 31, 2009057). As a result, the ordered and porous graphene nanostructures have been formed. In addition, metal inclusions of various nature, formed during laser processing, increased the physical and mechanical performance of the resulting material.

In this work, we developed a novel approach towards laser treatment of UiO-66 thin films immobilized on a nonconductive PET substrate. The structure of the composite material was evaluated using various techniques (XRD, FTIR, Raman, UV-Vis, XPS, SEM-EDX etc.), (Figure 1).

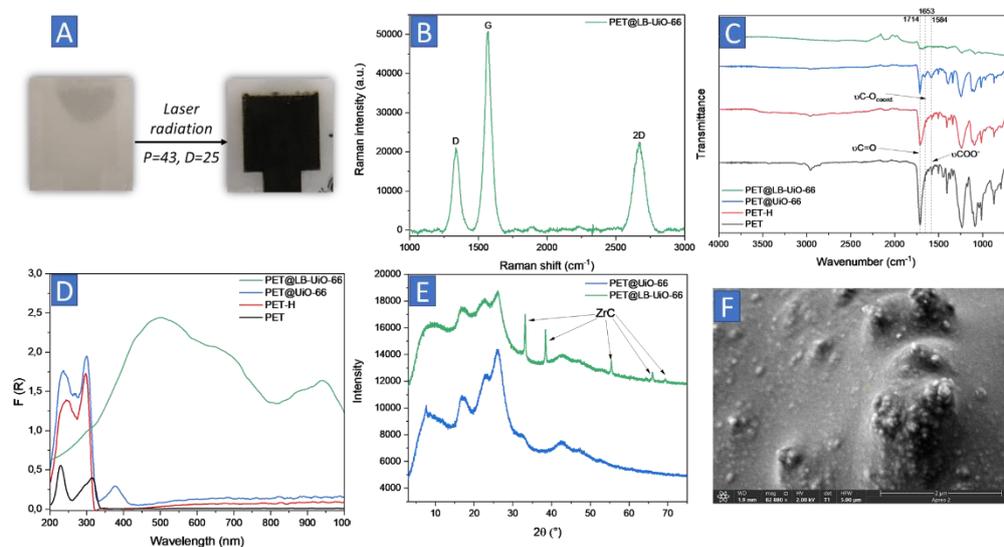


Figure 1 – (A) Images of PET@UiO-66 before and after laser radiation; (B) Raman spectra of PET@LB-UiO-66; (C) FTIR spectra of PET, PET-H, PET@UiO-66 and PET@LB-UiO-66; (D) UV-Vis spectra of PET, PET-H, PET@UiO-66 and PET@LB-UiO-66; (E) XRD pattern of PET@UiO-66 and PET@LB-UiO-66; (F) SEM image of PET@LB-UiO-66

Acknowledgement

This research was supported by PHC Kolmogorov № 075-15-2022-244.

KTiPO₄F and α -TiPO₄ as electrode materials for metal-ion batteries

Nikita Luchinin^{*}, Stanislav Fedotov^{**}

Skolkovo Institute of Science and Technology, 121205, Moscow, Russia

*E-mail: Nikita.Luchinin@skoltech.ru, **E-mail: S.Fedotov@skoltech.ru

Nowadays, 3d-metal phosphates are considered as promising electrode materials for metal-ion batteries (MIB). A phosphate group increases working potential of the M^{n+1}/M^{n+} redox pair and provides higher electrochemical and thermal stability that contribute to a longer life of electrodes up to several thousand charge/discharge cycles. Typically titanium redox transitions are not used for cathode applications because of low operating potential. Among titanium transitions Ti^{4+}/Ti^{3+} and Ti^{3+}/Ti^{2+} , the latter is supposed to demonstrate a lower working potential which is preferable for anode materials, however, due to the side conversion reactions, such examples are extremely rare. The d^1 electronic configuration of titanium (III) compounds is more preferable due to the higher electronic conductivity. Titanium reagents are comparable in cost with those of manganese, are produced widely and everywhere, non-toxic, and can be easily recycled, making titanium an attractive element for the industry.

Recently, our research group has developed several Ti(III) fluoride phosphates. One of them, KTiPO₄F, adopting the KTiOPO₄ (KTP)-type structure is a new compound, which was obtained in one stage via hydrothermal synthesis. Since, potassium and ammonium cations have the near ionic radius and crystallize in the same KTP structural type during the hydrothermal reaction, a new composition NH₄TiPO₄F can be prepared using ammonium salts by the same way as KTiPO₄F. Moreover, the similarity between the KTP and α -CrPO₄ structural types which enabled preparation of a new TiPO₄-compound with the α -CrPO₄ structure during the thermal decomposition of NH₄TiPO₄F.

Electrochemical investigation has shown the reversible activity of the KTiPO₄F/C electrode material in the potassium half-cell in the potential range from 2.0 to 4.0 V vs. K⁺/K. For the Ti^{4+}/Ti^{3+} couple, anomalously high potentials of the de/intercalation process were observed, reaching 3.6 V vs. K⁺/K, that can be explained by a combination of structural effects, as well as the inductive effect of the phosphate and fluorine-anionic groups. It should be noted that 3.6 V is still the record value of K⁺ de/intercalation for Ti^{4+}/Ti^{3+} redox transition. α -TiPO₄ shows reversible de/intercalation of Li⁺ at specifically high potentials for this Ti^{3+}/Ti^{2+} couple.

The report will consider in detail the peculiarities of hydrothermal synthesis of new Ti³⁺-containing compounds, the regularities of phase formation in the KTiPO₄F and α -TiPO₄ systems, as well as a detailed analysis of mechanisms of electrochemical de/intercalation of ions in the structure of the studied compounds.

Acknowledgements

This research was supported by RFBR (grant #21-53-12039).

A morphological study of solvothermally grown SnO₂ nanostructures for application in perovskite solar cells

Zhuldyz Yelzhanova¹, Gaukhar Nigmatova², Damir Aidarkhanov¹, Bayan Daniyar¹, Bakhytzhan Baptyayev³, Mannix P. Balanay⁴, Askhat N. Jumabekov⁵ and Annie Ng^{1*}

¹Department of Electrical and Computer Engineering, School of Engineering and Digital Sciences, Nazarbayev University, Kabanbay Batyr Ave. 53, Nur-Sultan 010000, Kazakhstan;

²Department of Chemical and Materials Engineering, School of Engineering and Digital Sciences, Nazarbayev University, Kabanbay Batyr Ave. 53, Nur-Sultan 010000, Kazakhstan;

³National Laboratory Astana, Kabanbay Batyr Ave. 53, Nur-Sultan 010000, Kazakhstan;

⁴Department of Chemistry, School of Sciences and Humanities, Nazarbayev University, Kabanbay Batyr Ave. 53, Nur-Sultan 010000, Kazakhstan;

⁵Department of Physics, School of Sciences and Humanities, Nazarbayev University, Kabanbay Batyr Ave. 53, Nur-Sultan 010000, Kazakhstan;

*E-mail: annie.ng@nu.edu.kz

SnO₂ is considered as one of the most effective electron transport materials used in solar cells. It has promising intrinsic properties such as wide bandgap, high electron mobility, high carrier transportation, and chemical stability. The majority of perovskite solar cells (PSCs) based on SnO₂ electron transport layers (ETL) is in the form of SnO₂ nanoparticles or quantum dots. The PSCs based on other SnO₂ nanostructured ETL show a large discrepancy in power conversion efficiency (PCE). One of the reasons is that the preparation of nanostructures is very sensitive to different growth factors, resulting in low reproducibility. Thus, the aim of this work is to empirically investigate the growth parameters of solvothermally grown SnO₂ nanorod arrays (NAs). It is noteworthy that the processing parameters such as growth pressure, substrate orientation, deionized (DI) water-to-ethanol ratio, types of seed layer, amount of acetic acid, and growth time have strong correlations with each other. For this reason, every parameter should be individually optimized. This work demonstrates the morphological control of solvothermally grown SnO₂ NAs by the systematic investigation of various growth parameters. This presentation will show the trend of morphological changes of SnO₂ nanostructure based on the obtained results. The outcomes present information, which provides the direction for future preparation of more reproducible SnO₂ nanomaterials for PSCs.

Acknowledgement

This research was supported by A. N. thanks Scientific Research Grant from Ministry of Education and Science of the Republic of Kazakhstan (grant no. AP08856931); Collaborative Research Grant from Nazarbayev University (grant no. 021220CRP0422) and the social policy grant. A. N. J. acknowledges Nazarbayev University Collaborative Research Grant (grant no. 021220CRP1922)

Switchable membrane materials based on electroactive polyazines

Ivan Prikhno^{1*}, Maria Komkova², Dmitry Petukhov^{1,2}, Andrei Eliseev^{1,2}

¹Department of Materials Science, Moscow State University, Moscow, Russia

²Department of Chemistry, Moscow State University, Moscow, Russia

*E-mail: ivan_prikhno@mail.ru

Rigid microporous polymers, such as PIM-1, are characterized by rather high selectivities in n-butane/methane pair (up to 58) together with high performance, useful for membrane gas separation for oil refineries. Electropolymerized azine dyes can be viewed as analogs of such polymers from the point of view of their microstructure. Electroactivity of these polymers allows one to hope for a possibility of switchability of properties of such membranes by external electric potential. So, the goal of the present work was to synthesize and study transport properties of membranes based on polyazine dyes.

Novel membrane materials based on polyazines were formed by electropolymerization of monomeric azine dyes on the surface of membranes of anodic alumina, having pores 40 nm in diameter, with sputtered golden conducting layer, in cyclic electrodeposition regime. Porosity and thickness of the polymer film were controlled by sweep rate and a number of cycles respectively.

According to electron microscopy studies continuous ultrathin layers with a thickness from 50 nm can be controllably grown. Membranes based on polyazines are shown to be selective for n-butane and water: poly(methylene green) membrane, obtained at a sweep rate of 50 mV/s, revealed an ideal separation factor of 73 for n-butane/methane pair. Poly(neutral red) membrane, obtained at the same sweep rate illustrated an ideal separation factor of 283 for water vapor/nitrogen pair. An effect of microstructure of polymers on selectivity of the layers was elaborated.

It is shown that selectivity of gas separation with electropolymerized polyazine membranes is determined by sorption selectivity of the polymer. Absorption characteristics of poly(methylene green) films on quartz microbalance showed significantly high solubility of n-butane in electropolymerized layers.

Application of electric potential, switched between -0,2 and 0,2 V, to poly(methylene green) membrane has made possible control of water vapor flux through membrane. Switch of potential from 0,2 to -0,2 V enables controlling water vapor flux from 4,0 to 2,3 m³/(m²*h).

Polyazine membranes, first described in the present study, illustrate strong potential for gas dehumidification, while their electroactivity allows controlling their permeability by application of electric potential.

Acknowledgement

This research was supported by RSF project №20-79-10205.

Composite aluminosilicate material based on halloysite and MCM-41 as a support for highly efficient hydrotreating catalysts

Nikolai Vinogradov^{1,2*}, Aleksandr Glotov², Aleksey Pimerzin^{1,2,3}

¹*Samara State Technical University, Samara, Russia, Molodogvardeyskaya st. 244*

²*Gubkin Russian State University of Oil and Gas, Moscow, Russia, 65 Leninsky Prospekt*

³*Gazprom Neft-Industrial Innovations LLC, Russia, St.Petersburg, Doroga v Kamenku st. 74*

*E-mail: nikkodym@gmail.com

Modern oil refining faces two important tasks: meeting the ever-increasing demand for high-quality motor fuels that meet stringent environmental requirements. No less important is the problem of processing heavy and residual raw materials, the quality of which does not allow obtaining products that meet modern requirements. The hydrotreatment process makes it possible to effectively remove undesirable components from the processed raw materials, in particular, sulfur-containing substances. The main direction of increasing the efficiency of the hydrotreatment process is the improvement of the applied catalytic systems.

Traditional hydrotreating catalysts are based on Co(Ni) and Mo(W) metals deposited on a porous support - γ -Al₂O₃. One of the ways to improve catalysts is to use modified composite supports. The promising material for catalysts modifying is halloysite - aluminosilicate nanotubes with a number of features: large mesopore size - 20-50 nm, chemical anisotropy of the surface and internal cavities of the material. This material can be modified in many ways, in particular on the surface or inside the tubes, a silicate material of the MCM-41 type can be obtained.

In this work, sulfide CoMo catalyst on traditional and composite halloysite supports were investigated. The obtained materials were characterized by a wide range of physical-chemical methods: TPR, Porosimetry, TEM, XPS, XRD. Prepared catalysts were investigated in the hydrotreatment of straight-run diesel fraction and mixed feedstock with up to 40% vol. light catalytic cracking gas oils. The influence of technological parameters on the efficiency of the process was investigated.

As a result, an increased efficiency of catalysts based on halloysite nanotubes was shown. The main reason may be the improvement of diffusion properties due to the system of large transport pores. indicated. The increased activity of halloysite catalysts in hydrogenation can be associated with increased dispersity of sulfide particles, caused by a weakening of the interaction between the active phase and the support.

Acknowledgement

This research was supported by the Russian Science Foundation, grant 19-79-10016.

High-power and inexpensive organic negolyte for redox flow battery based on anthraquinone sulfo-derivatives mixture

Dmitry Chikin¹, Lilia Abunaeva¹, Artem Glazkov¹, Kirill Karpenko^{1,2}, Mikhail Petrov^{1*}

¹Mendeleev University of Chemical Technology of Russia, Moscow, Russia

²N. D. Zelinsky Institute of Organic Chemistry of RAS, Moscow, Russia

*E-mail: mikepetrov@gmail.com

In recent years, various highly efficient energy storage devices have become popular as an efficient replacement for peak power plants. Redox flow batteries (RFB) and especially vanadium redox flow batteries (VRFB) are considered as an especially promising large-scale energy storage devices. VRFB have already been commercialized but it's further spread is limited by the high cost of energy storage with the main contribution of vanadium electrolyte price. In this regard, new types of electrolytes are being actively developed and researched, which can not only provide both high power and capacity but also be inexpensive.

One of the most promising options is anthraquinone-bromine RFBs (ABRFBs), which demonstrate high key characteristics and use only abundant raw compounds (bromine and various anthraquinone sulfo-derivatives). But most works is dedicated to single and expensive anthraquinone sulfonated derivative 2,7-AQDS used as a negolyte while it can be obtained in a mixture with other derivatives (2,6-AQDS disulfo-derivative and monosulfo-2-AQS) due to the anthraquinone sulfonation reaction with oleum. It has been shown that this mixture can be used as ABRFB negolyte without significant damage to key metrics. To optimize the composition of this mixture a series of syntheses was carried out with a change in key parameters - temperature, duration, mass ratio of reagents.

The redox behavior of the resulting mixtures was characterized using cyclic voltammetry, chronoamperometry, and square wave voltammetry. Also, the synthesized mixtures were tested as a negolyte of an anthraquinone-bromine redox flow battery. Polarization curves were obtained for various SOC and a series of charge-discharge tests were also carried out. The methods of electrochemical impedance spectroscopy and synchronous spectroelectrochemistry were also used. Redox stability of the synthesized mixtures was characterized using a symmetrical discharge cell. Finally, using reference electrodes based on Luggin capillaries, the polarization curves of the anode and cathode half-cells were determined, which made it possible to estimate the structure of energy losses arising during the operation of the flow battery. Obtained data shows that, according to the main metrics, the composition based on the synthesized mixture is comparable to single 2,7-AQDS.

Acknowledgement

This research was financially supported by the Russian Science Foundation (project 21-73-30029).

Effects of climate variability and climate change on wind power integration into power systems

Ekaterina Fedotova^{1, 2*}, Julia Kozlova^{1, 2}

¹*Moscow Power Engineering Institute, Moscow Krasnokazarmennaya 14*

²*Institute of Energy Куьуфксп Russian Academy of Science, Moscow Nagornaya 31*

*E-mail: e.v.kasilova@gmail.com

Intermittence associated with the very nature of renewable energy sources determines a fundamentally new class of problems related to account for climatic and meteorological characteristics when planning the development of energy systems. That leads to a need for a detailed study of the temporal and spatial variability of the renewable energy climate factors. Particularly, the wind speed is known to be significantly influenced both by the climate change and the multidecadal natural variability while a gap in understanding details of these processes still exists for many regions around the world.

The presented work was aimed to investigate the long-term dynamics of the wind speed field across the Northern Eurasia looking for options to facilitate wind power integration into the existing power systems. The latest generation climate datasets were validated against direct measurements data and used for further calculations. A detailed analysis considering the spatial structure of the wind speed fields has been fulfilled with consecutive evaluation of the long-term wind power potential dynamics.

The representative samples of the climate data were established to be utilized as inputs into the energy models. An approach has been proposed towards optimizing working conditions of the wind power units taking an advantage of the wind speed spatial features found before. It has been shown that proper accounting for the wind variability allows for a noticeable increase of an average wind power capacity utilization. The most pronounced effects on wind power integration is reached for the episodes of very high and very low speed values.

A forecast approach has been developed to assess a combined effects of the energy load evolution and the long-term wind speed changes on the power systems. The main fundamental challenges and opportunities have been identified in integration of the wind power considering the Northern Eurasia macro-region and taking into account the climate change impacts under realistic assumptions.

Acknowledgement

This research was supported by the Russian Science Foundation (project No. 18-79-10255).

Composite-track etched membranes for environmental applications

Anastassiya Mashentseva

The Institute of Nuclear Physics of the Republic of Kazakhstan, 050032 Almaty, Kazakhstan

E-mail: a.mashentseva@inp.kz

The photocatalytic removal of various classes of organic and inorganic pollutants is one of the most widely used methods due to its high efficiency, low cost and simplicity. The current research in this area is aimed at developing new technologies for producing high-performance and low-cost catalysts. Various types of composite materials have attracted much research attention in the field of photocatalysis owing to their advantages, such as their design flexibility, improved physical and chemical properties and stability.

The photocatalytic removal of various classes of organic and inorganic pollutants is one of the most widely used methods due to its high efficiency, low cost and simplicity. The current research in this area is aimed at developing new technologies for producing high-performance and low-cost catalysts. Various types of composite materials have attracted much research attention in the field of photocatalysis owing to their advantages, such as their design flexibility, improved physical and chemical properties and stability.

In this study a composite TeMs based on metals of the copper subgroup demonstrated high catalytic activity for removal of different classes of water pollutant i.e dyes, nitrophenols, pesticides. Cu and CuO-based composites have been shown to exhibit high efficiency in the sorption of As(III) and Pb(II) ions. Some important advantages of such catalysts and sorbents are their ease of use, low cost and ease of production, as well as the possibility for multiple reuses without additional activation and regeneration procedures.

Acknowledgement

This research was supported by the Ministry of Education and Science of the Republic of Kazakhstan (grant No AP08855527)

P-doped coffee ground-derived hard carbon for boosting sodium-ion batteries

Madina Kalibek^{1*}, Aishuak Konarov^{2**}, Zhumabay Bakenov³

¹*School of Engineering and Digital Sciences, Nazarbayev University, 53 Kabanbay Batyr Ave., Nur-Sultan 010000, Kazakhstan*

*E-mail: madina.kalibek@nu.edu.kz, **E-mail: aishuak.konarov@nu.edu.kz

The paper proposed the facile and successful preparation of P-doped coffee ground-derived hard carbon using H₃PO₄ as a dopant material for sodium-ion batteries. The manipulation with 1-3 M of H₃PO₄, contributed to finding the optimal concentration for the maximum incorporation of phosphorus ions into the carbon framework. The use of 2 M of H₃PO₄ dopant material for hard carbon as anode for sodium-ion battery delivers promising electrochemical performance. P-doped coffee ground-derived hard carbon carbonized at 1300 °C exhibits a high reversible capacity of 341 mAh g⁻¹ at 20 mA g⁻¹ (83 % retention upon 100 cycles). This excellent electrochemical performance of P-doped hard carbon can be attributed to microporous structure, large interlayer spacing, and the formation of C-P bonds.

Acknowledgment

This work was supported by the Ministry of Education and Science of the Republic of Kazakhstan Grant (AP09259165), “Utilization of the biowaste-derived carbon and enhancement of its electrochemical performance via doping”.

Reduced form of Prussian Blue (Prussian white) cathode material for application in two electrode systems

Olzhas Kaupbay*, Fyodor Malchik, Kaingali Maldybayev, Tatyana Kan, Saule Kokhmetova, Andrey Kurbatov, Alina Galeyeva, Marzhan Kyatova,
al-Farabi Kazakh National University, Center of Physical-Chemical Methods of Research and Analysis, Almaty, 050012, Kazakhstan

*E-mail: rustyryan799@gmail.com

With an increasing annual demand for energy storage devices there is a progressive attention on the research for rechargeable batteries. Even though traditional lithium-ion batteries offer great performance, they are unable to satisfy huge consumption worldwide, since the limits on availability of lithium resources. Sodium-ion batteries can be potential substitute for LIBs owing cost-effectivity and abundance of sodium salts.

Since cathode material of a battery has a great impact on the final performance of the battery, more and more researches are progressively focused on optimizing their properties to enable them for practical use. One of the promising cathode materials are representatives of Prussian Blue analogues, owing to their high energy density, wide range of working potentials and chemical and electrochemical stability. Their common representative – $\text{Na}_2\text{FeFe}(\text{CN})_6$ offers good discharge capacity and long cycling life, owing two RedOx reaction with both iron atoms ($\text{Fe}^{2+} \leftrightarrow \text{Fe}^{3+}$). However during traditional synthesis methods – straightforward precipitation, the product always comes in half-charged (half-oxidized) state – $\text{NaFe}^{\text{III}}\text{Fe}^{\text{II}}(\text{CN})_6$ due to its ease of oxidation of outer iron ion (for example by air oxygen). It is cause for only half of full capacity during 1st charge and does not seem to be a problem for three-electrode systems, where counter electrode has capacity in a huge excess. However, for two-electrode systems, where working and counter electrodes are ought to be balanced (at first cycle) in terms of loading mass and capacities, it is a problem.

Herein, the synthesis of PBA with reduced form (Prussian white) is presented and compared electrochemically with precipitation synthesis method.

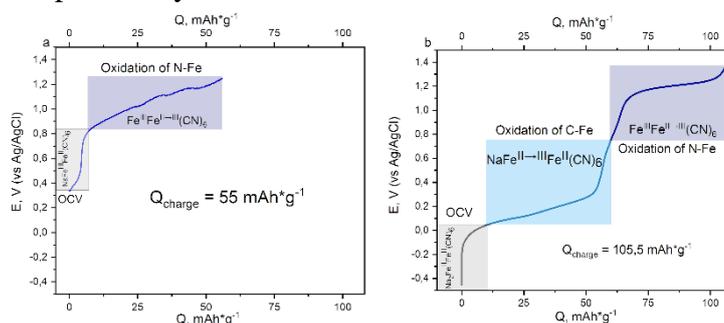


Figure 1 – First charges of PB materials synthesized by different methods

Acknowledgement

This research was supported by Science Committee of the Ministry of Education and Science of the Republic of Kazakhstan (Grant No. AP08856725).

Boosting MXene capacity by self-oxidation in air atmosphere for water-in-salt electrolyte-based supercapacitor

Fyodor Malchik^{*1}, Kairgali Maldybayev¹, Tatyana Kan¹, Saule Kokhmetova¹, Andrey Kurbatov¹, Alina Galeyeva¹, Olzhas Kaupbay¹, Marzhan Kiyatova¹, Netanel Shpigel²

¹*al-Farabi Kazakh National University, Center of Physical-Chemical Methods of Research and Analysis, Almaty, 050012, Kazakhstan*

²*Department of Chemistry and BINA – BIU Center for Nanotechnology and Advanced Materials, Bar-Ilan University, Ramat-Gan 5290002, Israel*

*E-mail: Frodo-007@mail.ru

The use of $\text{Ti}_3\text{C}_2\text{T}_x$ (MXene) electrodes for energy storage applications is gaining momentum in recent years. The ability of the MXene to host a large variety of mono and multivalent ions regardless of their charge or ionic radius makes it an attractive anode for aqueous and non-aqueous batteries and supercapacitor devices.

In this work, we demonstrate controllable $\text{Ti}_3\text{C}_2\text{T}_x$ oxidation in an ambient atmosphere with the formation of TiO_2 nanoparticles which serve as electrochemically active (battery type material) while preserving MXene electrochemical properties (capacitive type) utilizing water-in-salt (WIS) (14 M LiCl) electrolyte. There are several advantages of the proposed hybrid $\text{TiO}_2/\text{Ti}_3\text{C}_2\text{T}_x$ anode for water-based devices: 1) uniformly distributed TiO_2 nanoparticles in the MXene matrix open the space between MXene flakes causing faster ion penetration and increasing the rate capability of the hybrid anode; 2) in the spot synthesized TiO_2 serves as source of additional energy storage material with maximum negative value (for water-based electrolytes) of intercalation/deintercalation potential; 3) MXene serves as a matrix for battery material with the possibility to create flexible free-standing electrode without additional binding components, moreover providing fast electronic conductivity. Precise control of MXene suspension oxidation by air oxygen doesn't require any additional oxidizers and elevated temperature and allows to create of the adjusted amount and lateral size of TiO_2 with ideally uniform distribution.

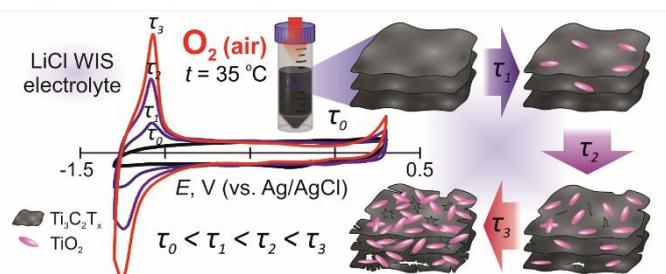


Figure 1 – Sketch of $\text{Ti}_3\text{C}_2\text{T}_x$ air oxidation process and its subsequent CV response in WIS electrolyte.

Acknowledgement

This research was supported by Science Committee of the Ministry of Education and Science of the Republic of Kazakhstan (Grant No. AP09058354).

Ti doped ZnO films deposited by magnetron sputtering for gas sensors

Yerkebulan Kadyrov¹, Baktiyar Soltabayev^{1,2*}, Zhumabay Bakenov³, A.Mentbayeva⁴

¹*National Laboratory Astana, Nazarbayev University, Nur-Sultan, Kazakhstan.*

²*School of Engineering, Nazarbayev University, Nur-Sultan, Kazakhstan*

*E-mail: baktiyar.soltabayev@nu.edu.kz

The use of semiconducting metal oxides to develop highly sensitive CO₂ gas sensors remains an important approach in the field of gas sensing applications. Zinc oxide (ZnO) as semiconducting metal oxide is considered as the promising resistive-type gas sensing material [1]. In this research, we describe the synthesis, characterization, and application of a very promising CO₂ gas sensing material ZnO doped with different concentration of Ti and synthesized by magnetron sputtering [2] method. The structural, morphological and optical characteristics of the synthesized specimens were studied. Using a gas sensing measurement device, the CO₂ sensing capabilities of different concentrations of Ti in ZnO structures were evaluated. The sensitivity, operating temperature, and response/recovery time were systematically investigated based on the change in electrical resistance of the materials in the presence of CO₂ gas. Experimental results confirmed that 60W of Ti (DC) power of TZO showed a maximum (100 ppm) response to CO₂ gas at 200°C operating temperature. The sensing mechanism of the TZO films with different concentration of Ti is discussed in detail. We believe that the Ti-doped, columnar ZnO nanostructure is a potential material for semiconductor-oxide-based CO₂ gas sensors.

Acknowledgement

This research was supported by the research grant 021220FD2201 “Development of highly sensitive MOS based nano-film gas sensors” from Nazarbayev University. References

Catalytic Effects of Different Loadings of Ni nanoparticles Encapsulated in Few Layers N-doped Graphene and Supported by Ndoped Graphitic Carbon in Li-S batteries

Nurzhan Baikalov^{1*}, Almagul Mentbayeva², Aishuak Konarov², Yongguang Zhang³, Zhumabay Bakenov^{1,2**}

¹National Laboratory Astana, School of Engineering and Digital Sciences, Nazarbayev University, NurSultan, Kazakhstan

²School of Engineering and Digital Sciences, Nazarbayev University, Nur-Sultan, Kazakhstan

³School of Materials Science and Engineering, Hebei University of Technology, Tianjin 300130, China

*E-mail: nurzhan.baikalov@nu.edu.kz, **E-mail: zbakenov@nu.edu.kz

Lithium-ion batteries (LIB), despite the fact that they have opened up new opportunities for the rapid development of modern portable devices, mainly use intercalation cathodes represented by transition metal oxides and phosphates as cathodes, which are unable to meet the requirements of electric vehicles and high energy storage systems and have several disadvantages associated with the high cost of materials and safety problems. In this regard, Lithium-Sulfur batteries (Li-S) have been considered as promising next generation energy storage systems due to high theoretical energy density (2600 Wh kg⁻¹) with sufficient operating voltage potential of ~2.1 V (vs Li/Li⁺) alongside its low cost and non-toxicity. Moreover, sulfur has low cost, considerably less environmental impact and abundant resources. However, the implementation of Li-S batteries is hindered due to a number of drawbacks such as low conductivity of sulfur, shuttle of soluble intermediates (polysulfides, LiPS), poor reaction kinetics, dendrite growth on lithium anode and volumetric expansion of cathode upon reduction to Li₂S₂/Li₂S which leads to structural degradation and lower the cycle life of batteries. Several works introduced the application of carbon-based materials decorated with transition metals/electrocatalysts as potential polysulfides trapping systems. However, the use of transition metal nanoparticles is complicated due to lower stability and tendency to aggregation upon cycling. In this regard, it is important to physically separate metal nanoparticles with a uniform distribution and protect them from aggregation and air oxidation. Given that Ni nanoparticles improved reaction kinetics and showed a large potential catalytic effect, it would be worthwhile to comprehensively understand the role of metal loadings in Li-S electrochemistry, which was rarely reported in previous literature. In the present research catalytic effects of Ni nanoparticles encapsulated in N-doped graphene supported by layers of graphitic carbon as electrocatalysts were investigated.

Acknowledgement

This research has been funded by the Science Committee of the Ministry and Science Education of Republic of Kazakhstan (Grant No. AP09259764).

A study of Cu-doping effects in Na₂Mn₃O₇ layered cathode material for Sodium-ion battery

Lunara Rakhymbay^{1*}, Aishuak Konarov^{1**}, Zhumabay Bakenov¹

¹*School of Engineering and Digital Sciences, Nazarbayev University, 53 Kabanbay Batyr Ave., Nur-Sultan 010000, Kazakhstan*

*E-mail: lunara.rakhymbay@nu.edu.kz, **E-mail: aishuak.konarov@nu.edu.kz

In recent years, sodium-ion batteries (SIBs) attracted great attention owing to their rich Earth-abundant resources, environmental friendliness, low cost, and high energy efficiency. To be compared to lithium-ion batteries the developing advanced cathodes play a key role in enhancing the performance of SIBs. Layered transition metal oxides Na_xMO₂ (M = Co, Mn, Fe, Ni, etc.) are one of the promising cathodes for SIBs due to the variable composition, abundant active center, and good electrochemical performance. Among these layered transition metal oxides, layered manganese oxide-based materials have been attracted because of the nontoxicity of manganese, economical price of precursors, and high capacity. Metal atom doping was extensively studied in layered cathodes for the purpose of enhancing the performance of SIBs. By means of doping can result in improvement of structure stability and capacity retention.

This research investigates developing Cu-substituted P1-type Na₂Mn₃O₇ in order to improve electrochemical performance. The Cu-substituted Na₂Mn₃O₇ was synthesized via the solid-state method in an oxygen atmosphere. The XRD, SEM, TEM, and electrochemical studies were employed to systematically investigate crystal structure, surface morphology, and cyclability.

Acknowledgment

This work was supported by the Ministry of Education and Science of the Republic of Kazakhstan Grant (AP08856179), "Boosting the electrochemical performance of the cathode material for beyond lithium-ion batteries" and by the Nazarbayev University Faculty-development competitive research grant (080420FD1914) "Rational design of new anionic-redox based active material for rechargeable sodium-ion batteries"

Rosatom state atomic energy corporation capacities and technologies in hydrogen energy

Ekaterina* S. Solntseva, Miron V. Borgulev, Vassily L. Konstantinov
Science and Innovations Private Enterprise, Rosatom State Atomic Energy Corp.

Moscow, Russia.

*E-mail: EkSeSolntseva@rosatom.ru

Rosatom State Atomic Energy Corporation is one of leaders in hydrogen energy development in Russia. The goal of Rosatom is to become one of drivers of hydrogen energy sector of Russia and technology leader and developer of hydrogen energy projects.

Rosatom State Atomic Energy Corporation takes part in implementation of the Schedule of measures on hydrogen energy development in Russian Federation until 2024 [1], Concept of hydrogen energy development in Russian Federation [2], and in preparing of Russian Federation Ministry of Energy Complex program of low-carbon hydrogen economy development.

R&D program on hydrogen energy and decarbonisation is implemented at Rosatom managed by Science and Innovations Private Enterprise. In February, 2022, Rosatom Strategic program on hydrogen energy development was approved. This Strategic program sets the priority of development of scientific research and own technologies of low-carbon energy including all the process flow of hydrogen energy and decreasing of carbon footprint [3].

Development of own import independent technologies on all the stage of hydrogen energy process flow including CCUS during hydrogen production from natural gas leads to establishing of a new sector of national economy with high export potential. Gathered for decades experience provide State Corporation with prominent technological and R&D potential in development in hydrogen energy technologies.

Rosatom State Atomic Energy Corporation provides R&D and technology promotion in the following fields:

- Nuclear power and technology plant for hydrogen production based on high-temperature gas-cooled reactor;
- Hydrogen production via methane pyrolysis, water electrolysis and aluminium-water interaction technology;
- Development of steam methane reforming technology for hydrogen production at the nuclear power and technology plant for hydrogen production based on high-temperature gas-cooled reactor;
- Materials and technology development for solid oxide, proton exchange polymer and alkaline electrolytic and fuel cells;
- Development of proton exchange membranes for electrolytic and fuel cells;
- Production of composite pressure vessels for hydrogen transportation and storage;
- Materials development for metal hydride hydrogen storage.

Wide experience in nuclear power plants hydrogen safety leads Rosatom to a wide range of research on hydrogen energy facilities safety. Rosatom take parts in Rosstandart Technical committee No. 29 and is ready to take part in development of Eurasian Economic Commission interstate standards.

Rosatom State Atomic Corporation is ready to develop R&D cooperation with in the above-mentioned fields.

Obtaining cellulose fibers from the fallen leaves

Gaukhar Smagulova^{1,2*}, Azamat Taurbekov^{1,2**}, Bayan Kaidar^{1,2}, Akniyet Baltabay^{1,2}, Zulkhair Mansurov^{1,2}

¹*Al Farabi Kazakh National University, Al-Farabi avenue 71, Almaty, Kazakhstan*

²*Institute of Combustion Problems, 172 Bogenbay batyr str, Almaty, Kazakhstan*

*E-mail: smagulova.gaukhar@gmail.com, **E-mail: a.taurbek@gmail.com

Cellulose and its derivatives are the most common polymers in nature. The wide range of products made from cellulose determines the need for constant growth of its production.

Cellulose is composed of beta-1,4-linked glucopyranose groups, which form a linear homopolymer, where the monomers are unfolded 180° relative to each other. It is an important structural component of the cell walls of various organisms of plant materials. To extract cellulose from plant biomass, it is necessary to free it from other plant tissue substances - hemicellulose, resins and fats by means of chemical heat treatment. The main component that they want to get rid of when making cellulose is lignin. The process of removing lignin from chopped wood is called delignification. Depending on how completely lignin and hemicellulose will be dissolved in the process of chemical - thermal treatment, the properties of cellulose fibers change. Thus, the quality indicators of cellulose depend both on the choice of raw materials and on the methods and conditions of its processing, which make it possible to provide a different degree of removal of lignin and other substances accompanying cellulose.

In the work, we used fallen leaves selected in the autumn of 2021 on the territory of the University of KazNU named after al-Farabi in Almaty. Chemical-thermal treatment was used for the production of cellulose: washing, grinding, homogenization, , extraction, washing, ultrasonic treatment, drying.

After chemical-thermal treatment, the content of cellulose increased to 92.5%, and the content of amorphous lignin decreased to 4.8%. The average fiber diameter after processing is 20 µm. As a result, during alkaline chemical-thermal treatment, the destruction of intermolecular ether bonds, which are stitched with hemicelluloses and lignin, occurs. Also, the effect of alkali on cellulose microfibrils reduces the degree of cellulose polymerization and cellulose swells, this leading to an increase in its fibers.

Acknowledgement

The Ministry of Education and Science of supported this work the Republic of Kazakhstan through the project AP13068375 «Obtaining cellulose materials based on vegetable wastes and mineral additives».

Obtaining compositional fibers via electrospinning method

Bayan Kaidar^{1,2*}, Gaukhar Smagulova^{1,2**}, Aigerim Imash², Zulkhair Mansurov^{1,2}

¹*Al Farabi Kazakh National University, Al-Farabi avenue 71, Almaty, Kazakhstan*

²*Institute of Combustion Problems, 172 Bogenbay batyr str, Almaty, Kazakhstan*

*E-mail: kaydar.bayan@gmail.com, **E-mail: smagulova.gaukhar@gmail.com

Carbon fibers can be defined as fibers composed of 90 % or more carbon atoms. Due to their unique physical, chemical and mechanical properties, carbon fibers and composites based on them occupy a special place among carbon materials.

This research presents the results of the synthesis of carbon-NiO and PAN/CTP/Fe₃O₄ composite fibers. Fibers doped with metal oxides nanoparticles are of practical interest for applications in sensors, energy storage systems, photocatalysts, etc. Three-component initial fibers based on polyacrylonitrile (PAN), coal tar pitch (CTP), and metal oxide (NiO or Fe₃O₄) nanoparticles were obtained. CTP was obtained by thermal treatment of coal tar, NiO by solution combustion synthesis and Fe₃O₄ by chemical condensation. PAN and CTP are a source of carbon, but each of them plays its own specific role. PAN is the basis of carbon fibers and a fiber-forming material, CTP is a technogenic waste added to replace polymer particles. The fibers were obtained using the electrospinning method, which makes it possible to use complex suspensions and obtain fibers of various diameters. PAN:CTP:NiO fibers were obtained. Next, the processes of stabilization and carbonization of the fibers were carried out. The fibers at each stage were examined by scanning electron microscopy and EDAX. The result of the synthesis was carbon/NiO fibers with a diameter of 100-300 nm and PAN/CTP/Fe₃O₄ with a diameter above 100 nm. The resulting fibers are promising for practical applications due to the one-dimensional structure of the fibers and better adhesion between the fiber and metal oxides nanoparticles.

Acknowledgement

The research was conducted as part of the grant OR11465430 under the special-purpose funding program on the topic «Development of New Structural Composites to Develop the Innovation Industry of the Republic of Kazakhstan» under the subprogram «Development of Carbon Fiber Production Technology and Carbon Fiber Application as Sensors and Carbon Fiber Reinforced Plastics».

Maximizing specific capacity of nutty hard carbon: Impact of treatment conditions on structural and electrochemical properties

Nardana Bazybek*, Maksat Maratov, Aishuak Konarov

School of Engineering and Digital Sciences, Nazarbayev University, Kabanbay Batyr Ave. 53, Nur-Sultan, 010000, Kazakhstan

*E-mail: nardana.bazybek@alumni.nu.edu.kz

Hard carbon (HC) has attracted tremendous attention in sodium ion batteries (SIBs) as promising negative electrode material due to its low cost, environmental friendliness and stable cycling performance. However, due to the limited capacity and low initial columbic efficiency (ICE), the actual full cell application of HC faces significant obstacles. Therefore, preparation process was optimized to investigate the impact of the pre-treatment conditions and degree of graphitization on electrochemical performance and to resolve abovementioned problems. By increasing the carbonization temperature, a high degree of graphitization was attained along with increased reversible capacity and decreased ICE. Additionally, a substantial correlation was shown between the pre-oxidation with structural characteristics and electrochemical performance. A higher specific capacity was achieved by obtaining HC with large domain sizes, low surface areas, and porosities, as shown by structural characterization. The walnut shell derived HC with pre-oxidation of 300°C and carbonization temperature of 1400°C delivered a high reversible capacity of 360 mAh/g with good capacity retention in a Na cell. Moreover, this research illustrated that the pre-oxidation increased the amount of C=O bond which improved the adsorption capacity of sodium ions and further increased the specific capacity.

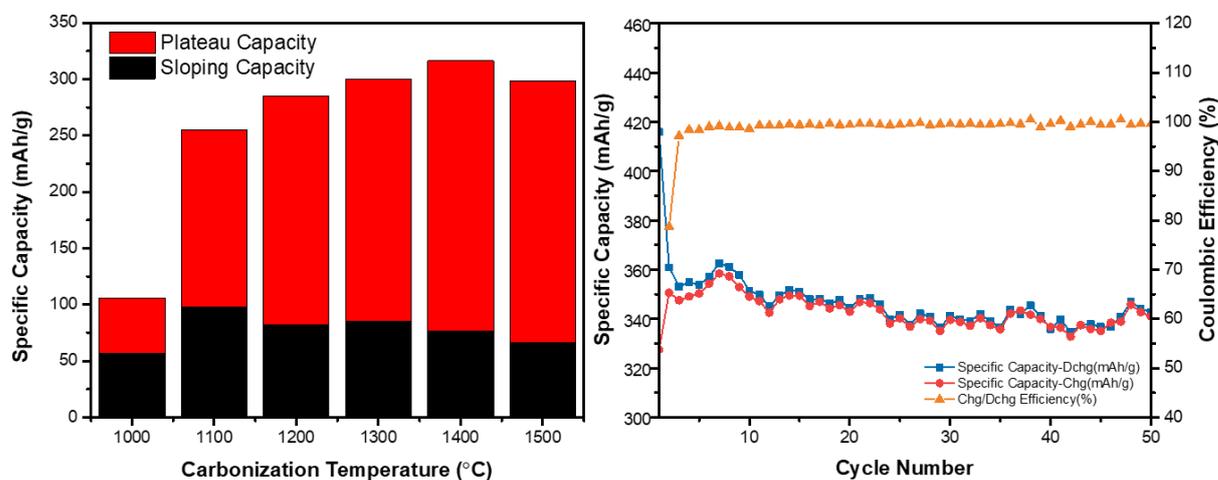


Figure1: The electrochemical performances of obtained hard carbon.

Acknowledgment

This research was supported by the Ministry of Education and Science of the Republic of Kazakhstan Grant (AP09259165) “Utilization of the biowaste - derived carbon and enhancement of its electrochemical performance via doping”.

Structural-phase state and properties of the Cr-Al-Co-Y composite coating as a result of thermal exposure

Assel Zhilkashinova^{1*}, M. Skakov², A. Gradoboyev³, Al. Zhilkashinova¹

¹ Sarsen Amanzholov East Kazakhstan University, Ust-Kamenogorsk, Kazakhstan

² National Nuclear Center, Kurchatov, Kazakhstan

³ National Research Tomsk Polytechnic University, Tomsk, Russia

*E-mail: assel2462@mail.ru

One of the urgent problems is the development of technologies for the strength and performance properties of materials responsible for the details of power plants.

Methods for studying foundations and properties of facades are quite widespread in the scientific literature. Coming with large incomes highlighted by profitable research, there are reviews of works on this topic, author's monographs, textbooks and reference books. However, the above studies were mainly based on coating methods, while studies in terms of the structural-phase state and the relationship between the structure and properties of the coating were not studied in full.

The study of composite coatings is of great scientific interest. The microstructure of a film can differ significantly from the structure of a bulk material of the same composition, and the properties of thin films are largely determined by their morphology. Structural defects in bulk materials, which do not have a significant effect on the properties, in thin films can radically affect their behavior. Surface roughness practically does not affect the characteristics of bulk materials, while for film materials it can be a factor that determines many parameters. Therefore, in the study of thin-film materials, it is possible to discover new phenomena and regularities, which can become the basis for the creation of fundamentally new technologies and devices.

Thus, the subject of this work is aimed at studying the structural-phase state and properties of the Cr-Al-Co-Y composite coating.

Synthesis of ZnO based gas sensing fiber material by electrospinning technique for detecting hazardous gases analysis

Aizhan Rakhmanova^{1,2*}, Sandugash Kalybekkyzy^{1,2}, Baktiyar Soltabayev^{1,2}, and Almagul Mentbayeva^{1,2**}

¹ Department of Chemical and Materials Engineering, School of Engineering and Digital Sciences, Nazarbayev University, Nur-Sultan, 010000, Kazakhstan

² National Laboratory Astana, Nazarbayev University, Nur-Sultan, 010000, Kazakhstan

*E-mail: aizhan.rakhmanova@nu.edu.kz, **E-mail: almagul.mentbayeva@nu.edu.kz.

In recent years air pollution has risen dramatically, therefore detecting hazardous gases is becoming increasingly important. Hazardous gas detection is critical for system and process control, as well as safety monitoring and environmental protection. Nowadays metal oxide-based gas sensors are in high demand due to these advantages such as being affordable to manufacture, easy to miniaturize, durable, dependable, and can be made to work in a variety of environments. Among metal oxides, zinc oxide (ZnO) is an eminent semiconductor material owing to its good electrical, mechanical, and unique optical properties. ZnO has a wide direct bandgap width (3.37 eV), a huge excitation binding energy (60 meV), as well as various distinctive qualities, including high electron mobility and transparency. This research is devoted to the development of gas sensors using the electrospinning technique to fabricate ZnO-based gas sensing material. Fiber spinning parameters were established and under these conditions, ZnO-based fibers were collected at the electrode. Finally obtained gas sensing material was morphologically and structurally characterized by scanning electron microscopy (SEM), transmission electron microscopy (TEM), Fourier-transform

infrared spectroscopy (FTIR), thermogravimetric analysis (TGA), and X-ray diffraction (XRD) analysis. In addition, electrical and gas sensing measurements were performed for the obtained samples. ZnO-based fiber gas sensing with precise control of size and morphology can be fabricated using the electrospinning method. I-V and gas measurements of the gas sensing materials from room to 100 °C showed positive responses.

Acknowledgment

This research was supported by the research grant 021220CRP0122 “Development of highly sensitive MOS based nano-film gas sensors” from Nazarbayev University.

Biomass-derived graphite as an anode material for high-performance Li-ion batteries at low temperature

Nurbolat Issatayev^{1*}, Kazna Tassybay¹, Gulnur Kalimuldina², Arailym Nurpeissova³, Zhumabay Bakenov^{1,3}

¹*Department of Chemical and Materials Engineering, Nazarbayev University, Kabanbay batyr ave. 53, Nur-Sultan, RK*

²*Department of Mechanical and Aerospace Engineering, Nazarbayev University, Kabanbay batyr ave. 53, Nur-Sultan, RK*

³*National Laboratory Astana, Nazarbayev University, Kabanbay batyr ave. 53, Nur-Sultan, RK*

*E-mail: nurbolat.issatayev@nu.edu.kz, **E-mail: zhumabay.bakenov@nu.edu.kz

Nowadays the demand for lithium-ion batteries with properties such as fast charging, high energy density and wide operating temperature range has attracted considerable attention. Graphite constitutes the first and most widely used anode in commercial LIBs owing to its remarkable cyclic stability, low potential vs. Li/Li⁺ (0.1 V) and high initial Coulomb efficiency. On the other hand, its rate characteristics are usually poor, particularly at sub-zero temperatures. Furthermore, high current can promote lithium plating and dendrite growth on the graphite surface, resulting in poor battery performance and a potential safety risk.

In this study, we purpose alternative biomass-derived porous graphitic carbon from date seeds as anode material for a low-temperature lithium-ion battery. The as-obtained graphite was characterized by X-ray diffractometry, scanning electron microscope, Raman scattering and X-ray photoelectron spectroscopy. The honeycombed structure of graphite shortens the diffusion path and provides excellent anode properties, showing high specific capacity at low temperatures.

Acknowledgement

This research was supported by the research grants OPFE2021001 “New materials and devices for defense and aerospace applications” from the Ministry of Digital Development, Innovations and Aerospace Industry of the Republic of Kazakhstan.

First-principles study of Ga-N co-doped graphene nanostructures

Dinara Akhmetsadyk^{1**}, Nazim Guseinov², Arkady Ilyin³

¹*a National Nanolaboratory, Al-Farabi Kazakh National University, 050000, Almaty, Kazakhstan*

²*a National Nanolaboratory, Al-Farabi Kazakh National University, 050000, Almaty, Kazakhstan*

³*a National Nanolaboratory, Al-Farabi Kazakh National University, 050000, Almaty, Kazakhstan*

*E-mail: d.akhmetsadyk@gmail.com

Graphene's physical properties have made it interesting and used in a range of fields of science and technology, such as medicine, nanoelectronics, sensors, and desalination. A simple method for manufacturing graphene with scotch tape was discovered in 2004. Graphene is a two-dimensional material, one carbon atom thick. The structure of graphene is provided as a hexagonal lattice, where the carbon atoms are linked by sp^2 bonds.

Graphene would be a good material for sensors. Single molecules of a chemical can be easily detected by using sensitive sensors. Graphene has the advantages of large surface area, high chemical and thermal stability. However, pristine graphene does not have excellent ability to detect gas molecules.

It is well known that the modification of graphene with various elements leads to a change in its chemical activity.

Based on this, in our work, a modification of graphene is provided by replacing carbon atoms with gallium and nitrogen atoms in order to change the chemical activity.

Acknowledgement

This research was supported by the National Nanolaboratory, Al-Farabi Kazakh National University, Kazakhstan. I deeply appreciate the laboratory's staff, including the supervisor, discussing the results with me.

Flexible strain sensor and energy storage devices based on MXene/polymer nanocomposites: Review

Haruna Abba Usman¹, Gulnur Kalimuldina¹, Reza Montazami^{1,2}, Zhumabay Bakenov², Sherif Araby^{1*}

¹*Department of Mechanical and Aerospace Engineering, School of Engineering and Digital Sciences, Nazarbayev University, Nur-Sultan 010000, Kazakhstan*

²*Department of Mechanical Engineering, Iowa State University, Ames, IA, 50011, USA*

³*Department of Chemical and Materials Engineering, National Laboratory Astana, Institute of Batteries LLP, Nazarbayev University, Nur-Sultan 010000, Kazakhstan*

*Email: Sherif.gouda@nu.edu.kz

MXene – first discovered in 2011– is a new family of two-dimensional (2D) transitional metal carbides or nitrides. It is rich in surface functional groups with excellent ion exchange and hydrophilic properties. Due to its resemblance to graphene, MXene has recently attracted attention in forming functional nanocomposites by adding to organic and non-organic materials. Integration of MXene with polymeric materials unlocks many possibilities for advanced functional polymer nanocomposites with enhanced electrical and thermal conductivity, dielectric properties, electromagnetic shielding, and flame retardancy. Plethora studies reported the application of MXene as an effective filler in a flexible matrix for various sensors and electronic applications. In this review, synthesis methods, morphology and structure, and its polymer-based nanocomposites are introduced. In this review, we have studied the application of MXene-based polymer nanocomposites as flexible strain sensors. A comprehensive discussion on the synthesis of strain sensors from MXene-based polymer nanocomposites is provided; morphology, mechanical and

electromechanical properties are reviewed and discussed. Recent progress in flexible electronics – e.g., supercapacitors – based on polymer/MXene composites are also discussed. Moreover, MXene-carbon nanomaterial hybrids, integrated with polymeric materials for flexible strain sensor applications are also attended. Lastly, current challenges and future directions of MXene research and its application in flexible electronics are presented.

Perovskite solar cells with structured and planar SnO_2 electron transport layers

Assylan Akhanuly^{1*}, Iliyas Dossayev¹, Erik Shalenov², Karlygash Dzhumagulova², and Askhat Jumabekov^{1**}

¹*Department of Physics, Nazarbayev University, Nur-Sultan, 010000, Kazakhstan*

²*Institute of Experimental and Theoretical Physics, al-Farabi Kazakh National University, Almaty, 050040, Kazakhstan*

*E-mail: assylan.akhanuly@nu.edu.kz, **E-mail: askhat.jumabekov@nu.edu.kz

Solar cell devices made using perovskites have reached the power conversion efficiency values (PCEs) as high as 25.7% for single-junction devices and 29.9% for silicon/perovskite tandem solar cell devices. This is a remarkable improvement in the performance of perovskite solar cells (PSCs) considering that the PCE of the first solar cell devices that employed methylammonium lead iodide (MAPbI_3) perovskite as a photo-absorber layer in perovskite dye-sensitized solar cells was only 3.9%.

The performance of perovskite solar cells (PSCs) with nanorod-based SnO_2 electron transport layers (ETL, hereon referred to as ‘structured’) and MAPbI_3 -based perovskite layer are investigated using computer simulation methods and contrasted with the performance of PSCs with planar SnO_2 (hereon referred to as ‘reference planar’) ETLs. The numerical simulations are conducted for different aspect ratios and density of SnO_2 nanorods, considering optimum electronic parameters of the materials selected for the device functional layers. For each geometrical configuration of the structured ETLs, the exact optical response of the corresponding devices are calculated to account for the photonic effects originating from the particular geometric dimensions of the structured ETLs. The underlying discrepancies in the device performance of PSCs with reference planar and structured ETLs are explained through the analysis of electric field and current density distributions in the devices.

Acknowledgement

This research was supported by the Nazarbayev University Faculty Development Competitive Research Grant (Grant Number: 110119FD4512), Nazarbayev University Collaborative Research Grant (Grant Number: 021220CRP1922), Young Scientist Grant from the Ministry of Education and Science of the Republic of Kazakhstan (Grant Number: AP08052412).

Optimization of Back-Contact Metal-Semiconductor-Metal Perovskite Solar Cells

Iliyas T. Dossayev^{1*}, Assylan Akhanuly¹, Erik O. Shalenov², Askhat N. Jumabekov^{1**}

¹*Department of Physics, Nazarbayev University, Nur-Sultan, 010000, Kazakhstan*

²*Institute of Experimental and Theoretical Physics, al-Farabi Kazakh National University, Almaty, 050040, Kazakhstan*

*E-mail: iliyas.dossayev@nu.edu.kz , **E-mail: askhat.jumabekov@nu.edu.kz

Currently, hybrid organic-inorganic halide perovskites are the most promising low-cost materials for solar cell fabrication with decent photovoltaic properties compared to the widely preferred crystalline silicon. Conventionally, perovskite solar cells (PSCs) have multi-layer structure, in which the perovskite layer is sandwiched between two charge-transporting layers. This structure demands a high level of precision and accuracy in fabrication to achieve a reasonable level of performance.

Herein we present a theoretical analysis of back-contact metal-perovskite-metal PSC, which intends to simplify the fabrication process. The electrical and optical properties of the two-dimensional model of devices are investigated numerically in accordance with the experimental results reported by other groups. The geometrical parameters of devices such as the thickness of the perovskite film, the distance between metallic contacts, and the width of metallic contacts are varied in search for the device structure that yields the best photovoltaic performance. An unexpected drop in the device current obtained when the width of metallic contacts are too small. The analysis of electric field distribution in the devices revealed the underlying reasons for this phenomenon. Based on the computer simulation experiments, it is found that a theoretical power conversion efficiency of 6.2% could be achieved for metal-perovskite-metal back-contact PSCs with the methylammonium lead iodide perovskite layer.

Acknowledgement

This research was supported by the Nazarbayev University Faculty Development Competitive Research Grant (Grant Number: 110119FD4512), Nazarbayev University Collaborative Research Grant (Grant Number: 021220CRP1922), Young Scientist Grant from the Ministry of Education and Science of the Republic of Kazakhstan (Grant Number: AP08052412).

Structural and mechanical properties of heat resistant titanium alloys of the Ti-24.5Al-24.5Nb (at.%) system

Nuriya Mukhamedova^{*}, Arman Miniyazov, Yernat Kozhakhmetov^{**}

Institute of Atomic Energy Branch of the National Nuclear Center of the Republic of Kazakhstan, 10 Beybit Atom str., Kurchatov, Republic of Kazakhstan

*E-mail: bakayeva@nnc.kz, **E-mail: kozhahmetov_e@nnc.kz

Heat resistant titanium alloys with various types of microstructure and homogeneous distribution of components were obtained using high-energy processing of powder mixtures in a planetary mill, followed by spark plasma sintering (SPS). Isothermal sections of the Ti-24,5Al-24,5Nb (at.%) system at SPS (1000, 1200 and 1300°C, 1550) were studied using X-ray diffraction, scanning electron microscopy and energy-dispersive spectral analysis. Three-point bending mechanical tests were carried out at room temperature on Instron 5966 universal testing machine.

Based on the study of the phase composition of mechanically activated powder compositions, it was found that during the high-energy treatment of powder mixtures, most of the aluminum component dissolves in the Ti and Nb lattices by interpenetration, forming solid solutions (Ti, Al) and (Nb, Al) and various intermediate compounds.

After SPS of mechanically activated powder mixtures for all sintered samples at 1000, 1200 and 1300°C, the presence of unreacted Nb and β /B2 phases was found. But, with an increase in the sintering temperature, the content of unreacted Nb sharply decreases, while the content of the β /B2 phase increases with transformation into the main matrix structure up to 1300°C. The microstructure of alloys of the Ti-24.5Al-24.5Nb system, in addition Nb and β /B2 phases, is characterized by the presence of γ , α_2 and O phases, the morphology and quantitative content of which varies depending on the exposure temperature.

It has been determined that alloys of the Ti-24.5Al-24.5Nb system, regardless the SPS temperature are characterized by low strength and ductility. Precipitation and large number of brittle α_2 -phases on the borders of particles are one of the main reasons for the low value of the strength properties of titanium alloys.

Acknowledgement

The research was carried out within the framework of STP “Development of nuclear power in the Republic of Kazakhstan for 2021-2023” on the topic “Study of the influence of various time-temperature parameters of heat treatment on the formation of a set of properties of alloys based on orthorhombic titanium aluminide” (URN No. BR09158470).

Solution-processed SnO₂ quantum dots electron transport layer for flexible printed perovskite solar cells

Muhammad Salman Kiani^{1*}, Zhandos T. Sadirkhanov¹, Alibek G. Kakimov¹, Annie Ng², and Askhat N. Jumabekov^{1**}

¹*Department of Physics, Nazarbayev University, Nur-Sultan 010000, Kazakhstan*

²*Department of Chemical Engineering, Nazarbayev University, Nur-Sultan 010000, Kazakhstan*

* E-mail: muhammad.kiani@nu.edu.kz , ** E-mail: askhat.jumabekov@nu.edu.kz

Flexible perovskite solar cells (PSCs) fabricated on lightweight plastic substrates have many excellent potential applications in emerging new technologies including wearable and portable electronics, the internet of things, smart buildings, etc. To fabricate flexible PSCs, all functional layers of devices should be processed at low temperatures. One of the best metal oxide materials to employ as the electron transport layer (ETL) in PSCs is tin oxide. One of the limitations of its use in flexible electronics is its high annealing temperature, which is unsuitable for heat-sensitive flexible substrates. Herein, the preparation and application of SnO₂ quantum dots (QDs) as an ETL for flexible PSCs are demonstrated.

SnO₂ QDs have been synthesized via a solvothermal method and processed to obtain aqueous and printable ETL ink solutions with different QD concentrations. PSCs are fabricated using a slot-die coating method on flexible plastic substrates. For this purpose, a vectorSC (FOM Technologies, Denmark) coating system has been used. All the functional layers including ETL are deposited at room temperature with annealing temperatures < 150 °C. Morphological analysis confirms the uniformity and crystallinity of SnO₂ QDs ETL. The thickness of the SnO₂ QDs ETL is observed to be around 25 nm. The solar cell performance and spectral response of the obtained devices are characterized using a solar simulator and an external quantum efficiency measurement system. The ETL ink solutions with 2.0 wt.% SnO₂ QD concentration yielded a high average power conversion efficiency (PCE) of 7.23 % along with 10% PCE for the champion device. The work presented in this paper can be used in the future for the synthesis of SnO₂ QDs and also for its use as an efficient ETL for rigid as well as heat-sensitive flexible substrates.

Acknowledgement

This research was supported by the Nazarbayev University Faculty Development Competitive Research Grant (Grant Number: 110119FD4512), Nazarbayev University Collaborative Research Grant (Grant Number: 021220CRP1922), Young Scientist Grant from the Ministry of Education and Science of the Republic of Kazakhstan (Grant Number: AP08052412).

Influence of mechanical stresses on recombination processes in flexible and printed perovskite solar cells

Hryhorii Parkhomenko^{1*}, Yerassyl Yerlanuly¹, Viktor V. Brus¹, and Askhat N. Jumabekov^{1**}

¹*Department of Physics, Nazarbayev University, Nur-Sultan 010000, Kazakhstan*

*E-mail: hryhorii.parkhomenko@nu.edu.kz , **E-mail: askhat.jumabekov@nu.edu.kz

In recent years, solar cells based on organic-inorganic perovskites have gained wide popularity among scientists in the PV research community. In a relatively short time, the laboratory samples of perovskite solar cells (PSCs) reached power conversation efficiency values as high as 25.7 %. In addition, the manufacturing technology of PSCs is simple and relatively cheap. There are, however, certain challenges associated with the use of perovskites as an active layer in flexible solar cells. Due to its crystalline nature, the perovskite layer in flexible and printed PSCs is prone to gradual degradation when devices are subjected to various mechanical stresses. This leads to corresponding performance deterioration in devices. Thus, the investigation of charge carrier recombination losses in the perovskite layer would be one way to characterize and quantify the impact of mild mechanical stresses on the properties and performance of flexible and printed PSCs. In this work, the analysis of photovoltaic properties and recombination losses are carried out for flexible and printed PSCs before and after mechanical stresses. A combination of methods is applied to obtain a detailed understanding of recombination dynamics in flexible and printed PSCs. The obtained results indicate that a significant trap-assisted recombination occurs. An analytical model is applied to describe the total recombination density of the current originating from bimolecular as well as bulk and surface mechanisms of recombination with the help of traps. The recombination coefficients for bimolecular and bulk recombination before and after mechanical stresses are obtained. In turn, based on the obtained experimental results, the dependence of the extraction coefficient as a function of thickness is calculated. It is shown that one of the ways to increase the efficiency of this type of solar cell is to reduce the perovskite thickness.

Acknowledgement

This research was supported by the Nazarbayev University Faculty Development Competitive Research Grant (Grant Number: 110119FD4512), Nazarbayev University Collaborative Research Grant (Grant Number: 021220CRP1922), Young Scientist Grant from the Ministry of Education and Science of the Republic of Kazakhstan (Grant Number: AP08052412).

The effects of different electron transport layer materials on the photovoltaic properties of flexible and printed perovskite solar cells

Yerassyl Yerlanuly^{1*}, Hryhorii P. Parkhomenko¹, Viktor V. Brus¹, Askhat N. Jumabekov^{1**}

¹*Department of Physics, Nazarbayev University, 010000 Nur-Sultan, Kazakhstan*

*E-mail: yerassyl.yerlanuly@nu.edu.kz , **E-mail: askhat.jumabekov@nu.edu.kz

One of the promising photovoltaic devices for converting power is perovskite solar cells (PSCs). To date, PSCs have achieved a certified power conversion efficiency (PCE) of 25.7%. This is due to the unique properties of perovskites, such as low-temperature solution processing and the use of various deposition methods to print thin perovskite films on different types of rigid and flexible substrates. These features of perovskites afford large-scale production of cost-effective and fully printable and flexible PSCs (FPSCs). However, there is a number of urgent problems and tasks that need to be addressed to transition the manufacturing of FPSCs from laboratory to industrial scale.

This work is dedicated to fabricate PSCs on the surface of flexible polyethylene terephthalate with a layer of transparent conducting indium-tin-oxide (PET/ITO) using a slot-die coating method and studying the effect of different electron-transporting layers materials on the performance of FPSCs. Fabrication of partially printed (printing the main functional layers and applying the top metallic electrodes by thermal evaporation) FPSCs with the architecture PET/ITO/ETL(SnO₂ or PCBM)/Perovskite(MAPbI₃)/HTL (Spiro-OMeTAD)/Au is carried out using a slot-die coater (NanoRoll, FOM Technologies, Denmark). All three device functional layers are printed in air with the temperature and relative humidity of 18-21 °C and ~27%, respectively. After the completion of the device fabrication process, the photovoltaic properties of printed FPSCs are studied. As a result, printed FPSCs with the PCEs of 11.7% using SnO₂ and 8% using PCBM are obtained. According to statistical data, on average the FPSCs with SnO₂ ETL yield a PCE value of 7.68%, whereas the device with PCBM ETL shows around 6% for a PCE value.

Acknowledgement

This research was supported by the Nazarbayev University Collaborative Research Grant (Grant Number: 021220CRP1922), Young Scientist Grant from the Ministry of Education and Science of the Republic of Kazakhstan (Grant Number: AP08052412).

Photodetectors made of carbon nanowalls transferred on Si and CdTe

Rakhymzhan Zhumadilov^{1,2,3*}, Yerassyl Yerlanuly^{1,2,3}, Hryhorii P. Parkhomenko³, Askhat N. Jumabekov^{3**}

¹*Al-Farabi Kazakh National University, 050040 Almaty, Kazakhstan.*

²*Kazakh-British Technical University, 050000 Almaty, Kazakhstan.*

³*Department of Physics, Nazarbayev University, 010000 NurSultan, Kazakhstan.*

*E-mail: rakhymzhan.zhumadilov@nu.edu.kz , **E-mail: askhat.jumabekov@nu.edu.kz

Carbon nanowalls (CNWs) are few-layer graphene nanosheets standing vertically on a substrate. CNWs can be synthesized on various metallic, semiconductor and insulator substrates using various techniques. CNWs demonstrate unique structure and special optoelectronic properties, which makes them a promising material for various optoelectronic applications.

In this study, plasma-enhanced chemical vapor deposition (PECVD) is used to synthesis CNWs on copper foil. The surface morphology and quality of the CNWs are analyzed using a scanning electron microscope (SEM) and a Raman spectrometer. The photodetectors were fabricated by transferring the synthesized CNWs films onto Si (n-type) and CdTe substrates. Our simple CNWs/Si and CNWs/CdTe Schottky-junction photodetectors exhibits a high responsivity of 190 mA/W at 950 nm light and 82 mA/W at 710 nm light, respectively. Another important parameter of photodetectors called external quantum efficiency (EQE) is measured from the responsivity of devices. The CNWs/Si photodetector demonstrates the EQE of ~25%. The CNWs/CdTe device exhibits the EQE of 15.7%. The responsivity and EQE can be further improved by changing the bias voltage. The detectivity values of 4.8×10^{11} and 2.1×10^{11} Jones are obtained for the CNWs/Si and CNWs/CdTe, respectively. Because of the high light absorption, the CNWs photodetector based on Si has higher responsivity than the CNWs/CdTe device. The photocurrent of both photodetectors changes with the applied reverse bias and increases with the intensity of incident light. Our study shows that the CNWs is a promising material for high-performance photodetectors.

Acknowledgement

This research was supported by the Nazarbayev University Faculty Development Competitive Research Grant (Grant Number: 110119FD4512), Nazarbayev University Collaborative Research Grant (Grant Number: 021220CRP1922), Young Scientist Grant from the Ministry of Education and Science of the Republic of Kazakhstan (Grant Number: AP08052412).

Structural and phase state of carbidized layer tungsten obtained in a beam-plasma discharge

Arman Miniyazov^{1*}, Mazhyn Skakov², Viktor Baklanov¹, Gainiya Zhanbolatova^{1**}, Igor Sokolov¹,
Yernat Kozhakhmetov¹, Timur Tulenbergenov¹, Ol'ga Bukina¹

¹*"Institute of Atomic Energy" Branch of the National Nuclear Center of the Republic of Kazakhstan, Kurchatov,
Republic of Kazakhstan*

²*National Nuclear Center of the Republic of Kazakhstan, Kurchatov, Republic of Kazakhstan*

*E-mail: miniyazov@nnc.kz , **E-mail: kaiyrdy@nnc.kz

The use of tungsten (W) for areas with high ion and heat fluxes does not adequately resolve the problems accompanying interaction between plasma and divertor surface. These circumstances determine the concern in continuing to use graphite and carbon-graphite materials as plasma-faced ones. However, erosion and transport of sputtered graphite and carbon-graphite materials (C) will lead to simultaneous irradiation of W with hydrogen isotopes, C atoms, and hydrocarbon molecules, which will lead to the formation of a mixed W–C surface layer.

This paper provides research results of the structural and phase state of near-surface tungsten layers after irradiation with a methane ion beam. Based on interaction with an electron beam, gaseous methane decomposes into fragments such as H^+ , H^{2+} , C^+ , CH^+ , CH^{2+} , CH^{3+} and CH^{4+} , which enables simulating the conditions of local transfer of C atoms along surfaces wetted by plasma by means of hydrocarbons.

The structural and phase state of the near-surface tungsten layers was researched using SEM, TEM, and XRD methods. The temperature dependence of microstructural evolution and phase transformations has been determined. Carbide phase generation was recorded after irradiation at 1000°C. Three phases of tungsten carbide (WC, W_2C and WC_{1-x}) were observed, mainly as mixtures of two phases (WC, W_2C). According to the results of microstructural analysis, it was found that presence of a carbon coating as a continuous film is observed on the sample surface during the interaction between tungsten and methane. Thermally unstable carbon film is destroyed under high temperatures and carbon is already chemically bounded forming tungsten carbide phases, as XRD results evidence.

Acknowledgement

The work was carried out at the National Nuclear Center of the Republic of Kazakhstan within the framework of a scientific and technical program on the topic "Investigation of the interaction of plasma with a carbidized tungsten surface".

Modeling of sandwich and quasi-interdigitated back-contact perovskite solar cells

Erik Shalenov^{1,3*}, Karlygash Dzhumagulova^{1,3}, Yeldos Seitkozhanov¹, Annie Ng², Constantinos Valagiannopoulos³, Askhat Jumabekov^{3**}

¹*Institute of Experimental and Theoretical Physics, al-Farabi Kazakh National University, Almaty, 050040, Kazakhstan*

²*Department of Electrical and Computer Engineering, Nazarbayev University, Nur-Sultan 010000, Kazakhstan*

³*Department of Physics, Nazarbayev University, Nur-Sultan, 010000, Kazakhstan*

*E-mail: Shalenov.erik@physics.kz, **E-mail: askhat.jumabekov@nu.edu.kz

To date, the hybrid halide perovskite solar cells (PSCs) exhibit a record power conversion efficiency (PCE) of 25.7% for single-junction and 29.1% for monolithic perovskite/silicon tandem solar cells, which outperform other thin-film PV technologies (e.g., CIGS, CdTe, and so forth), and are comparable to well-established solar technologies such as crystalline silicon solar cells.

A numerical simulation method is used to investigate the optical and electrical properties for both conventional sandwich and quasi-interdigitated back-contact (QIBC) PSCs. The results reveal the fundamental physics of PSCs with different architectures, exhibiting their difference in working principles and device properties. A two-dimensional optical model, which takes into account both electromagnetic and electronic properties of various device layers, is selected to accurately describe the device optical properties and to achieve more comprehensive simulations of solar cells properties at different device working conditions. Different carrier recombination mechanisms for two kinds of PSC architectures are also compared. The conditions under which the electrical properties of the perovskite photo-absorber layer enable QIBC PSCs to operate competitively or exhibit better device performance compared to the sandwich PSCs are examined in detail. The case of QIBC PSCs with various combinations of charge selective layers are analyzed to provide insight in materials selection for high-efficiency QIBC PSCs. It is found that PCEs more than 25 % can be potentially achieved for CH₃NH₃PbI₃ based QIBC PSCs after careful optimization of material selection and device fabrication.

Acknowledgement

This research was supported by the Nazarbayev University Faculty Development Competitive Research Grant (Grant Number: 110119FD4512), Nazarbayev University Collaborative Research Grant (Grant Number: 021220CRP1922), Young Scientist Grant from the Ministry of Education and Science of the Republic of Kazakhstan (Grant Number: AP08052412).

Information and analytical system as a method for scientific information processing

Nuriya Mukhamedova*, Alexandr Vurim, Yuliya Baklanova

*Institute of Atomic Energy Branch of the National Nuclear Center of the Republic of Kazakhstan, 10 Beybit Atom str.,
Kurchatov, Republic of Kazakhstan*

*E-mail: bakayeva@nnc.kz

Effective management of the large flows of various information cannot be organized without the use of computer information systems (IAS). In scientific and technical applications, the IAS is of particular value, which provide deep analytical processing of data from previous studies or experiments and predicting parameters of new experiments as well as processing and analyzing of their results.

For more than 30 years, the IAE Branch RSE NNC RK has been conducting studies to justify NPP safety. During this time, a large amount of experimental data and research results have been gained obtained when modeling the processes that take place while developing severe accidents at nuclear reactors.

The goal of this study is to provide quick access to the necessary experimental data, to create a single mathematical apparatus for calculation of input parameters and a method for comprehensive analysis of output parameters.

The main component of the IAS is an analytical unit with the following functions: determination of time-temperature parameters that depend on a set power and heating rate, comparison of experiments and their results, output of only necessary data tracing.

Due to quick access to the necessary data and research results, the ability to calculate input parameters using a single mathematical apparatus and a comprehensive analysis of output parameters, speed and volume of processed data and reliability of compared parameters will be increased, number of errors in planning experiments will be decreased, and repeatability of the results required for analysis will be increased.

Acknowledgement

The study was carried out within the framework of grant financing for 2021-2023 (MES RK) AP09260704 on the topic “Information and analytical system of data obtained from experimental modeling of severe accident processes at a nuclear reactor”.

Joint growth of BiOI and BiSI films in the chemical deposition process

Xeniya Leontyeva^{1,2*}, Darya Puzikova^{1,3**}, Gulnur Khussurova¹, Polina Panchenko¹

¹“D.V. Sokolsky Institute of Fuel, Catalysis and Electrochemistry” JSC, Almaty 050010, Kazakhstan

²“Al-Farabi Kazakh National University”, Faculty of Chemistry and Chemical Technology, Almaty 050040, Kazakhstan.

³“Al-Farabi Kazakh National University”, Faculty of Physics and Technology, Almaty 050040, Kazakhstan.

*E-mail: leontyeva.xeniya@mail.ru , **E-mail: d.s.puzikova@mail.ru

The chemical synthesis of BiOI and BiOI/BiSI semiconductor films for photoelectrochemistry application has been carried out. The influence of the process duration on the films composition and morphology has been studied.

Bismuth-containing films were synthesized on preliminarily prepared FTO substrates by complete immersion in a solution heated to 105°C. The deposition time varied from 15 to 60 minutes. After deposition the films were dried at 90°C for 15 minutes in air.

According to the SEM image and the elemental analysis results, the BiOI films have a flower-like morphology formed by a combination of 1-2 μm flake-shaped particles. As the deposition time is increased to 45 minutes, there is also an ubiquitous formation of smaller needle

sphere-shaped BiSI particles, which increase in number as the deposition time increases to 60 minutes.

The results of structural studies confirm the BiOI crystal structure formation and followed by the joint growth of BiOI/BiSI crystals with an increase in the deposition time.

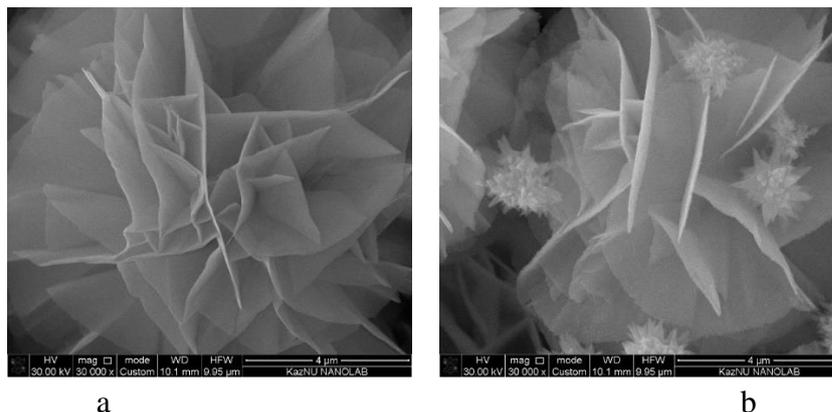


Figure 1 – SEM-images of BiOI and BiOI/BiSI films:
(a) 15 minutes; (b) - 60 minutes

Acknowledgement

This research was supported by the Science Committee of the Ministry of Education and Science of the Republic of Kazakhstan (AP08856338 «Photoelectrochemical solar cells based on thin-film semiconductor bismuth compounds»).

Effect of cyclic thermal load on beryllium

M.K. Skakov¹, I.A. Sokolov^{2**}, Ye.Ye.Sapatayev², A.Zh. Miniyazov²

¹National Nuclear Center of the Republic of Kazakhstan, Kurchatov, Republic of Kazakhstan

²“Institute of Atomic Energy” Branch of the National Nuclear Center of the Republic of Kazakhstan, Kurchatov, Republic of Kazakhstan

*E-mail: sokolov@nnc.kz

The aim of this work is obtaining of experimental data on the behavior of beryllium at the boundary between the gaps of the tiles of the ITER first wall as a result of thermal load effect.

Thermal effects lead to the destruction of the material. Therefore, predicting changes in the structure and properties of beryllium under these operating conditions is important for ITER.

Thermal loads were experimentally simulated in vacuum conditions under the influence of an electron beam. As a result, HP-56 beryllium was irradiated in the form of pellets with a diametrical gap when the temperature of beryllium surface was ~360 °C, ~800 °C and ~1200 °C, according to thermal simulation. The number of pulses was 1, 10 and 100 with the duration of each pulse – 500 s.

According to the results of the conducted research, the following can be distinguished:

- assessment of the surface profile of beryllium samples showed that there is an increase in the depth of the eroded layer, namely, at the edges of beryllium, which is confirmed by smoothed gap angles.

– a decrease in the mass of beryllium samples irradiated in the temperature range of 800 °C – 1200 °C consistently revealed. This tendency increases with increasing of thermal effect cycles.

– the SEM analysis showed that the structure of the samples after testing at ~360 °C is almost the same as the original sample. Significant changes in the structure occurred at ~ 800 °C and above, which, with increasing of cycles, are expressed by merging of point voids up to 10 μm in size

into single ones and increasing of their depth. After irradiation at ~ 1200 °C highly dispersed pores with a diameter of ~ 10 μm are more pronounced, which increased with an increasing in the number of effect cycles.

Finally, it can be said that the beryllium coating is quite resistant to the standard operating conditions of ITER, but at temperatures of 800 °C and above, over the time of operation of the thermonuclear facility, critical destruction of the material and further plasma contamination with beryllium impurities are possible. And as a result, it was found that a significant effect on the change in the structure of the irradiated beryllium surface as a result of thermal effects is caused by an increase in temperature, rather than an increase in the number of cycles.

Acknowledgments

This research has been/was/is funded by the Science Committee of the Ministry of Education and Science of the Republic of Kazakhstan (Grant No. AP08856026)

Influence of carbamide and thioamide additives on photostability & performance of MAPbI₃

Mayuribala Mangrulkar^{1*}, Pavel Troshin², Keith Stevenson^{1**}

¹*Skolkovo Institute of Science and Technology, Moscow, Russia*

²*Institute for Problems of Chemical Physics Russian Academy of Sciences, Chernogolovka, Moscow, Russia*

*E-mail: mayuribala.mangrulkar@skoltech.ru, **E-mail: mayuribala.mangrulkar@nu.edu.kz

The certified efficiencies of perovskite solar cells (PSC) have reached beyond 25% since the first reported PSC. This improvement in efficiency is further comparable to existing photovoltaic technology. This makes PSCs a potential candidate for commercial application. This is especially because of the benefits of easy and low-cost manufacturing technology used for fabrication of PSC. Unfortunately, perovskite absorber materials tend to degrade in presence of moisture, air, elevated temperature and light. In practical terms, these conditions are unavoidable for the operation of solar cells. Thus making PSC unstable extrinsically as well as intrinsically.

To overcome these stability challenge scientists have suggested to perform additive engineering. Studies have shown that the addition of carbamide and thioamide additives act as Lewis bases that can coordinate with lead atoms. Thus, it can form an intermediate phase which delays the crystallization process in perovskite film; in turn, increases the lifetime and enhances the photovoltaic properties, further passivates defects at grain boundaries.

Following the approach, herein, we used urea and thiourea additive into MAPbI₃ precursor solution and investigated the impact onto photostability of MAPbI₃ thin films and onto the performance of solar cells. Our investigation suggests that addition of urea enhances the intrinsic photostability of the absorber layer and remains stable over 1400 h under the light intensity of 70-80 mW cm⁻² at 50-60 °C. Further, the champion device exhibits PCE of 17%. Thus, our study demonstrates a scope of overcoming the stability challenges associated with perovskite light absorber materials.

Acknowledgement

This research was supported from the Ministry of Science and Higher Education of the Russian Federation (project no. 0089-2019- 0010/AAAA-A19-119071190044-3) at IPCP RAS (Institute for Problems of Chemical Physics of the Russian Academy of Sciences).

Quantum efficiency of water splitting on the surface of nanoporous layers of silver and copper iodides and copper oxide

Pavel Bezrukov^{1*}, Aleksandr Sidorov^{1,2}, Nikolay Nikonorov¹

¹*ITMO University, Kronverksky Pr. 49, bldg. A, Saint-Petersburg, 197101, Russia*

²*Ioffe Institute, Politekhnicheskaya St., Saint-Petersburg, 194021, Russia*

*E-mail: pawqa1@yandex.ru

The use of solar energy offers solutions to many problems, consistent with energy and ecology trends. Photocatalytic decomposition of water is one of the ways to obtain gaseous hydrogen and oxygen, which can be used in other areas of industry.

The main element of a photocatalytic cell is a photocathode, a material capable of absorbing radiation energy in a wide range of the spectrum. Nanoporous films of copper and silver iodide and copper oxide have a developed surface area. This method of obtaining films is characterized by the ability to quickly scale up in industry.

Nanoporous films of copper and silver iodides films were synthesized by a reaction of iodide vapour with copper and silver thin layers. Nanoporous films of copper oxide were synthesized by a heat treatment at 300 °C. This surface morphology contributes to the concentration of photogenerated electrons at the ends of dendrites - on quantum dots.

The quantum efficiency of water decomposition shows the ratio of the number of photogenerated electrons to the number of electrons absorbed by the photocathode surface. This is one of the main characteristics of the photocatalytic material

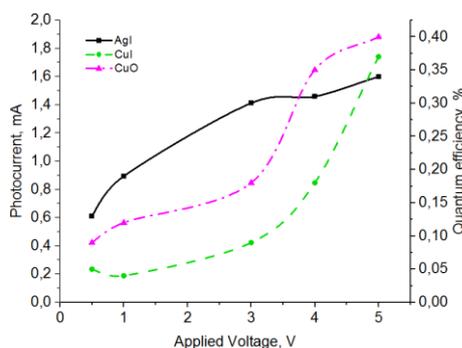


Figure 1 – The dependence of the photocurrent and the quantum efficiency of water splitting on the applied voltage

With an increase in the applied applied voltage, the photocurrent and the quantum efficiency of the photocatalytic decomposition of water in thin nanoporous copper and silver films increase as shown in this work (fig. 1).

Acknowledgement

This research was supported by Russian Science Foundation (project # 20-19-00559).

Evaluation of the strength characteristics of steel grade 35X by testing miniature samples SPT

Yerzhan Sapatayev, Yerkhat Daulet Khanov*, Nurkhat Orazgaliyev, Yersin Aryngazy, Bauyrzhan Orazymbekov.

Institute of Atomic Energy Branch of the National Nuclear Center of the Republic of Kazakhstan, 10 Beybit Atom str., Kurchatov, Republic of Kazakhstan

*E-mail: daulet Khanov@nnc.kz

The experimental procedure for traditional testing of materials adapted to assess the mechanical properties includes the use of traditional “full-size” samples. In the case of irradiated materials, the use of such samples requires handling large quantities of radioactive materials. In addition, the dimensions of the structural components do not allow the production of standard samples. These limitations prevent sufficient data from being obtained using traditional tests. To overcome these limitations, various attempts have been made towards developing methods for testing miniature specimens that require a small amount of irradiated material to determine the mechanical properties.

The SPT (small punch test) method, using samples in the form of miniature disks (8 mm in diameter and 0.5 mm thick), is an effective alternative to traditional tensile tests. The SPT method is based on pressing a hemispherical punch, or a flat punch with a hard spherical ball at the end, through a miniature sample until it is deformed.

This paper investigates the effect of heat treatment under various conditions on the mechanical properties of 35X structural alloy steel using the SPT miniature test method. Heat treatment of the samples was performed by quenching (at 860°C) and subsequent tempering at various temperatures of 200°C, 300°C, 400°C, 500°C. For the SPT test, from the head of the failed tensile test specimens, miniature specimens were made in the form of a disc with dimensions of $\varnothing 8 \times 0.5$ mm. Miniature SPT tests were carried out on an Instron 5966 universal testing machine using the developed test device with a punch loading rate of 0.2 mm/min and continuous recording of load-displacement curve data.

According to the results of testing miniature samples, characteristic zones of elastic, elastic-plastic and plastic deformation were determined. After analyzing the load-displacement curves, the load values P_y/t^2 were determined using the $t/10$ method, which is similar to the method for determining the yield strength $\sigma_{0.2}$ (0.2% displacement) in standard tensile tests. Between the actual values of the yield strength $\sigma_{0.2}$ (tensile test) of the material of steel grade 35X and the value of P_y/t^2 (SPT method), a correlation dependence with a high level of correlation ($R^2 = 0.99$) was established.

Acknowledgement

The research was carried out within of STP “Development of nuclear energy power in the Republic of Kazakhstan for 2021-2023” on the topic “Determination of the strength properties of structural materials for nuclear and thermonuclear energy using the methodology for testing miniature samples” (URN No. BR09158470).

On the use of lithium-containing layers to study the sputtering of lithium into noble gas via bombardment by an electron beam

Kuanysh Samarkhanov^{1*}, Mendykhan Khasenov^{1,2}, Yuriy Gordienko¹, Yevgeniy Tulubayev¹, Vadim Bochkov¹, Yekaterina Martynenko¹

¹*Institute of Atomic Energy Branch of the National Nuclear Center of the Republic of Kazakhstan, 10 Beybit Atom St., 071100, Kurchatov, Republic of Kazakhstan*

²*School of Science and Humanities, Nazarbayev University, 53 Kabanbay Batyr Ave., 010000, Nur-Sultan, Republic of Kazakhstan*

*E-mail: samarkhanov@nnc.kz

Currently, there are plenty methods to pumping gaseous active laser medium. The most widespread are various forms of gas discharge, electron and ion beams, nuclear pumping, chemical pumping, pumping by electromagnetic radiation, et. al.

This paper presents in sufficient detail the procedure for obtaining a lithium-containing layer, the main object of research, intended for conducting experiments to study the sputtering of lithium into noble gas upon excitation by a nanosecond electron beam. The possibility of using solid lithium hydride instead of lithium in the liquid phase in a surface excitation source is discussed.

To simulate the processes during excitation of noble gas atom and lithium by ${}^6\text{Li}(n,\alpha){}^3\text{H}$ nuclear reaction products, a lithium target was fabricated, stabilized in the matrix of the capillary-porous structure, which allows conducting the measurements up to 900 K. The lithium CPS target was located in the irradiation chamber of the experimental setup based on a pulsed electron accelerator. Spectral properties of luminescence of noble gases and lithium sputtering in noble gas was recorded by QEPro-abs spectrometer (Ocean Optics). The integration time of the spectrometer was 15 s, within 12 electron-beam pulses passed through. Light collecting implemented by a quartz lens, mounted directly close to a quartz window, and connected with 2 m long fiber-optic cable.

Acknowledgement

This research was supported by the Ministry of Energy of the Republic of Kazakhstan (Program “Development of nuclear energy in the Republic of Kazakhstan for –2023 years”).

Development of a methodology for conducting experiments with a sample of lithium capillary-porous structure at a plasma-beam installation

Yevgeniy Tulubayev^{**}, Yuriy Ponkratov, Kuanysh Samarkhanov, Igor Sokolov, Gainiya Zhanbolatova, Vadim Bochkov

*Institute of Atomic Energy Branch of the National Nuclear Center of the Republic of Kazakhstan,
10 Beybit Atom St., 071100, Kurchatov, Republic of Kazakhstan*

***E-mail: tulubayev@nnc.kz*

In recent years, one of the important directions in the development of fusion facilities is research related to the use of lithium and liquid lithium systems as plasma-facing material. The use of liquid lithium as a plasma-facing material in most cases is realized through the use of a capillary-porous structure (CPS) as a stabilizing matrix. Experiments on the use of liquid lithium as a plasma-facing-material (PFM) are carried out at operating plasma-physical facilities, such as T11-M (Troitsk, Russia), FTU (Frascati, Italy), NSTX (Princeton, USA), EAST (Hefei, China) and at the TJ-II stellarator (Barcelona, Spain). A review of the modern scientific literature within the field of fusion shows that other operating facilities are also conducting research with lithium and liquid-lithium systems. Due to establishing the KTM research materials science tokamak in the Republic of Kazakhstan, the Institute of Atomic Energy Branch of the National Nuclear Center of the Republic of Kazakhstan is conducting research on the possibility of using lithium CPS as in-vessel elements of FR. Thus, in previous years were implemented works on the development and testing of the mockup of a lithium divertor (LDM), which, in turn, is planned to be used in the KTM tokamak as one of the removable parts of the receiving divertor device. The specific feature of the LDM is that a lithium CPS is used as a plasma-facing material, which is mounted on the receiving surface of the divertor element. In order to obtain data on the optimal operating modes of a lithium device in the conditions of real operation of a KTM tokamak, there is a need for a full-scale verification of the concept of using lithium technologies, in particular, the study of the behavior of lithium CPS in conditions of high thermal, radiation and plasma loads.

This paper presents a description of the procedure for testing a lithium CPS sample during irradiation experiments at a plasma-beam installation (PBI). The design of the target assembly was developed, the procedure for manufacturing lithium CPS samples during placement in the PBI target assembly was described, and the optimal temperature modes and vacuum conditions during irradiation were determined.

Acknowledgement

This research was supported by the Ministry of Energy of the Republic of Kazakhstan (Program “Scientific and technical support of experimental research at the Kazakhstan Material Testing tokamak KTM).

Development of a methodology for conducting experiments with a sample of tin-lithium eutectic at a plasma-beam installation

Vadim Bochkov^{*}, Yuriy Ponkratov^{**}, Yuriy Gordienko, Kuanysh Samarkhanov, Yevgeniy

Tulubayev, Timur Tulenbergenov, Igor Sokolov, Yekaterina Martynenko

Institute of Atomic Energy Branch of the National Nuclear Center of the Republic of Kazakhstan,

10 Beybit Atom St., 071100, Kurchatov, Republic of Kazakhstan

**E-mail: bochkovv@nnc.kz , **E-mail: ponkratov@nnc.kz*

Nowadays, intensive research activities around the globe are aimed to study the possibility of using liquid metals and liquid metal systems as plasma-facing materials (PFM) as part of the creation of new controlled thermonuclear fusion units. In the course of promoting this idea, the fusible metals such as lithium, gallium, tin, and indium were considered, but lithium is superior to other low-melting metals in almost all respects (low nuclear charge, good thermo-physical properties, corrosion interaction with structural materials of fusion reactors). Therefore, most experiments on tokamaks and stellarators were conducted specifically with lithium. As these studies progressed, it was recorded that during experiments with lithium in-vessel elements, an intensive process of lithium evaporation takes place, which subsequently condenses on almost all internal surfaces of the vacuum chambers of plasma-physical facilities. Therefore, many researchers focused on lithium alloys with low-melting metals. The requirement for the selection of such an alloy is to find a compromise between the thermo-physical properties and the processes of vaporization, that is, without significantly affecting the heat capacity of the alloy, it is necessary to significantly reduce the pressure of saturated vapor. Tin-lithium alloys they are interesting primarily due to liquid state of tin has very low saturated vapor pressure. Due to aforementioned, there is a need to carry out calculations and experiments to determine the possibility of using tin-lithium alloys as PFM in fusion facilities.

This paper presents a description of the procedure for testing a tin-lithium eutectic sample during irradiation experiments at a plasma-beam installation (PBI). The design of the target assembly was developed, the procedure for manufacturing lithium CPS samples during placement in the PBI target assembly was described. Thermophysical calculations were conducted for a target with a sample of tin-lithium eutectic, its temperature field was determined, and optimal temperature modes were selected for irradiation experiments.

Acknowledgement

This research was supported by the Ministry of Energy of the Republic of Kazakhstan (Program “Development

Fabrication of the Ag/DMAEMA@PET composites for efficiency removal of As(III) ions

Nursanat Parmanbek^{1,2}, Barsbay Murat³, Anastassiya Mashentseva¹, Zhanar Jakupova²

¹*Institute of Nuclear Physics of the Republic of Kazakhstan, Almaty, Kazakhstan*

²*ENU*

³*Hacettepe University, Ankara, Turkey*

Reversible addition-fragmentation chain transfer (RAFT) polymerization is considered as the most promising synthetic route to prepare well-controlled structures with enhanced performance in specialized applications. Polymers synthesized by controlled free-radical polymerization (CRP) techniques process well-defined molecular architectures and are used in many applications such as drug-delivery, special sensing materials, molecular imprinting, polymer-protein conjugates, development of cylindrical, spherical, hyper-branched polymers, pH or temperature responding smart polymers, etc. These studies prove the versatility of CRP techniques for answering the requirements of highly functional complex polymeric architectures due to the advantages of well-defined and controllable properties achieved by these methods.

Grafting of PET track-etched membranes (TEMs) was carried out in certain ratios of 2-Dimethylaminoethyl methacrylate (DMAEMA) and xanthate-based RAFT agent, O-ethyl-S-(1-methoxycarbonyl) ethyl dithiocarbonate (RA) ([DMAEMA]/[RA]=500, 1000) in a total volume of 10 ml solution prepared using four different solvents such as water, acetone:water, ethanol:water, and ethanol. Based on the obtained data, the optimal experimental conditions were chosen: monomer concentration - 20%, solvent - acetone:water in a ratio of 1:1. All further studies were carried out under these optimal conditions.

The stabilization of Ag/DMAEMA@PET was studied as a function of loaded composites and stabilization time (it varied from 30 to 1440 min). When studying the effect of loading mass of Ag nanoparticles on the efficiency of stabilization time the mass of nanoparticles was varied from 4.7 mg/cm² to 7.6mg/cm², and the suitable stabilization time in all experiments was about 300min. Structure and composition of prepared composite TEMs were elucidated using SEM, XRD, EDX techniques.

As (III) is known as a toxic metal in aqueous media because of a high toxicity that is potentially dangerous for both human body and the environment. Therefore, development of new type of sorbents for efficient removal of toxic pollutant is an urgent task. The solution's PH was 4, the time of mixture exposure in all experiments was 600 min. The effect of removal amount of Ag/DMAEMA@PET on Arsenic solution had reached about 90 % as well that means it has acceptable potential for the removal of arsenic (III) from aqueous medium.

Acknowledgement

The research titled "Development of Functionalized Composite Track-Etched Membranes for Environmental Applications" (grant No AP08855527) was funded by the Ministry of Education and Science of the Republic of Kazakhstan.

Adsorption and displacement of methane in graphene-based microstructures: insight from molecular simulations

Dias Bekeshov^{1*}, Sultan Ashimov¹, Yanwei Wang^{1,2*} and Lei Wang^{3,4}

¹*Department of Chemical & Materials Engineering, School of Engineering and Digital Sciences, Nazarbayev University, Nur-Sultan 010000, Kazakhstan*

²*Laboratory of Computational Materials Science for Energy Applications, Center for Energy and Advanced Materials Science, National Laboratory Astana, Nur-Sultan 010000, Kazakhstan* ³*College of Energy, Chengdu University of Technology, Chengdu 610059, China*

⁴*School of Mining and Geosciences, Nazarbayev University, Nur-Sultan 010000, Kazakhstan*

*E-mail: dias.bekeshov@nu.edu.kz (D.B); yanwei.wang@nu.edu.kz (Y.W.)

Shale gas and coalbed methane are alternative energy sources that partly or even mainly consist of methane stored in an adsorbed state in pores of organic-rich rock and coal seams. This study employed a combination of Grand Canonical Monte Carlo (GCMC) and Molecular Dynamics (MD) simulations to investigate the mechanisms of gas adsorption and displacement of methane in coal microstructures, which were modeled as slit pores with the slit walls modelled by graphene layers. The adsorption of various gases (CO₂, CH₄, N₂) in such microstructures were quantified at different pore sizes and temperature-pressure conditions. The following findings were obtained: (1) The minimum slit pore size at which molecules can penetrate the pore was found to be ~0.7 nm, and as expected, the amount of methane adsorption increased with the increase of the slit width, and the structure of the adsorbed methane transitioned from a single adsorption layer to multiple adsorption layers; (2) the amount of adsorption for all three cases (CO₂, CH₄, N₂) was found to increase with increasing pressure, and for most cases, the amount of adsorption increased with decreasing temperature; and (3) The comparison of the amount of adsorption of gas molecules provided the following order, CO₂ > CH₄ > N₂, at 298 K and atmospheric pressure and a pore size of 1 nm. Enhancing methane recovery was also investigated by injecting CO₂ or N₂ gas to displace the adsorbed methane. This study provides a preliminary understanding of the competitive adsorption mechanisms of methane, carbon dioxide, and nitrogen in organic nanopores common in shale gas and coalbed methane reservoirs

Acknowledgement

This research was supported by the “Simulation of sour gas injection EOR in tight carbonate reservoirs coupling capillarity and geomechanics” project (Grant Award Number 080420FD1918) and the “Development of cryogenic fracturing technology for coalbed methane production in Karaganda Coal Basin, Kazakhstan” project (Grant Award Number 021220CRP2022).

Electromagnetic particles" are elementary energy carriers

Akmaral Utelbayeva^{1*}, Nurlan Zhangabay¹, Essen Suleimenov²,
Bolysbek Utelbayev^{2**}

¹*M. Auezov South Kazakhstan University, Shymkent*

²*Kazakhstan - British Technical University, Almaty*

*E-mail: mako_01-777@mail.ru , **E-mail: b.utelbayev@mail.ru

The purpose of this work is to study and elucidate the nature of the chemical bond in the atomic structure of substances. It is well known that during the course of chemical, biochemical, electrochemical reactions between atoms, the initial bonds are broken and new chemical bonds are formed, which are accompanied by energy manifestations. At the same time, the release (absorption) of heat and light, where their elementary carriers, respectively, are "theplotrons" and photons, mean their participation in chemical bonding. To bind atoms consisting of nuclear-electronic structures "theplotrons" and photons must have a subdipole structure. The flow of photons, "theplotrons" and other particles representing the sun's rays, are the result of thermonuclear transformations in the main proton-proton cycle, i.e., charged particles. Based on this, it is assumed that in the course of the evolution of the Universe, subelementary dipoles were formed during collisions of charged electrical matters. The connection between the polar parts of the subdipoles is carried out by means of magnetic bipoles. The combination of electrical and magnetic components forms an "electromagnetic particle", which is a creation of Nature (Fig. 1).

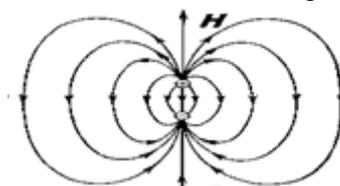


Figure 1. Conventional diagram of the "electromagnetic particle"

The intensity of the electromagnetic interaction between electrical matters is determined by the electric potential of the charge. Depending on the nature of the process, "electromagnetic particles" create an electromagnetic field, transfer energy in the form of heat, light, magnetism and other phenomena. The electrical and magnetic components of "electromagnetic particles" fluctuations create a picture of a standing wave taken for particle-wave duality of the particle. The frequency of fluctuations of the poles of "electromagnetic particles" determines the thermal, optical, magnetic and electrical properties of the "chemical individual" of substances". Thus, the nature of the chemical bond between atoms is "electromagnetic particles", where "theplotrons" and photons represent their variety.

Methoxy-substituted naphthothiophenes – single molecules' vs. condensed phase properties and prospects for organic electronics applications

Anatoly Botezatu^{1*}, Andrey Khoroshutin², Sergey Tokarev¹, Dmitry A. Lypenko³, Alexey Tameev³, Olga Fedorova¹

¹INEOS RAS, Russia, Moscow, Vavilova St. 28

²Lomonosov Moscow State University, Faculty of Chemistry, Russia, Moscow, 1-3 Leninskiye Gory

³A.N. Frumkin Institute of Physical Chemistry and Electrochemistry, Russian Academy of Sciences, Russia, Moscow, Leninsky Prosp. 31, bld.4.

*E-mail: tolik.botezatu98@gmail.com

In this work, a series of tricyclic naphthothiophenes – photocyclization products (8-methoxynaphtho[1,2-b]thiophene (**1a**); 6,7-dimethoxynaphtho[1,2-b]thiophene (**1b**); 8-methoxynaphtho[2,1-b]thiophene (**2a**)) have been studied. All compounds possessing similar structures demonstrated the close optical, electrochemical characteristics. Spectroelectrochemical investigation showed that **1b** and **2a** are able to form stable radical particles at 1.55 V. In case of **1a**, the formed at 1.55 V radical is short-living.

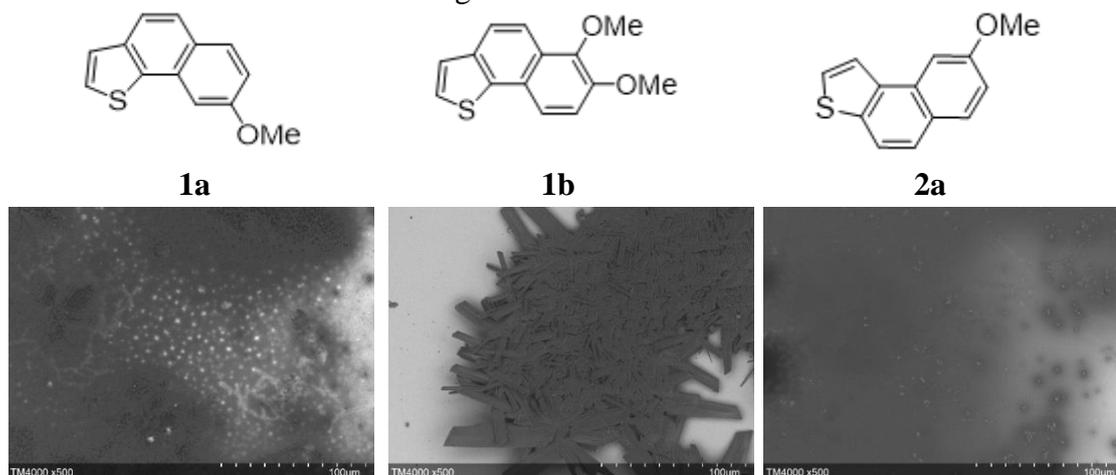


Fig.1 SEM image of **1a**, **1b**, **2a** film (thickness – 200 nm).

We have demonstrated, that due to differences in the morphology thin films of **1a** and **2a** exhibit the charge carriers mobilities ($10^{-4} \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$) one order of magnitude higher than that of **1b**. The **1a** and **2a** layers predominantly consist of an amorphous phase incorporated with microcrystals (Fig. 1). On the contrary, **1b** layers are formed only by microcrystals. Poor contacts between individual microcrystals limit the transport of charge carriers in such a polycrystalline medium. At the same time, the charge carrier mobility of **1a** in crystal form reaches high values ($0.09 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$). This indicates that these substances may serve a good starting point for the search for a new prospective organic semiconductors.

Acknowledgements. The reported study was funded by RSF according to the research project № 17-73-30036

The SOH and the SOC assessment of NCR18650 PANASONIC cylindrical battery through the entropymetry

Yerkin Serik^{1*}, Desmond Adair^{1,2}, Zhumabay Bakenov^{1,2,3}, Berik Uzakbaiuly^{1,2,3**}

¹*Institute of Batteries LLC, Kabanbay Batyr Ave 53, S4, 511, Nur-Sultan, Kazakhstan*

²*Nazarbayev University, Kabanbay Batyr Ave 53, Nur-Sultan, Kazakhstan*

³*National Laboratory Astana, Kabanbay Batyr Ave 53, S2, Nur-Sultan, Kazakhstan*

*E-mail: yerkin.serik@nu.edu.kz , **E-mail: berik.uzakbaiuly@nu.edu.kz

As the demand for the li-ion batteries increases in various areas, the precise and reliable assessment of the state of health (SOH) and the state of charge (SOC) of the battery become more important in the battery management system (BMS). The main goal of this research work is to create the model for the assessment of the SOH and SOC of the NCR18650 PANASONIC cylindrical battery based on thermodynamics parameters such as, enthalpy and entropy.

There are a lot of the SOH and SOC assessment methods in the market such as, the electrochemical, the equivalent circuit, and the machine learning models based methods. In this research work, it was used the Universal Battery SOC Theory proposed by Rachid Yazami in which α , β , γ coefficients depend on the SOH and nature of the battery.

$$\text{SOC} = \alpha + \beta(K \cdot \text{mol}) / J \Delta S + \gamma \text{mol} / J \Delta H$$

The mode of aging of the battery is divided into a calendar and cycling aging. Calendar aging is the decreasing the SOH of the battery without applying current. Cycling aging is the decreasing the SOH of the battery by charging and discharging of the battery. In this research work, the influence of the calendar aging was neglected by a continuous cycling of the battery. Cycling aging depends on the various parameters of cycling such as, the number of cycles, C-rate, the depth of discharge (DOD) , and the temperature.

To determine the dependence of the SOH of the battery to α , β , γ coefficients, it was analyzed the thermodynamics parameters of the NCR18650 PANASONIC cylindrical battery at various C-rate, DOD, and the number of cycles. But the influence of the temperature to the aging was extracted by cycling the battery at ambient temperature.

Acknowledgement

This research was supported by Institutte of Batteries LLC under Grant AP09261149.

Biomass-based biochar obtained by low-temperature pyrolysis in the presence of metal oxides: preparation, characterization and future applications

Aigerim Aitbayeva¹, Aitolkyn Uali^{1*}, Rustam Shlyapov¹, Alexey Vishnyakov², Shamshiya Amerkhanova^{1**}

¹*L.N.Gumilyov Eurasian National University, K. Munaitpassov St., 13, Nur-Sultan, Kazakhstan*

²*Skolkovo Institute of Science and Technology, Nobel St., 1, Moscow, Russia*

*E-mail: ualiaitolkyn@gmail.com , **E-mail: amerkhanovashk@gmail.com

Biochar, which is material obtained from biomass by thermochemical decomposition, is an environmentally friendly replacement for carbon materials. Its applications range from heat and energy production, agriculture and livestock farming to analytical chemistry and analysis. This carbon-enriched material can be obtained by using microwave-assisted pyrolysis, hydrothermal carbonization, pyrolysis, and gasification, thus changing the product's structure and properties. This research presents an environmentally and economically beneficial method for biochar synthesis from pine wastes in the presence of mineral additives and low-temperature pyrolysis. An increase in carbonization temperature leads to decreased product yield accompanied by increased pyrolysis co-product, bio-oil. The contents of O and H reduced are 12.90% and 11.00%, 7.60% and 3.60%, 2.67% and 1.98% for temperatures of 250, 350 and 400°C, respectively. Accordingly, the O/C and H/C molar ratios reduce with increasing temperature. It is shown that biochar produced at higher temperatures is more aromatic and less hydrophilic. Herein, the sample obtained at 300°C has a C-content of 76.59%; thus, its bulk polarity index [(O+N)/C] of 11.08 is the highest one among all samples investigated. Based on this, it is most likely that this biochar indicates lower aromatic nature and higher polarity of biochar. The FT-IR spectroscopy shows the carbonyl groups (C=O/C-O-C), carboxyl groups (-COOH), and hydroxyl groups (-OH) on the biochar surface. Regarding phase composition, the XRD confirms the presence of dolomite [CaMg(CO₃)₂], calcite CaCO₃, and quartz SiO₂ in the biochar bulk. Besides this, it includes Fe by EDS analysis. Based on materials characterization results, demonstrating the high carbon content, high polarity index, and the nature of surface functional groups, this biomass-derived biochar is most likely to be used as a sorbent, soil amendment, and even as shown redox activity.

Hydrodeoxygenation of guaiacol on transition metal phosphides formed *in situ*

Mariyam Mukhtarova*, Maria Golubeva, Anton Maximov

TIPS RAS, Russia, Moscow, Leninsky prospekt, 29

*E-mail: mariyam_99.02@mail.ru

Nowadays, catalysts based on transition metal phosphides can provide competition with traditional hydroprocessing catalysts due to their high catalytic activity and low cost. Transition metal phosphides poorly known and need more work in the hydrodeoxygenation of bio-oil phenolic compounds—biomass fast pyrolysis products.

This work is devoted to the catalysts based on molybdenum and tungsten phosphides generated *in situ* from metal carbonyls and triphenylphosphine in a stainless-steel batch reactor during the hydrodeoxygenation of bio-oil model compound - guaiacol. *In situ* formed molybdenum and tungsten phosphides are amorphous that was found by XRD. The molar Mo/P in MoP and W/P in WP ratios calculated from energy dispersive X-ray analysis were 1.3 and 1.1, respectively.

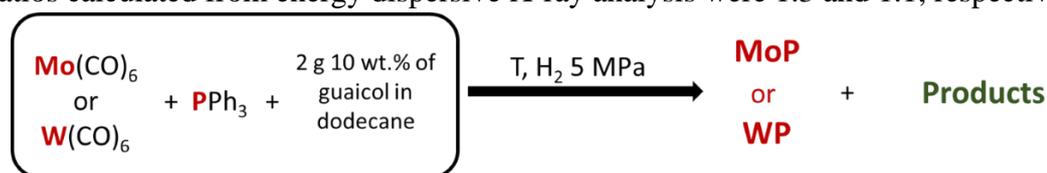


Fig. 1. Scheme of *in situ* production of catalysts based on molybdenum and tungsten phosphides

It was shown that conversion of guaiacol was 89–91 % and 80–86 % on MoP and WP respectively at 320–380°C, 5 MPa H₂, after 6 hours of reaction. The main hydrodeoxygenation product of guaiacol was phenol; anisole, cresols, and toluene were also formed. The highest selectivity for phenol on MoP was reached 80% at 360°C (5 MPa H₂, 6 hours). The highest selectivity for phenol on WP was 72% (340°C, 5 MPa, 6 hours). The recycling test of molybdenum and tungsten phosphides formed *in situ* from triphenylphosphine and metal carbonyls in the hydrodeoxygenation of guaiacol led to a slight decrease in catalytic activity. It should be noted that the selectivity for phenol remained unchanged.

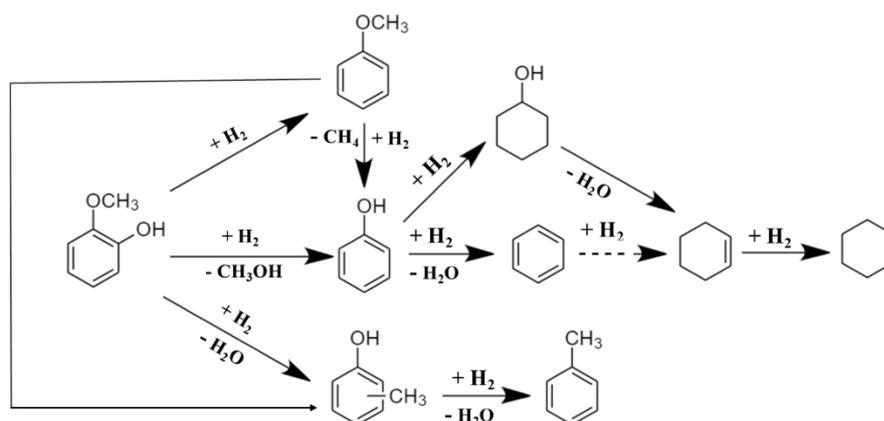


Fig. 2. Proposed reaction pathways of guaiacol hydrodeoxygenation in dodecane on *in situ* generated molybdenum and tungsten phosphides based catalyst

Experimental and numerical studies of rheological behavior of non-spherical powders

Asset Aliyev^{1*}, Zhazira Berkinova¹ and Boris Golman^{1**}

Chemical and Materials Engineering Department, Nazarbayev University, Nur-Sultan, KZ

*E-mail:asset.aliyev@nu.edu.kz , **E-mail:boris.golman@nu.edu.kz

Particles of irregular shapes have wide industrial applications in powder processing such as mixing, powder packing, conveying, fast feeding etc. Particle shape has an extreme influence on bulk powder flow performance which should be considered during powder processing. Powders used in industries have not only spherical shapes, but mostly non-spherical shapes from simple cylindrical to complex elongated geometries. The aim of the work is to study of rheological behavior of irregularly shaped aluminum oxide Al₂O₃. In this work, the Freeman FT4 powder rheometer was used to experimentally characterize the flow behavior of irregular shaped alumina. Flow behavior of alumina powders based on parameters such as basic flow energy, specific energy, flow rate index was analyzed. Non-spherical particle flow was simulated using Discrete Element Method (DEM) by filling and withdrawing particles from the hopper. After a heap was formed its angle of repose was measured using the ImageJ software to assess the powder flowability.

Keywords: Non-spherical particles, FT4 Rheometer, DEM, Angle of repose, flowability

Acknowledgement

This research is funded by the Science Committee of the Ministry of Education and Science of the Republic of Kazakhstan (Grant No. AP09260422).

Synthesis of 1,4-dihydropyridine derivatives in microwave flow reactor

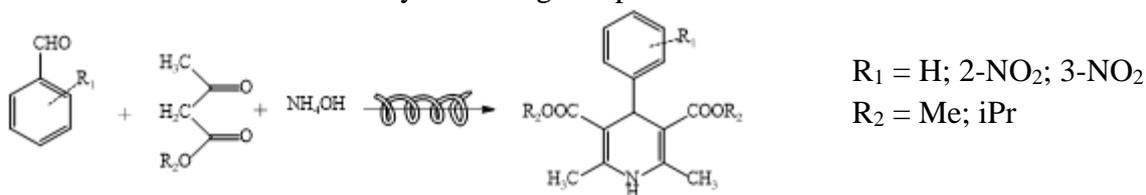
Anastassiya Khrustaleva^{1*}, Dmitriy Khrustalev^{1**}, Azamat Yedrissov², Marlen Mustafin¹

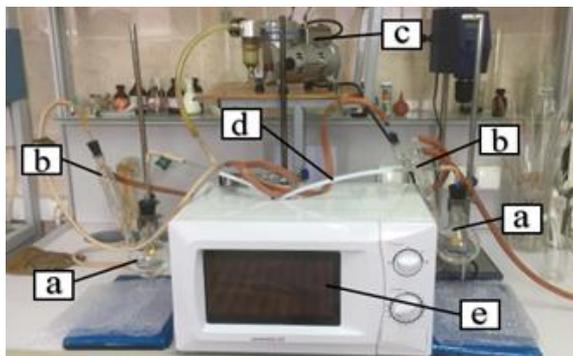
¹Medical University of Karaganda, 100000, Karaganda, Kazakhstan

²Nazarbayev University, 010000 Nur-Sultan, Kazakhstan

*E-mail: anasteishin_2009@mail.ru , **E-mail: khrustalev@bk.ru

1,4-Dihydropyridine derivatives (e.g. Nimodipine, Nifedipine, Nitrendipine), which belong to the group of calcium channel blockers, serve as effective drugs in the treatment of cardiovascular diseases. According to the World Health Organization (WHO), this disease class ranks first in terms of the number of deaths worldwide. Considering the unfavorable statistics of mortality from cardiovascular diseases, which is about 17 million people per year, the development of unique, cost-effective methods of obtaining 1,4-dihydropyridine derivatives is an urgent task. The previously developed method for effective Nifedipine and Nitrendipine synthesis in a microwave bath reactor is only suitable for the synthesis of small amounts of the product since attempting synthesis in large amounts results in loss of microwave irradiation benefits. The implementation of the process in a microwave flow reactor is the key to solving this problem.





- a. Reservoirs;
- b. Reverse refrigerators;
- Pump;
- d. Reactor;
- e. Energy source

The use of a microwave flow reactor for the synthesis of 1,4-dihydropyridine derivatives is an effective method that not only increases the reaction rate but also enables its large-scale production.

Acknowledgement

The study was conducted as part of the grant "Development of full synthesis of Aciclovir and Abacavir under microwave activation conditions"(2022). Karaganda Medical University. Scientific advisor- D.Sc. (Chemistry) Khrustalev D.P.

Synthesis of anti-tuberculosis drugs in a microwave flow reactor

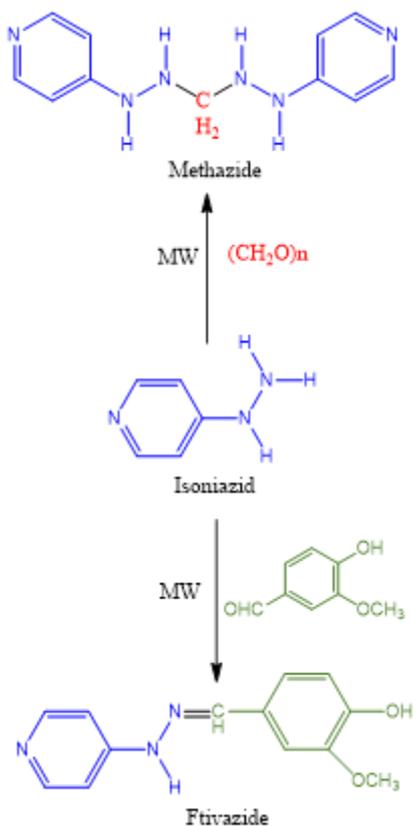
Azamat Yedrissov¹, Dmitriy Khrustalev², Anastassiya Khrustaleva², Marlen Mustafin²

¹Nazarbayev University, 010000 Nur-Sultan, Kazakhstan

²Medical University of Karaganda, 100000, Karaganda, Kazakhstan

*E-mail: aedrisov@gmail.com , **E-mail: khrustalev@bk.ru

According to the World Health Organization, one in every third person in the world is infected with Koch's bacillus. About 10 million people contract tuberculosis every year and about 1 million die from it. Therefore, the development of efficient and cost-effective ways to produce anti-tuberculosis drugs remains an urgent task. In our previous studies, highly efficient methods for the synthesis of such high-demand anti-tuberculosis drugs as Metazide and Ftivazide in microwave bath reactors have been developed. For the development of an industrial method for the production of Metazid and Ftivazid, we have developed an advanced technology for their synthesis in a microwave flow reactor.



The use of a microwave flow reactor has demonstrated the efficiency and prospects of industrial-scale production of Methazide and Ftivazide.

Acknowledgement

The study was conducted as part of the grant "Development of full synthesis of Aciclovir and Abacavir under microwave activation conditions"(2022). Karaganda Medical University. Scientific advisor- D.Sc. (Chemistry) Khrustalev D.P.

Design of low-silica zeolites based on natural halloysite nanotubes

Maria Rubtsova*, Aleksandr Glotov, Vladimir Vinokurov,

Gubkin Russian State University of Oil and Gas, Moscow, Russia

*E-mail: artemovamai@gmail.com

In this work, application of a natural halloysite nanoclay as a source of silicon and aluminum atoms for the synthesis of various low-silica zeolites has been proposed.

Halloysite with the chemical formula of $\text{Al}_2\text{Si}_4\text{O}_5(\text{OH})_4 \cdot n\text{H}_2\text{O}$ is formed by rolled aluminosilicate sheets, giving nanotubes with an inner diameter of 10-25 nm. An outer surface of halloysite nanotubes (HNT) comprises of siloxane groups (-Si-O), while inner – of aluminol groups (-Al-OH). Such structure makes it possible to modify HNT by various methods. In particular, treatment of HNT with acid/alkaline agents allows to remove selectively silicon or aluminum atoms, thus changing Si/Al ratio.

Within this study, HNTs were subjected to preliminary thermal and chemical (acid) treatment with further recrystallization into zeolites under hydrothermal conditions. Since acid treatment is not the only way to regulate Si/Al, an experiment was carried out in which halloysite was recrystallized in the presence of tetraethoxysilane (TEOS) as an additional source of silicon. The influence of organic templates addition was investigated.

According to X-ray diffraction data, zeolites obtained from thermally activated HNT possessed SOD structure, while those synthesized from acid etched halloysite had ANA structure, both demonstrated spherical morphology of the crystals (fig. 1a). The sample obtained with TEOS also possessed ANA structure, however, it had unique pompon-like morphology (fig. 1b).

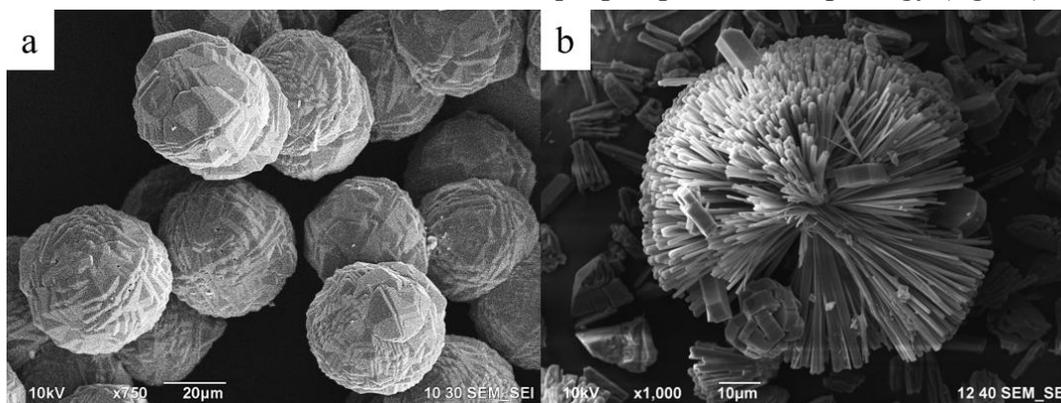


Figure 1. SEM images of the obtained halloysite-based materials

Based on the results obtained, it can be assumed that both HNT and TEOS act as co-templates responsible for the mesopores and crystals of unusual configuration formation.

Acknowledgement

This research was supported by the Ministry of Education and Science of the Russian Federation, project number FSZE-2020-0007 (0768-2020-0007).

Calibration-free Coulometric Sensors for Vanadium Redox Flow Battery Imbalance Monitoring

Pavel Loktionov^{1,2*}, Roman Pichugov¹, Mikhail Petrov¹, Anatoly Antipov^{1,2}, Dmitry Konev^{1,2**}

¹*Mendeleev University of Chemical Technology of Russia, Moscow, Russia*

²*Institute of Problems of Chemical Physics of RAS, Chernogolovka, Russia*

*E-mail: paul.loktionov@gmail.com , **E-mail: dkfrvzh@gmail.com

The vanadium redox flow battery (VRFB) technology is gradually filling a niche in the stationary energy storage market. In recent years, great progress has been made in increasing the discharge characteristics and energy capacity of electrolytes, but the problem of a gradual decrease in the available capacity during its long-term operation has not yet been solved. The main reason of the VRFB capacity fade is the gradual increase in the average oxidation state (AOS) of the negolyte due to electrochemical and chemical side reactions. This problem is proposed to be solved by carrying out periodic rebalancing of electrolytes – in this case, partial electrochemical reduction of posolyte is carried out in a special membrane-electrode assembly (MEA) cell. Ideally, such a process can fully restore the battery capacity to its nominal value. However, the efficiency of such a process is highly dependent on the accuracy of information about the composition of both VRFB electrolytes and their AOS. The literature presents many methods for analyzing the composition of vanadium electrolytes, but all of them have their drawbacks. The presented methods are either relevant only for a specific composition of supporting electrolyte, or for dilute solutions, or demonstrate low accuracy in the analysis under the electrolyte imbalance conditions.

In this work, we propose a unique method for assessing the vanadium electrolytes AOS - in-situ coulometry. According to this method, the electrolysis of the studied sample of vanadium electrolyte is carried out in a special symmetrical cell of the MEA. In this case, the investigated sample is first electrooxidized to VO_2^+ , and then electroreduced to V^{+2} . Based on the amount of charge spent in both steps, the AOS is estimated. The proposed sensors were tested for the analysis of the composition of 1 and 1.6 M vanadium electrolytes. AOS estimates were verified by 3 methods - conventional coulomb-counting, spectrophotometry and ex-situ coulometric titration. The sensors showed good accuracy both in ideal conditions of a single charge of electrolytes and in conditions of long-term battery cycling under the unbalance conditions. The data obtained confirmed that during cycling, the negolyte AOS increases due to the appearance of a side electrochemical process of hydrogen evolution during charging at high voltage. It has been shown that the proposed in-situ coulometric titration cells can be successfully used for laboratory studies of VRFB, as well as integrated with an electrolyte rebalancing system for obtaining stable long-duration battery cycling.

Acknowledgement

This research was financially supported by the Russian Science Foundation (project № 21-73-30029).

Optical features of Ag/Au-WO_{3-x} plasmonic composite thin films

Yerzhan Mukhametkarimov*, Nazim Gusseinov, Renata Nemkayeva, Ulantay Dosseke, Madi Aitzhanov

Al-Farabi Kazakh National University, 71 al-Farabi Ave., 050040 Almaty, Kazakhstan

*E-mail: yerzhan.mukhametkarimov@kaznu.kz

Tungsten oxide (WO₃) is a wide gap semiconducting material, well known as a functional element of smart windows, electrochemical electrodes for water splitting reactions, etc. One of the ways to extend the practical application of WO₃ is the modification of its electronic properties by chemical doping and formation of composites.

In this work, plasmonic composite thin films based on tungsten oxide (WO₃) matrix and Ag/Au nanoparticles (NPs) were deposited by RF magnetron sputtering. As deposited thin films have amorphous substoichiometric WO_{3-x} matrices with isolated noble metal NPs with average sizes of about ~3 nm. The resonance absorption peak is located at 580±10 nm and 430±10 nm for Au and Ag doped WO_{3-x} thin films, respectively. Depending on Ag/Au ratio, composite films demonstrate tunable plasmonic resonance absorption peak.

Acknowledgement

This research was supported by the Science Committee of the Ministry of Education and Science of the Republic of Kazakhstan Grant No. AP09258922.

Optoelectronic properties of layered gallium sulfide crystals

Nazim Gusseinov*, Yerzhan Mukhametkarimov**, Renata Nemkayeva, Madi Aitzhanov

Al-Farabi Kazakh National University, 71 al-Farabi Ave., 050040 Almaty, Kazakhstan

*E-mail: solar_neo@mail.ru , **E-mail: yerzhan.mukhametkarimov@kaznu.kz

Gallium Sulfide (GaS) layered crystal is a binary compound with excellent nonlinear optical and semiconducting properties. The energy band gap of GaS bulk crystals is ~2.6 eV, while it can reach up 3.3 eV in monolayer. In recent years, GaS two-dimensional crystals are considered as one of the perspective materials for the flexible electronics.

In this work, optoelectronic properties of gallium sulfide (GaS) crystals obtained by melting were investigated. In particular, it has been produced metal/semiconductor/metal photodetector based on micromechanically exfoliated GaS two-dimensional flakes. The photodetector demonstrates high responsivity in the near UV light range. The value of the on/off ratio of photocurrent is up to 10⁵ for 365 nm light with ~1 mW/cm² intensity. Obtained results indicate that GaS crystals are one of the most perspective materials for optoelectronic application in UV region among the other two-dimensional semiconductors due to the high response time, stability and on/off ratio value.

Acknowledgement

This research was supported by the Science Committee of the Ministry of Education and Science of the Republic of Kazakhstan Grant No. AP08052085.

Is azo-coupling of p-nitrothiophenol a good reaction for the evaluation of plasmon catalysis mechanism?

Alina Gorbunova^{*}, Oleg Semyonov, Pavel Postnikov, Olga Guselnikova^{**}

Research School of Chemistry and Applied Biomedical Sciences, Tomsk Polytechnic University

*E-mail: aag84@tpu.ru , **E-mail: guselnikovaoa@tpu.ru

The excitation of plasmon resonance on noble metals nanostructures delivers practical outcome in sensorics, photocatalysis. In plasmon-induced transformations, plasmon excitation allows to overcome the limitations of classical catalysis, such as high temperatures, pressures, and the use of complex catalytic systems. A model reaction for studying the mechanistic aspects of the plasmon-induced catalysis is the azo coupling of nitro- or -aminothiophenols. However, the nature of bonding between thiols and plasmonic metals is considered as chemisorption, which may be reversible – one thiophenols can be replaced by other molecules. Thiols can desorb from the substrate surface at elevated temperature and pressure, different pH values. This calls into question the validity of using the azo coupling reaction to assess the mechanism of plasmon catalysis. Therefore, we were faced with the task of evaluating the possibility of using this reaction in mechanistic studies.

We performed a detailed study about the stability of thiols-metal layer under the excitation of plasmon resonance. The elemental composition and chemical state (sulfur and nitrogen) were evaluated on the surface of nanoparticles during the azo coupling reaction. The azo coupling reaction of nitrothiophenol was carried out on the surface of gold nanoparticles with a size of 13 nm under excitation of plasmon resonance by illumination of 660 nm (corresponding to the maximum of plasmon resonance) for 1, 3, 6 hours. The reaction control was performed by Raman spectroscopy and X-ray photoelectron spectroscopy (XPS). The elemental composition and chemical state of the atoms were verified by XPS. We found that during irradiation, the oxidation and desorption processes were observed on S2p XPS spectra. This calls into question the validity of using the azo coupling reaction to study the mechanistic aspects of plasmon catalysis.

Acknowledgement

This research was supported by PHC Kolmogorov № 075-15-2022-244.

Improvement of light harvesting in optoelectronic devices by amphiphilic carbon dots

Sergei Cherevkov^{*}, Evgenia Stepenidenko, Elena Ushakova^{**}

ITMO University, 14, Birzhevaya linya V.O., St. Petersburg, Russia

*E-mail: s.cherevkov@gmail.com , **E-mail: el.ushakova@gmail.com

The development of strategies to compensate for losses in light harvesting is important in further improvements in the efficiency of solar cell devices. This can be achieved by development of multilayer active materials, which are composed of layers with efficient absorption in different spectral regions. To date, one of the promising materials for solar energy harvesting is metal-halide perovskites, whose major drawback is the destruction under UV irradiation. To decrease the influence of UV irradiation, it is proposed to use an additional layer, which will efficiently absorb in that spectral region and convert it to lower-energy emission. For that, luminescent carbon nanoparticles as efficient light absorbers in the range of 200–400 nm are attractive. Carbon dots are functional nanostructured composites whose structural parameters and physicochemical properties can be precisely controlled with photophysical characteristics that are not inferior to those of semiconductor nanostructures. The obtained nanostructures have a great potential due to the low toxicity of both precursors and the final product. They are usually synthesized in polar media, and

thus are hydrophilic. However, solution-processible optoelectronics demands hydrophobic inks, including conductive polymers; thus, further applications of carbon dots in such devices are highly limited. In this work, the amphiphilic carbon dots are developed and proposed to convert the UV spectral range of sun radiation into visible light via energy down-conversion.

The amphiphilic carbon dots were synthesized by solvothermal method using amines and organic acids as precursors dissolved in acetylacetone. In this case, the solvent not only facilitates the reaction of the precursors as media, but also participates in the formation of carbon dots. The morphology and optical properties of synthesized carbon dots were studied in detail. These nanoparticles can be efficiently redissolved in a set of polar and nonpolar solvents such as tetrachloromethane, chloroform, isopropanol, and water. The energy of optical transitions while changing the solvent is almost the same; moreover, the photoluminescence quantum yield is largest for nonpolar solvents. This observation opens an opportunity to use these carbon dots to fabricate photoactive functional films based on them for the improvement of the working parameters of optoelectronic devices based on perovskites.

Acknowledgement

This research was supported by Priority 2030 Federal Academic Leadership Program and the Russian Science Foundation (RSF22-13-00294)

Structure and electronic properties of layered Ge-Sb-Te based alloys

Zhandos Tolepov^{*}, Oleg Prikhod'ko, Alibek Zhakupov, Yernar Tursyn, Assyltas Rakhi.

Al Farabi Kazakh National, al-Farabi 71, Almaty.

*E-mail: tolepov.zhandos@kaznu.kz

Currently, with the increasing demands for modern storage media, such as flash memory (flash-memory) and hard disks based on magnetic recording, there is a failure of these types of storage media. This is mainly due to the insufficient number of write and erase cycles, the speed of writing and reading information, low radiation resistance, etc. [1-3]. In this regard, the expected receiver of a new generation of information carriers are non-volatile phase memory elements (PCM - Phase Change Memory) based on chalcogenide glassy semiconductors (CGS) [4].

Chalcogenide glassy semiconductors have unique properties. One of these properties is the ultrafast reverse phase transition of their structure from an amorphous to a crystalline state under the action of an electric or light pulse, which differ significantly in electrical and optical properties. It is known that chalcogenide semiconductors of the Ge-Sb-Te system of compositions $\text{Ge}_1\text{Sb}_2\text{Te}_4$, $\text{Ge}_2\text{Sb}_2\text{Te}_5$, $\text{Ge}_3\text{Sb}_2\text{Te}_6$ in the crystalline state have a layered structure with a van der Waals force of interaction between layers, which allows them to be exfoliate into two-dimensional crystals with a controlled number of layers [5,6].

In this work, an integrated approach was applied to study the structure and electronic properties of layered systems based on the Ge-Sb-Te compound.

Development of core-shell structured HCNF/Si anode material via coaxial electrospinning technique for new generation of lithium ion batteries

Nursultan Sapar^{1*}, Yerkezhan Yerkinbekova^{1,2}, Sandugash Kalybekkyzy^{1**}

¹National Laboratory Astana, Nazarbayev University, Nur-Sultan, Kazakhstan

²Department of Chemical and Materials Engineering, School of Engineering and Digital Sciences, Nazarbayev University, Nur-Sultan, Kazakhstan

*E-mail: nursultan.sapar@nu.edu.kz , ** E-mail: sandugash.kalybekkyzy@nu.edu.kz

Silicon hollow carbon nanofiber (HCNF) anode materials can be considered as a promising alternative for the conventional graphite electrode due to its 10 times higher theoretical capacity (4200 mAh g⁻¹ vs 372 mAh g⁻¹). However, it suffers from the fast capacity loss and limited cycle life because of volume expansion of Si at the lithiation process, therefore a considerable amount of Li ions is irreversibly trapped in the Si active sides. Generally, HCNF with its unique structure could withstand large volume change of Si.

Nanofibers were obtained by coaxial electrospinning technique by using PMMA as core and PAN as shell polymers. Porous structured CNFs were produced by decomposition of PMMA after stabilization at 280°C followed by carbonization processes at 800°C in the Ar atmosphere. To the fabrication of hollow structure, CNFs were activated by KOH. The SEM image in Fig.1a shows the HCNF have pores, while the TEM image demonstrates that this hole is continuous inside the nanofibers and has nanovoids on the surface of fibers. Incorporation of Si within these voids by Si-PMMA core solution might be a promising solution for the volume expansion problem.

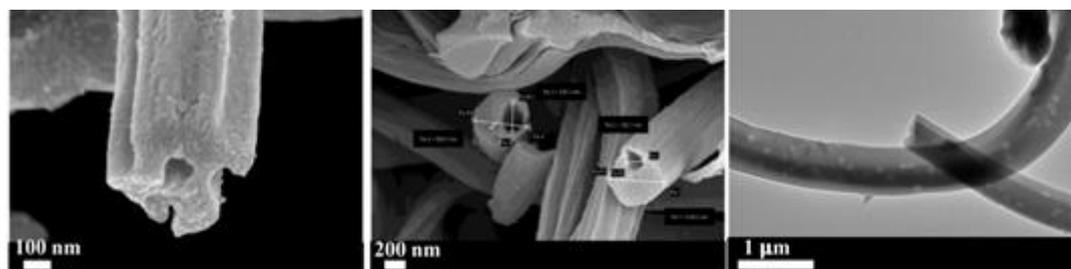


Figure 1. (a), (b) SEM image of HCNF, (c) TEM image of HCNF

Acknowledgement

This research was supported by the research grants #AP08855889 “Development of Flexible and Safe Next - Generation Li - Ion Batteries” from the Ministry of Education and Science of the Republic of Kazakhstan

Pt-free and efficient counter electrode with nanostructured MnCo₂S₄ for dye-sensitized solar cells

Diana Suleimenova^{1*}, Ayagoz Ibrayeva¹, Bakhytzhan Baptyayev², Yerbolat Tashenov^{1,3}, Mannix P. Balanay^{3**}

¹*L.N. Gumilyov Eurasian National University, Nur-Sultan, 010000 Kazakhstan*

²*National Laboratory Astana, 53 Kabanbay Batyr Ave., Nur-Sultan, 010000 Kazakhstan*

³*Department of Chemistry, School of Sciences and Humanities, Nazarbayev University, 53 Kabanbay Batyr Ave., Nur-Sultan, 010000 Kazakhstan*

*E-mail: www.lady.di@mail.ru , **E-mail: mannix.balanay@nu.edu.kz

In the past few years, the development of alternative and renewable energy sources has been one of the urgent and most important tasks due to the growing demand of the population for energy. Dye-sensitized solar cells (DSSC) firstly introduced by Grätzel and O'Regan are third generation photovoltaic devices that have distinctive advantages over silicon solar cells, such as low cost of materials used, ease of fabrication and eco-friendliness.

The development of an alternative counter electrode for dye-sensitized element (DSSC) using a simple and single method is an ad hoc research direction for problem solving used with an expensive Pt-based counter electrode. In this work, a MnCo₂S₄ counter electrode was developed directly on a fluorine-doped titanium oxide (FTO) coated glass substrate using a one-step and simple hydrothermal method. The MnCo₂S₄@FTO counter electrode has been characterized by several spectroscopic and microscopic methods and has also been assembled in a DSSC device to evaluate electrode performance.

The DSSC with MnCo₂S₄ counter electrode produced 97 % comparable efficiency with Pt-based electrode which shows its applicability as an alternative counter electrode owing to its reduced production cost and almost similar photovoltaic efficiency with the reference electrode.

Analysis of RIM-driven turbines: a literature review

Nursultan Jyeniskhan^{*}, Akezhan Zholdybayev, Chingiz Arystanbekov, Sherif Gouda^{**}

Nazarbayev University, Qabanbay Batyr Ave 53, Nur-Sultan 010000

^{*}E-mail: nursultan.jyeniskhan@nu.edu.kz , ^{**}E-mail: sherif.gouda@nu.edu.kz

One of the common and convenient methods for generating electricity from the marine environment is extracting energy from the water containing kinetic energy. Due to environmental concerns, rim-driven turbines are proposed, with several advantages such as efficiency due to compact design and reduced failure rates. This review paper aims to evaluate the various aspects of turbines to denote the necessity of applying Rim-driven turbines. In the first part of a review paper, the energy potential of the marine environment was discussed. The second part is focused on the importance of research and indicates both advantages and disadvantages of the design and utilization of Rim-driven propellers. Lastly, some literature has addressed blade cavitation, which is the main factor contributing to energy loss. Therefore, we discussed the literature that has addressed blade cavitation and studied the effect of cavitation on energy-generating efficiency. Then, we divided the literature according to its scope and indicated the drawbacks. In essence, they lacked experimental validation, contained high errors, or lacked higher-precision design models that are essential in developing energy-efficient energy systems. The results of this literature review could be used to address the drawbacks in the application of Rim-driven thrusters and initiate further research in the field.

Highly efficient bio-based carbonaceous counter electrode for dye-sensitized solar cells

Ademau Aliakbarova^{1*}, Yerbolat Tashenov^{2,3}, Bakhytzhan Baptayev⁴,
Mannix P. Balanay^{3**}

¹*Kazakh-British Technical University, Almaty, 010000 Kazakhstan*

²*L.N. Gumilyov Eurasian National University, Nur-Sultan, 010000 Kazakhstan*

³*Department of Chemistry, School of Sciences and Humanities, Nazarbayev University, 53 Kabanbay Batyr Ave., Nur-Sultan, 010000 Kazakhstan*

⁴*National Laboratory Astana, 53 Kabanbay Batyr Ave., Nur-Sultan, 010000 Kazakhstan*

^{*}E-mail: ademau@inbox.ru , ^{**}E-mail: mannix.balanay@nu.edu.kz

The use of platinum, an expensive and scarce element, in dye sensitized solar cells may affect the cost and commercialisation of the technology. In this regard preferable candidates would be materials which are abundant and cost effective. Carbonaceous materials are promising materials for being abundant and having many suitable characteristics such as porosity, conductivity, high surface area, chemical and thermal stability. We propose to use carbonaceous materials as counter electrode for dye-sensitized solar cells to replace Pt. The carbon electrocatalyst is prepared from organic waste such as apricot and/or walnut shells. The material is characterized by various techniques including XRD, SEM, EDS, FTIR. Also photovoltaic and electrochemical properties of solar cells based on novel counter electrode are measured.

Adsorption of polyethene glycol and propylene glycol onto the modified glass microspheres

Shamshiya Amerkhanova^{1*}, Alexey Vishnyakov², Dana Belgibayeva¹, Aitolkyn Uali¹, Rustam Shlyapov^{1**}

¹*L.N.Gumilyov Eurasian National University, K. Munaitpassov St., 13, Nur-Sultan, Kazakhstan*

²*Skolkovo Institute of Science and Technology, Nobel St., 1, Moscow, Russia*

*E-mail: amerkhanovashk@gmail.com , **E-mail: rustamshlyapov@gmail.com

Since polyethene glycol (PEG) and other derivatives of ethylene oxides are contained in the composition of medicinal and detergents, their large volumes enter water bodies. However, the issue of removing PEG and other polyatomic alcohols from the environment has not been solved yet. This research presents the adsorption of polyethene glycol (PEG) and propylene glycol (PG) on the surface of glass microspheres of the SVJ, SPJ and SMJ brands. The second virial coefficient B values in the Jones-Dole model have been calculated from the concentration dependence of dynamic viscosity for PEG and PG solutions. The strongest polymer-solvent interactions are observed in the concentration range up to 20 g/L for the initial PEG's aqueous solution. A further increase in the polymer fraction makes this interaction weaker due to a change in macromolecule configuration and the formation of overlapping areas of PEG chains. However, after adsorption on modified glasses, the strength of PEG macromolecule and water associates decreases as follows: SVJ (vinyl) > SPJ (phenyl) > SMJ (methacrylate). In the same series, the adsorption capacity of PEG varies symbiotically from 5.89 g/g (SVJ) to 0.099 g/g (SMJ). This fact can be explained by hydrogen atom mobility in the modifier's structure and the ability to form hydrogen bonds with the oxygen atom in the PEG chain. At the same time, for a PG solution, adsorbents form a series based on the degree of influence on the solute-solvent complex strength that is increasing as SMJ (methacrylate) > SVJ (vinyl) > SPJ (phenyl). However, the change in adsorption value is likely similar to that for PEG. The Jones Dole model, together with the polymer adsorption data, makes it possible to establish the priority of fixing the solute substance or solvent on the surface. To sum up, glass microspheres modified with the SVJ vinyl can be used to neutralize effluents containing polyethene glycol.

The SOH and the SOC assessment of $\text{LiNi}_{0.88}\text{Co}_{0.09}\text{Al}_{0.03}\text{O}_2$ cathode material for lithium-ion batteries through the entropymetry

Gulzat Nuroidayeva¹, Yerkin Serik¹, Berik Uzakbaiuly^{1,2,3*}, Zhumabay Bakenov^{1,2,3} Desmond Adair^{1,2}

¹*Institute of Batteries LLC, Kabanbay Batyr Ave 53, S4, 511, Nur-Sultan, Kazakhstan*

²*Nazarbayev University, Kabanbay Batyr Ave 53, Nur-Sultan, Kazakhstan*

³*National Laboratory Astana, Kabanbay Batyr Ave 53, S2, Nur-Sultan, Kazakhstan*

*E-mail: gulzat.nuroidayeva@alumni.nu.edu.kz , **E-mail: berik.uzakbaiuly@nu.edu.kz

Lithium-ion batteries (LIB) are widely used in new energy vehicles and energy storage. That is why the user should be aware of the state of charge (SOC) and the state of health (SOH) of the battery. The SOC in Battery Management System (BMS) provides the percentage of battery capacity, while the SOH measures the battery health. LIBs are met with significant challenges in saving capacity retention, becoming increasingly necessary to achieve a sustainable model. The main goal of this research is the accurate assessment of the SOH and the SOC of the battery cell to study the main electrochemical characteristics of the cathode material and measure the entropy to estimate the remaining useful life (RUL) of the battery. The object of the study is active materials based on $\text{LiNi}_{0.88}\text{Co}_{0.09}\text{Al}_{0.03}\text{O}_2$ (NCA) cathode powders. A series of NCA cathodes were tested to characterize the capacity fading mechanism through the thermodynamic characterization - entropy.

It is a powerful method to study the cycle life and safety of batteries. For this purpose, the Universal Battery SOC equation have been used: $SOC = \alpha + \beta(K \cdot mol)/J \Delta S + \gamma(mol/J) \Delta H$.

This paper reveals the capacity fading of NCA cathodes, largely stemmed from the anisotropic volume change, which was caused by the phase transition near the charge-end.

Acknowledgements

This research was funded by the Science Committee of the Ministry of Education and Science of the Republic of Kazakhstan (Grant No. AP09261149) and by the research grant #51763/IIIΦ-MLIPOAII PK-19 "New materials and devices for defense and aerospace applications" from MDDIAI Republic of Kazakhstan.

Application of biogenic zinc oxide nanoparticles in the degradation of organic dyes

Assel Alimkhanova^{1,2**}, Nurgulim Aimanova^{1,2}, Azamat Kitzhan^{1,2*}, Anastassiya Mashentseva^{1,2}

¹The Institute of Nuclear Physics of the Republic of Kazakhstan, Ibragimov str., 1, Almaty 050032, Kazakhstan;

²L.N. Gumilyov Eurasian National University, Satpaev str., 5, Nur-Sultan 010008, Kazakhstan

*E-mail: azamat1997kitzhan@gmail.com , **E-mail: aselalimkhanova645@gmail.com

Heterogeneous photocatalysis is one of the most popular methods among the variety of different technologies to purify environmental pollutant. The dye Rhodamine B and Alizarin Yellow R are used in many industrial applications and have side effect, when significant amount of the dye is washed off with the wastewater of production during the process, falling into surface reservoirs and destroying the ecosystem.

Metal oxides as a multifunctional material are non-toxic, biocompatible, and have high activity. Metal oxide semiconductors have good photocatalytic activity for decomposition of organic dyes. In particular, zinc oxide can be considered as the most important among all the various metal oxides because of the wide band-gap (3.36 eV) and high exciton binding energy (60 MeV) as well high thermomechanical stability.

This work investigated the possibility of using biogenic zinc oxide nanoparticles (NPs) ZnO as photocatalysts for the decomposition reaction of RhB and AYR dyes. The photoactivity of the catalyst in relation to the reaction of AYR and RhB was revealed: the effect of the dye concentration, temperature, and mass of catalysts were examined.

The photoreaction showed that the efficiency of dye removal increases with increasing irradiation time. The kinetics of the photodegradation reaction expressed a pseudo-reaction of the first order. An increase in the dye concentration reduced the efficiency of dye removal. The optimal mass of the RhB catalyst is 100 mg decomposition 98%, AYR 50 mg 97%, while the optimal concentration of dyes: RhB 5 mg/l reaction rate constant 0.0101 min⁻¹, AYR 10 mg/l k= 0.0204 min⁻¹. To study the effect of temperature on the efficiency of the decomposition of dyes, the experiment was carried out in the temperature range of 15-45 ° C. The activation energy for RhB was determined by Arrhenius equation to be equal to 12.3 kJ/mol, AYR E_a equal to 11.63 kJ/mol.

Determination of optimal synthesis conditions of the Cu@PET composites using Taguchi robust experiment design

Anastassiya Mashentseva^{*}, Maxim Zdorovets^{**},

The Institute of Nuclear Physics of the Republic of Kazakhstan, 050032 Almaty, Kazakhstan

**E-mail: a.mashentseva@inp.kz, **E-mail: mzdorovets@inp.kz*

In this task the Taguchi robust design was applied to optimize experimental parameters as well as to determine the optimal conditions for the electroless copper plating. Taguchi robust planning is widely used in the production and study of various technological processes and scientific research, including synthesis of nanomaterials and the study of their properties. Orthogonal array of L₂₇ type was applied as an experimental design to analyze the results and to determine optimum conditions for synthesis of copper microtubes loaded composite membranes. Four key process parameters – deposition temperature, amount of activation, amount of formaldehyde and concentration of carboxylic groups on the PET template surface – were considered for the optimization of Cu@PET composites as an efficient catalyst in the methylene blue decomposition reaction.

The signal-to-noise (S/N) ratio analysis is adapted to improve the statistical properties of the Taguchi design method used in this work to evaluate the conditions required to obtain composite TeMs with the highest photocatalytic activity. In this study, for measurable quality characteristics, the equation “larger-is-better” was used.

Optimal conditions for the sunthesis of Cu@PET composites according to obtained results were determined: carboxylic group concentration - 16.5 ± 1.5 nM/cm², deposition temperature – 25 °C, plating time – 20 min and reducing agent (formaldehyde) concentration – 5.95 ml/l.

Acknowledgement

This research was supported by International Atomic Energy Agency (IAEA) under coordinated research project F22070 (IAEA Research Contract No: 23152).

Fabrication of the free-standing Ni_xS_y microflowers for li-ion batteries

Assyl Adylkhanova^{1*}, Nurbolat Issatayev¹, Zhumabay Bakenov^{1,3}, and Gulnur Kalimuldina^{2**}

¹*Department of Chemical and Materials Engineering, School of Engineering and Digital Sciences, Nazarbayev University, Nur-Sultan 010000, Kazakhstan*

²*Department of Mechanical and Aerospace Engineering, School of Engineering and Digital Sciences, Nazarbayev University, Nur-Sultan 010000, Kazakhstan*

³*National Laboratory Astana, Nazarbayev University, Nur-Sultan 010000, Kazakhstan*

**E-mail: assyl.adylkhanova@nu.edu.kz, **E-mail: gkalimuldina@nu.edu.kz*

Flexible energy storage systems have attracted extensive attention owing to the rapid development of advanced technology. Among them, transition metal sulfides, particularly, nickel sulfides (Ni_xS_y), are considered prospective cathode materials for lithium-ion batteries due to their excellent energy storage performance. Herein, flexible three-dimensional Ni_xS_y cathodes were synthesized using a facile dip-coating method without surfactants and high temperatures. The as-prepared electrode composite demonstrates superior electrochemical performance with high specific capacitance. Ni_xS_y flower-like microspheres supported on nickel foam (Ni_xS_y@Ni) can benefit electrode stability and cycling performance. The structure and morphology of Ni_xS_y are characterized by X-ray photoelectron spectroscopy and scanning electron microscopy coupled with energy dispersive X-Ray spectroscopy. The porous structure of the nickel skeleton can hinder the volume expansion of the sulfur and enhance the ion/electron diffusion. In accordance with electrochemical tests, the obtained electrode demonstrates superior electrochemical performance

with a high specific capacitance of 420 mAh/g at a current density of 0.1 C, accompanied by a Coulombic efficiency of about 100% for 50 charge-discharge cycles.

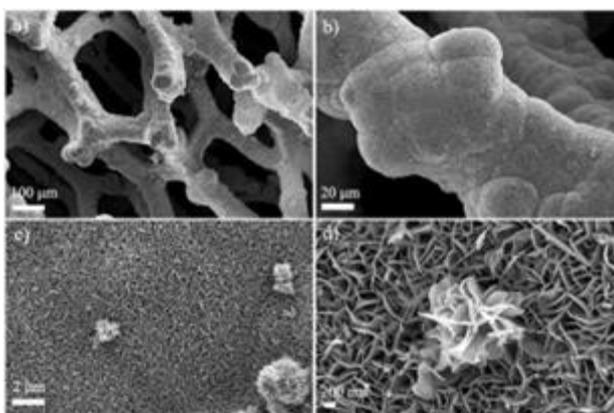


Figure 1a-d. SEM pictures of Ni_xS_y samples

Acknowledgment

This work was supported by the research project AP08052143 “Development of Wearable Self-Charging Power Unit” from the Ministry of Education and Science of the Republic of Kazakhstan.

Kinetics of sodium intercalation-deintercalation processes into an Eldfellite cathode material with a MoS_2 surface layer

Saule Kokhmetova*, Tatyana Kan, Fyodor Malchik, Alina Galeyeva, Andrey Kurbatov

*Center of Physical-Chemical methods of Research and Analysis, al-Farabi Kazakh National University 96A Tole bi Str.,
Almaty, Kazakhstan*

*E-mail: tornatore@mail.ru

Among the conditions for the occurrence of an electrochemical reaction on the electrode surface is the presence of electronic conductivity of the electrode material. Among the cathode materials for metal-ion batteries, there is a large group of polyanionic substances that have excellent energy performance, but have poor conductivity. To implement the intercalation-deintercalation of the cation into these materials, their conductivity is increased by creating a point carbon contact, which makes it possible to improve electrochemical characteristics only up to a certain limit. In this work, it was proposed to create a flat conductive layer on the surface of the working material to increase the area of charge transfer to the surface of the latter.

$NaFe(SO_4)_2$ with an eldfellite structure was used as a model cathode material with poor conductivity, which was coated by MoS_2 using long-term homogenization of both materials in a planetary mill in a hexane medium. The thickness of MoS_2 varied in the range of 5-125 nm.

It was found that with an increase in the thickness of the MoS_2 layer, the area of implementation of the electrochemical process increases due to a decrease in the electron transfer resistance. However there is also an increase in the resistance of sodium cation transfer from the electrolyte to the surface of the cathode material. All this ultimately leads to the fact that the process of cation transfer becomes limiting, leading to a decrease in the overall rate of the process with an increase in the coating thickness, as can be seen in the CV curves at different contents of MoS_2 . The same can be seen in the values of the diffusion coefficient of the reagent in the zone of the electrochemical reaction, passing through the corresponding maximum at a MoS_2 concentration in the mixture of 0.5 %. The dependence of the half-wave potential on the thickness of the MoS_2 layer

and the shift of the potential of the CV peaks are related to the ohmic contribution of the charge transfer in the coating phase to the total overvoltage of the process.

Acknowledgement

This work was supported by Ministry of Education and Science of the Republic of Kazakhstan [grant number AP09260371].

Establishing regularities of charge transfer through corrosive films on lithium

Yaroslav Zhigalenok*, Andrey Kurbatov

al-Farabi Kazakh National University, 71 al-Farabi Ave., Almaty 050040, Kazakhstan

*E-mail: yaroslav.zsv@gmail.com

Lithium metal is the highest energy intensive anode of all known materials. It cannot be commercially used at the moment due to poor cycle-to-cycle capacity retention as well as safety concerns. The main problem is the transition of lithium from a compact morphology to a dendritic one during battery operation. This problem is caused primarily by the heterogeneous structure of the solid electrolyte interphase layer, the film that is the product of lithium passivation in the organic electrolyte. Revealing the basic laws of charge transfer through such a film will make it possible to find an effective solution to the problem of dendrite growth.

In this work the charge transfer mechanism in the lithium-solid electrolyte interphase-electrolyte system is investigated. Lithium metal electrodes were fabricated, the surface of which was renewed just before their immersion in the electrolyte. For these electrodes anodic polarization curves were obtained with different corrosion times in the electrolyte. The obtained curves were analyzed by non-linear interpolation with six equivalent circuits representing paired combinations of three electric circuit elements. The absence of diffusion overvoltage at the lithium electrode in the investigated polarization interval was shown. It was shown that polarization of the lithium electrode is caused by the charge transfer stage through the volume of the solid electrolyte interphase. It was found that cation transfer in the film proceeds in parallel along the sections described by Ohm's law and the sections obeying Mott-Gurney's law, equation 1:

$$i = \frac{\eta}{R} + \frac{9\varepsilon\mu\eta^2}{32\pi L^3} \quad (1)$$

By numerical simulations it was shown that there is no influence of the charge transfer contribution across the interface on the total polarization. By simulation of voltammetric curves, the conditions of mixed kinetics of electrochemical process, i.e. conditions under which the rates of charge transfer through the interface and charge transfer through the film volume are comparable with each other, are found.

Selecting a membrane for supercapacitor batteries with water-based electrolyte

Kaiyrgali Maldybayev*, Fyodor Malchik, Tatyana Kan, Saule Kokhmetova, Andrey Kurbatov,
Alina Galeyeva, Olzhas Kaupbay.

al-Farabi Kazakh National University, Center of Physical-Chemical Methods of Research and Analysis, Almaty, 050012, Kazakhstan

*E-mail: Kaiyrgali.m.m@mail.ru

One of the important parts of the energy storage system is a separator, which has the function of separating the anode from the cathode. Despite the wide variety of existing materials, there are

still ongoing developments to improve membrane properties such as: ionic conductivity, high porosity, chemical and electrochemical stability in the electrolyte, as well as the thickness of the material. This study analyzes new materials courtesy of Nippon Kodoshi Corporation (pulp-and-paper separator TF4050 and VL100; Japan) and compares them with hydrophilic membrane filter made of PVDF (Durapore, Germany) and Whatman quality filter paper, Grade 1 (Whatman, UK).

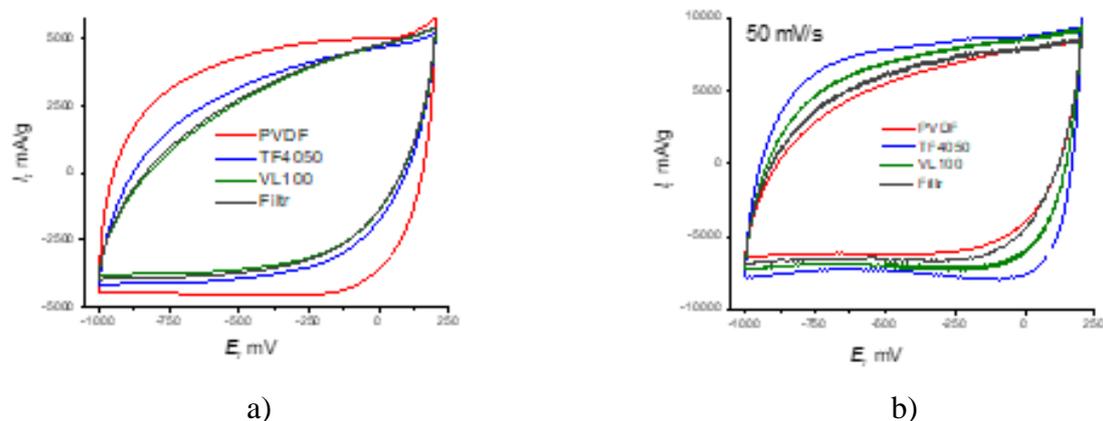


Figure 1 –CV curves in saturated a) LiCl and b) NaClO₄ electrolyte (scan rate is 50 mV/s).

Comparison was done by CV measurements (from 1 to 100 mV/s) using galvanostat/potentiostat Biologic SP-300. Cyclic voltammetry was provided on different membranes in saturated LiCl (14 M) and NaClO₄ (8.5 M) electrolytes where MXene, Carbon-cloth and Ag/AgCl were chosen as working, counter and reference electrode respectively. At low scan-rate (1-5 mV/s) there is no difference between CV shapes, since there are no limitations on membrane nature, however, on a higher scan rate, starting from 10 mV/s, the CV area as well as sweep angle differences can be noticed significantly. According to this, TF4050 based membranes have best response with NaClO₄ electrolyte and good response with LiCl electrolyte for kinetic properties which is very important for MXene type supercapacitor-electrode materials, where specific power is an important factor and requires fast charge-discharge abilities (or high scan rate).

For farther investigation of membrane properties for possible application in water-based electrolyte batteries and supercapacitors is necessity to check impedance spectroscopy and to evaluate mechanical properties of membranes. At this moment, investigated membranes are very suitable for this application.

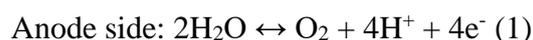
Establishment of regularities of the influence of factors that determine the electrochemical stability window of aqueous electrolytes for sodium-ion batteries

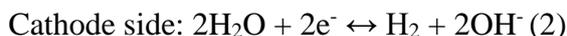
T.A. Akatay, A.P. Kurbatov, Kohmetova S.T.

Al-Farabi Kazakh National University, Almaty, Republic of Kazakhstan

Email: tlekakatay@gmail.com

The use of water as a battery electrolyte provides better ion migration. Also, an aqueous electrolyte is more environmentally friendly and safe, the low price of such electrolytes is also important, in addition, water is an excellent solvent for many salts. The main problem of aqueous electrolytes is a narrow electrochemical stability window, beyond which water decomposition begins:





In this work, we present a method for expanding of electrochemical stability window of aqueous electrolytes by coating the electrode with a hydrophobic layer. The resulting coatings were applied by soaking in solutions of various concentrations of paraffin in hexane and subsequent drying. The change in the stability window for coatings of various thicknesses, as well as the values of the electrode resistance and the thickness of the electrical double layer, were determined using electrochemical impedance. The effect on other electrochemical reactions was also investigated.

The resulting coating extended the stability window to 3.2 volts, compared to 2.9 volts in saturated sodium perchlorate. Coating to a greater extent window expanded in the anode region by 230 mV.

Acknowledgement

This research was supported by Science Committee of the Ministry of Education and Science of the Republic of Kazakhstan (Grant No. AP08856725).

Simulation of Intercalation Processes in Poorly Conductive Materials

Andrey Kurbatov*, Yaroslav Zhigalenok**, Saule Kokhmetova, Fyodor Malchik, Alina Galeyeva
*Center of Physical-Chemical methods of Research and Analysis, al-Farabi Kazakh National University 96A Tole bi Str.,
Almaty, Kazakhstan*

*E-mail: kurbatovap@gmail.com , **E-mail: knife6924@gmail.com

Currently, the search for new electrode materials for metal-ion batteries, based on the identification of crystal structures with ionic mobility and the ability for reversible intercalation process, often leads to materials with low conductivity, especially electronic. In fact, these are dielectric materials, a striking example of which are many polyanionic compounds. At the same time, these materials are often characterized by potentially attractive characteristics, such as low volume change during cycling, ease of synthesis, moderate values of specific capacity, and others.

However, the implementation of the intercalation process and especially its kinetics represent a significant difficulty for dielectric materials, despite their thermodynamic attractiveness. Even nanosized materials at low currents in the electrodes show low specific capacitance for this reason. The physical model includes a description of mass transfer and charge transfer in the phases of the electrode material and electrolyte, connected by the condition of transformation at the interface between them. A single-particle model using COMSOL Multiphysics was modeled to calculate the process of intercalation and accumulation of intercalation phase in the bulk of the initial active material phase. A distinctive feature of the model is considering the distribution of the intercalation process over the surface, in contrast to the dominant approach based on the use of the idea of particle surface equipotentiality. The influence of the number of electron contacts to the particle on the kinetics of the process is also considered.

Acknowledgement

This research has is funded by the Science Committee of the Ministry of Education and Science of the Republic of Kazakhstan (Grant No. AP09563408).

On electrochemical activity of $Zn_2(EDTA)(H_2O)$ in aqueous sodium-ion based electrolytes

Alena Starodubtseva^{1*}, Ivan Trussov^{1,2}, Alina Galeyeva¹, Andrey Kurbatov¹

¹*al-Farabi Kazakh National University, Almaty, 050040, Kazakhstan*

²*Skolkovo Institute of Science and Technology, Moscow, 121205, Russian Federation*

*E-mail: alena.a.rubanova@gmail.com

Metal-organic frameworks (MOFs) are a class of compounds consisting of metal ions or clusters coordinated to organic ligands to form one-, two-, or three-dimensional structures. Due to their high porosity and excellent adsorption and catalytic activity, as well as the ability to simultaneously implement different charge accumulation mechanisms (ions de/intercalation and adsorption/desorption), they can be considered as electrode materials for metal-ion batteries. However, a significant drawback is that most MOFs have low conductivity, and the obtaining of conducting MOFs is a costly, time-consuming and technically difficult process.

In this work, we present a method for synthesis of $Zn_2(EDTA)(H_2O)$ MOF composite and investigation of its electrochemical activity in aqueous sodium-ion based electrolytes. The structure of the synthesized substance was confirmed by X-ray diffraction analysis with subsequent Rietveld refinement method as well as by IR spectroscopy. Scanning electron microscopy has showed the porous structure of investigated material. Thermogravimetric analysis data indicates considerable stability of the material up to 500 °C and confirming stable bonding of coordination water with the zinc ion in the structure. Electrochemical characteristics of the studied MOF in 1-10M NaOH alkaline electrolytes as well as in $NaClO_4$ saturated aqueous electrolyte were evaluated by cyclic voltammetry and galvanostatic cycling. It was found that the studied compound does not give a satisfactory electrochemical response in aqueous electrolytes due to the strong degradation of the electrode material, which is associated with the high solubility of this MOF. The main driving force for dissolution is the replacement of carboxylate linkers by hydroxide ion\water, which competitively bind to zinc ions in the organic framework. Thus, this material is not suitable for use as an intercalation electrode material for sodium-ion batteries based on aqueous electrolytes. This conclusion is in a direct conflict with the work of Sangeetha S. Patel et al, published in the journal of Inorganic and Organometallic Polymers and Materials in 2020.

The obtained results have an importance by two reasons: 1) we have better understanding of behavior of EDTA based MOFs in aqueous electrolytes; 2) once again we understand that every piece of scientific knowledge must be cross-checked by various researchers.

Acknowledgement. This research was supported by Science Committee of the Ministry of Education and Science of the Republic of Kazakhstan (Grant No. AP09058322).

Impact of substrate surface preparation method on SEI formation regularities during electrochemical deposition of lithium

Margarita Ryabicheva^{*}, Andrey Kurbatov

al-Farabi Kazakh National University, Almaty 050040, Kazakhstan

*Email: maga050198@gmail.com

The use of lithium metal as an anode for batteries has undeniable advantages because this metal has the most negative reduction potential and the highest theoretical specific capacity. The reduction of lithium metal initially involves processes of solution components decomposition with the formation of SEI - a film of interfacial electrolyte, under which lithium is further deposited. Reversible lithium deposition requires it to have pure ionic conductivity and high mechanical strength.

In this work, the reproducibility of lithium separation on nickel and steel substrates with different preparation of their surfaces was evaluated. The electrodes were polished to a mirror finish, kept in an ultrasonic bath in a 5% KOH solution with 0.01% OP-10, washed with distilled water and dried under vacuum ($T = 70^{\circ}\text{C}$). Sandpaper (P3000) and a soft cloth were used as methods of cleaning the working surface after CV inside the chamber box (Ar atm.). Cleaning outside the box was carried out with soft cloth followed by washing and drying under vacuum.

Microscopic control of electrode surface along its polishing showed that "mirror shine" is achieved much earlier than ideal surface homogeneity, therefore, in the absence of surface quality control, its homogeneity is unlikely, as well as the reproducibility of obtained results.

A three-electrode cell was used for the electrochemical process of lithium deposition. 0.5 M LiClO_4 in propylene solution electrolyte was chosen as the electrolyte. The counter electrode was a platinum plate, and the reference electrode was lithium metal. The water content in the electrolyte did not exceed 50 ppm according to the Karl-Fischer titration method. Research was carried out by cyclic voltammetry (CV), potential sweep was carried out from open circuit potential to -0.2 and -0.4 V (vs Li/Li^+), the sweep rate was 0.1 V/s.

The CV curves obtained on polished substrates show electrolyte decomposition waves, peaks of cathodic deposition and anodic dissolution of lithium. The second cycle obtained without surface cleaning shows only the deposition peak on the curve.

On nickel, a reproducible curve can be obtained only by surface preparation with polishing, other methods do not lead to the necessary surface quality, which causes a significant change in the shape of the CV curve. On steel, the curves differ slightly from each other even with careful polishing, whereas cleaning with cloth outside the box results in sufficient visual surface purification, but the curve differs significantly from obtained on the polished electrode. In summary, the lack of careful control during substrate preparation makes it impossible to notice surface inhomogeneities critical for lithium electrodeposition.

Application of LiFePO₄ cathode on substrate by electrophoretic deposition technique

Nuray Zhalgas¹, Yerkebulan Kadyrov¹, Nurbol Tolganbek¹,
Zhumabay Bakenov^{1,2}, Almagul Mentbayeva^{1*}

¹*School of Engineering and Digital Sciences, Nazarbayev University, Nur-Sultan, Kazakhstan*

²*National Laboratory Astana, Nazarbayev University, Nur-Sultan, Kazakhstan*

*E-mail: almagul.mentbayeva@nu.edu.kz

There has been many research conducted on development of electrode materials for Li-ion batteries. One of the most utilized and stable cathodes, LiFePO₄ (LFP) olivine structured material depict its full capacity by providing practical discharge capacity of almost 100% of its theoretical one. In addition, olivine LFP has long cyclability up to 1000 times. Yet, a minor number of experimental works were dedicated to application of these materials on current collector.

One of the most interesting and promising approach to consume LFP cathode is coating it through electrophoretic deposition (EPD) method. The simplicity of the technique allows to obtain cathode material with various thickness by controlling applied voltage and current which opens many possibilities for various applications starting from thin film batteries.

The work presents facile EPD procedure for coating LFP on current collector. Obtained film were characterized through various physical, chemical and electrochemical analysis.

Acknowledgment

This research was supported by a Targeted Program Funding #51763/IIIQΦ-MIQOAPI PK-19 "New materials and devices for defense and aerospace applications" from Ministry of Digital Development, Innovation and Aerospace Industry of the Republic of Kazakhstan.

The deposition and electrochemical study of multilayered Li_xSn alloy anode for lithium-ion microbatteries

Assel Serikkazyeva, Berik Uzakbaiuly, Aliya Mukanova, Zhumabay Bakenov

School of Engineering and Digital Science, Nazarbayev University, Z05P4X0 Nur-Sultan, Kazakhstan

*E-mail: assel.serikkazyeva@nu.edu.kz , **E-mail: aliya.mukanova@nu.edu.kz

Li-ion microbatteries (LIMBs) are the most attractive topic for investigation due to the rapid growth of miniaturized electronic devices. In order to obtain superior performance of the microbattery, it is essential to achieve good rate capability and stable cyclability of materials. Lithium metal (Li) is one the most attractive anode materials, with high theoretical capacity (3860 mAh g⁻¹), low density, and low negative potential. However, Li anodes suffer from an uncontrollable dendritic growth during the repetitive charge-discharge process and have high reactivity with moisture, which can lead to the explosion. Tin metal also can be considered a promising candidate, due to the high theoretical specific capacity (992 mAh/g) compared with commercial graphite, high conductivity, abundance and low price. However, the main drawback of the Sn anodes is the high-volume expansion, leading to the structure collapse and causing capacity fading after a few initial cycles. The ready lithium-tin (Li_xSn) alloy-based anode, can reduce the problems of both Li and Sn materials providing a much higher theoretical specific capacity of 788 mAh/g and enabling fast Li-ion diffusion. To the best of our knowledge, the Li_xSn alloy was not investigated as an anode for microbatteries. However, the monolithic thin film can still experience the volume change and the amount of lithium is limited. In this point of view, the multilayered structure with the alternating Li_xSn and Li-rich layers can provide the highly diffusive media, buffer regions, and enough Li for reactions.

This study reports on the new thin-film anode based on Li_xSn alloy prepared by using magnetron sputtering and thermal evaporation techniques. X-Ray diffraction analysis confirmed the formation of an alloy phase Li_2Sn_5 . Alloy-based anodes with the multilayered structure of $\text{Sn}/\text{Li}/\text{Sn}/\text{Li}/\text{Sn}$ and various thicknesses (500, 1000, and 1500 nm) were investigated. The microcells were assembled with liquid electrolytes and tested. The developed anode with 1000 nm thickness demonstrated the most promising results, with an initial specific capacity of 1240 (mAh) and stable cyclability during 100 cycles. Moreover, lower overpotential during stripping plating measurements was determined. Finally, it can be concluded that the Li_xSn_y alloy-based anode material demonstrated significant results in terms of cyclability and stability, therefore can be promising anode material for next-generation LIMBs.

Acknowledgment

This research was supported by a Targeted Program Funding #51763/IIIQΦ-MIQPOAI PK-19 "New materials and devices for defense and aerospace applications" from MDDIAI RK.

Graphene-like porous carbons as a sulfur host for lithium-sulfur batteries

Fayil Sultanov^{1*}, Almagul Mentbayeva^{1,2}, Sandugash Kalybekkyzy^{1,2}, Askhat Danebayev¹, Azhar Zhaisanova¹, Zhumabay Bakenov^{1,2}

¹*Department of Chemical and Materials Engineering, Nazarbayev University, Kabanbay Batyr Ave. 53, Nur-Sultan, 010000, Kazakhstan*

²*National Laboratory Astana, Nazarbayev University, Kabanbay Batyr Ave. 53, Nur-Sultan, 010000, Kazakhstan*

*E-mail: fail.sultanov@nu.edu.kz

Lithium-sulfur batteries (LSBs) are recognized as the next generation energy storage systems due to their high theoretical capacity of 1675 mAh g^{-1} and energy density of 2600 Wh kg^{-1} . However, such disadvantages as low sulfur electrical conductivity, polysulfides shuttle effect and volume expansion are limiting their practical application.

Herein, the advantages of using bio-waste-derived graphene-like porous carbons (GPCs) as a carbon matrix for sulfur immobilization are discussed. GPCs were obtained by carbonization of pre-washed, dried and milled rice husk wastes at 500 °C in inert atmosphere and thermo-chemical activation (750 °C, Ar atmosphere) of the formed carbonaceous product by using KOH as an activator. According to peaks intensities of Raman spectrum, the prepared GPCs are characterized by presence of reduced graphene oxide in the structure, the ratio of intensities of 2D band to G band (I_{2D}/I_G) is equal to 0.74, corresponding to the formation of a few-layered graphene structure. Based on TEM observations, the GPCs are presented by flake-like hierarchical porous structure, the presence of disordered transparent and well-formed graphene layers, which lie on top of each other was observed. The sulfur was immobilized on the formed carbon matrix by melt-diffusion and mechanochemical methods. As a result, the sulfur content in the matrix was 68-70 wt%.

The electrochemical performance was studied by CV, which demonstrated the good reversibility of sulfur reduction and lithium polysulfides oxidation. Further research will be focused on the preparation of composite GPCs with various modifiers (MXene, metal oxides) to create the additional sites for chemical adsorption of polysulfides and reduce the shuttle effect.

Acknowledgement

This work was supported by the research grant #51763/IIIQΦ-MIQPOAI PK-19 "New materials and devices for defense and aerospace applications" from Ministry of Digital Development, Innovation and Aerospace Industry of the Republic of Kazakhstan.

Three-Dimensional modeling of all solid-state lithium-ion batteries

Yer-Targyn Tleukenov^{1*}, Arailym Nurpeissova¹, Gulnur Kalimuldina², Anar Arinova¹, Zhumabay Bakenov^{1,3}

¹National Laboratory Astana, 53 Kabanbay Batyr Ave., Nur-Sultan, 010000, Kazakhstan

²Department of Mechanical and Aerospace Engineering, School of Engineering and Digital Sciences, Nazarbayev University, 53 Kabanbay Batyr Ave., Nur-Sultan, 010000, Kazakhstan

³Department of Chemical and Materials Engineering, School of Engineering and Digital Sciences, Nazarbayev University, 53 Kabanbay Batyr Ave., Nur-Sultan, 010000, Kazakhstan

*E-mail: yertargyn.tleukenov@gmail.com

In recent years, lithium-ion batteries (LIBs) are used in a range of energy storage applications, such as portable electronic devices, and vehicles. Traditional LIBs, however, are based on porous electrodes and liquid electrolytes, making them prone to degradation and major safety concerns. In this instance, using 3D all-solid-state batteries (3DASSB) is a good option because these battery systems use solid electrolytes, which have greater thermal and electrochemical stability and avoid dangerous electrolyte leakage when compared to liquid electrolytes. In order to make further improvement in the technology of 3DASSB, an in-depth understanding of the electrochemical processes involved, and the ability to simulate these processes in LIBs is necessary. However, the measurements and evaluations of these batteries are very difficult due to the complicated structure of them. In this regard, the numerical simulation method is a powerful tool to realize the processes. Herein, the model of 3DASSB, where Ni/NiO is used as an anode, was developed by COMSOL Multiphysics in order to investigate solid polymer electrolyte interface and to describe the conductivity in the solid-state electrolyte. The aim of the modeling is to develop a mathematical model for all-solid-state Li-ion batteries, which includes all important physical and electrochemical characteristics and is capable of describing the basic functionality of these devices under a wide variety of operating conditions. Figure 1 shows the modeling results of complex processes on the interface between solid-state electrolyte and anode during the cycling charge process of the all-solid-state lithium-ion battery. The battery is charged up to 2.4 V.

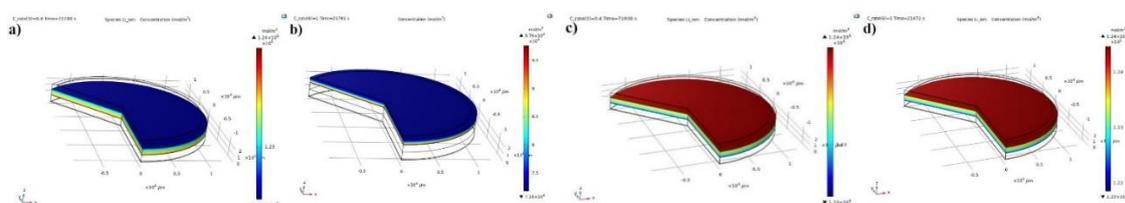


Figure 1. Concentrations of Li^+ ions in the electrolyte at the end of 0.4 (a) and 1.0 (b) C-rate discharge and at the end of 0.4 (c) and 1.0 (d) C-rate charge

Acknowledgement

This work was supported by the project 091019CRP2114 “Three-Dimensional All Solid State Rechargeable Batteries” from Nazarbayev University.

SnSe@porous carbon nanofibers as a free-standing anode for low-temperature lithium-ion batteries

Aiym Rakhmetova^{1*}, Arailym Nurpeissova², Gulnur Kalimuldina³, Zhumabay Bakenov^{1,2**}

¹*Department of Chemical and Materials Engineering, School of Engineering and Digital Sciences, Nazarbayev University, Kabanbay Batyr Ave. 53, Nur-Sultan 010000, Kazakhstan*

²*National Laboratory Astana, Nazarbayev University, Kabanbay Batyr Ave. 53, Nur-Sultan 010000, Kazakhstan*

³*Department of Mechanical and Aerospace Engineering, School of Engineering and Digital Sciences, Nazarbayev University, Kabanbay Batyr Ave. 53, Nur-Sultan 010000, Kazakhstan*

*E-mail: aiym.rakhmetova@nu.edu.kz . **E-mail: zbakenov@nu.edu.kz

Tin selenide-based materials are considered to be promising high-capacity anode materials for Li-ion batteries (LIBs) owing to their non-toxicity, earth-abundance, and chemical stability. However, SnSe suffers from a large volume expansion, which leads to poor cycling performance. In addition, it lacks in-depth research on low-temperature electrochemical performance. Here, SnSe@porous carbon nanofiber material was synthesized by the electrospinning method with consequent heat treatment and employed as a free-standing and slurry anode material at room and low temperatures. The pores in carbon nanofibers can help to suppress the volume change of SnSe during lithiation/delithiation as well as give additional insertion sites for lithium ions. X-ray diffraction (XRD) analysis and scanning electron microscope (SEM) observation were carried out to show the composition, diameter, and structure of synthesized SnSe@porous carbon nanofibers. The obtained material exhibits good mechanical flexibility and better electrochemical performance at low temperatures in comparison to commercially-available anode materials.

Acknowledgement

This research was supported by the research grant OPFE2021001 from the Ministry of Digital Development, Innovations and Aerospace Industry of the Republic of Kazakhstan

Low-temperature performance of Sn_xP/C composite nanofibers as free-standing anode materials for lithium-ion batteries

Ayaulym Belgibayeva^{1,2*}, Makpal Rakhatkyzy¹, Aiym Rakhmetova¹, Gulnur Kalimuldina³, Arailym Nurpeissova^{1,2}, Zhumabay Bakenov^{1,2**}

¹Department of Chemical and Materials Engineering, School of Engineering and Digital Sciences, Nazarbayev University, Kabanbay Batyr Ave. 53, Nur-Sultan 010000, Kazakhstan

²National Laboratory Astana, Nazarbayev University, Kabanbay Batyr Ave. 53, Nur-Sultan 010000, Kazakhstan

³Department of Mechanical and Aerospace Engineering, School of Engineering and Digital Sciences, Nazarbayev University, Kabanbay Batyr Ave. 53, Nur-Sultan 010000, Kazakhstan

*E-mail: ayaulym.belgibayeva@nu.edu.kz , **E-mail: zbakenov@nu.edu.kz

Graphite anode is admitted as one of the critical limiting factors for applying lithium-ion batteries (LIBs) in low-temperature (LT) environments. As an alternative, tin compounds, such as SnO₂, exhibit much better LT performance owing to the unique allotropic changes of tin and increased reversibility of lithiation-delithiation reactions at low temperatures. However, to the best of our knowledge, LT performance of Sn_xP as anode for LIBs has not been reported so far.

In this work, Sn_xP-based free-standing carbon composite nanofiber mats have been successfully synthesized by electrospinning with heat treatments and applied as anode materials for LT LIBs. The material, prepared under optimal conditions showed 6 times higher capacity (900 mAh g⁻¹) at 0 °C compared to commercial graphite anode and improved cycle stability than pure Sn at a current density of 50 mA g⁻¹.

Acknowledgement

This research was supported by the research grant OPFE2021001 from the Ministry of Digital Development, Innovations and Aerospace Industry of the Republic of Kazakhstan.

Enhancing the low-temperature characteristics of a Li/graphite half-cell by the comprehensive modification of electrolyte

Makpal Rakhatkyzy^{1*}, Arailym Nurpeissova^{1,2}, Gulnur Kalimuldina³, Ayaulym Belgibayeva^{1,2}, Zhumabay Bakenov^{1,2**}

¹Department of Chemical and Materials Engineering, School of Engineering and Digital Sciences, Nazarbayev University, Kabanbay Batyr Ave. 53, Nur-Sultan 010000, Kazakhstan

²National Laboratory Astana, Nazarbayev University, Kabanbay Batyr Ave. 53, Nur-Sultan 010000, Kazakhstan

³Department of Mechanical and Aerospace Engineering, School of Engineering and Digital Sciences, Nazarbayev University, Kabanbay Batyr Ave. 53, Nur-Sultan 010000, Kazakhstan

*E-mail: makpal.rakhatkyzy@nu.edu.kz , **E-mail: zbakenov@nu.edu.kz

The behavior of electrolytes with decreasing temperature generally affects the overall performance of lithium-ion batteries. Freezing of the electrolyte, increased viscosity, reduced ionic conductivity, and increased charge transfer resistance are the main limitations stemming from the electrolyte side. In particular, batteries with commercial electrolyte and a well-known graphite anode are recognized as poorly operated at low temperatures due to a large loss of capacity (more than 50% of its room-temperature capacity) even at zero degrees. In this work, a complex modification of the lithium salt and solvents was applied simultaneously to develop an optimal electrolyte system with improved low-temperature characteristics for the Li/graphite half-cell. Various concentrations of commercial and alternative lithium salts, dissolved in a mixture of solvents, are used as electrolytes to determine the best interaction with a graphite electrode at low temperature. A solvent mixture of non-carbonate organic ester with low freezing point and SEI-forming fluorinated co-solvent in a ratio of 9:1 is used to prevent freezing of the electrolyte and

ensure the formation of a more conductive SEI layer, respectively. The Li/graphite half-cell with the designed electrolyte system has retained about 90% of its room-temperature capacity at zero degrees, demonstrating a new perspective for the development of low temperature type electrolytes.

Acknowledgement

This research was supported by the research grant OPFE2021001 from the Ministry of Digital Development, Innovations and Aerospace Industry of the Republic of Kazakhstan.

Solid-state synthesis of nanostructured LiMPO₄ cathode materials for Li-ion batteries

Batukhan Tatykayev, Assylzat Aishova, Sandugash Kalybekkyzy, Almagul Mentbayeva,
Zhumabay Bakenov

Nazarbayev University, Nur-Sultan, Kazakhstan

E-mail: batukhan.tatykayev@nu.edu.kz

The energy sector is developing very rapidly, which requires the use of more efficient energy storage systems. Lithium-ion batteries (LIB) are the most common type of energy storage. However, materials that are currently used in these systems have a short lifespan and, moreover, are manufactured from limited environmentally toxic compounds. Thus, the demand for research into the development of more efficient and environmentally friendly materials for LIB is very high. LiMPO₄ (M = Mn, Fe, Co, and Ni) are promising and environmentally benign cathode materials for energy storage. Moreover, these materials are cost-effective and provide excellent thermal stability during battery operation^{1,2}.

In this research solid-phase synthesis of nano-sized olivine LiMPO₄ cathode materials is proposed. This method leads to the production of cathode materials with high thermal stability, specific capacity, and intrinsic conductivity. The proposed methodology consists of two stages, namely, mechanical activation (MA) of solid precursors in planetary ball mill and heat treatment in inert atmosphere at a relatively low temperature in the range of 500–600 °C. The synthesis was optimized by changing MA parameters and including solid diluent to the reaction system. The mixture of precursors FeC₂O₄ + Li₂CO₃ + NH₄H₂PO₄ and solid diluent (NH₄)₂CO₃ were used to prepare LiFePO₄/C cathode material. After mechanical activation and heat-treatment in the presence of sucrose as carbon source, nanoparticles with a size less than 100 nm were obtained. Electrochemical studies of the half-cell cell, where LiFePO₄ nanoparticles are used as a cathode show stable performance for 30 cycles with 130 mAh/g specific capacity and 100% coulombic efficiency.

Acknowledgements

This research was supported by the research grant #51763/IIIΦ-MIΠOAI PK-19 "New materials and devices for defense and aerospace applications" from MDDIAI Republic of Kazakhstan.

Obtaining nanostructured red phosphorus as an anode material for Li- and Na-ion batteries

Uldana Kydyrbayeva^{1*}, Didar Maushanova¹, Aliya Mukanova^{1,2**},
Zhumabay Bakenov^{1,2}

¹*Institute of Batteries, Z05P4X0, Kazakhstan, Nur-Sultan, 53, Kabanbay Batyr Avenue*

²*Nazarbayev University, Z05P4X0, Kazakhstan, Nur-Sultan, 53, Kabanbay Batyr Avenue*

*E-mail: kydyrbayevauldana@gmail.com , **E-mail: aliya.mukanova@nu.edu.kz

Phosphorus based materials, specifically red phosphorus(RP), has aroused growing concern as a promising anode material for both Li- (LIBs) and Na-ion batteries(NIBs), owing to its high theoretical capacity (2596 mA h g⁻¹) and appropriately low redox potential (~0.4 V). However, phosphorus has the poor electronic conductivity and large volume expansion during cycling which leads to low electrochemical activity and unstable cyclability. To solve the problem of its limit in practical application, phosphorus needs to be obtained in the most nanoscale powder from commercial red phosphorus by complex method such as the ball mill.

Therefore the aim of the work is to find the most effective way in obtaining nanostructured RP powder for its further use as anode material in LIBs and NIBs.

In this work, commercial RP powder with an average particle size 20-30 μm was ball milled. In order to prevent the oxidation of red phosphorus and to avoid the introduction of water impurities, the entire process was carried out in an inert atmosphere (Ar). The different time durations were compared and optimized. To analyze the structure and composition of the investigated powders XRD, Raman spectroscopy and SEM were carried out. According to the SEM data, the particles were a size of 140 nm to 5 μm. It was determined that the optimal ball mill time for RP is 10 h, longer times led to the aggregation of particles up to 20 μm.

The electrochemical tests were performed with the coin-type 2032 cell, soaked in a few drops of 1M LiPF₆ in EC:DEC:EMC as electrolyte, at a scanning rate of 0,1mVs⁻¹ with the anode based on obtained RP.

The experimental result and other details will be discussed at the conference.

Acknowledgments

Our group gratefully acknowledges funding by grant AP09260012 «Development of red phosphorus composite anodes for the next generation of lithium-ion and sodium-ion batteries» from the Ministry of Education and Science of the Republic of Kazakhstan.

I-V characterization of p-n heterostructures obtained by GLAD

Madina Sarsembina^{1*}, Amanzhol Turlybekuly¹, Almagul Mentbayeva¹, Baktiyar Soltabayev²,
Zhumabay Bakenov^{1,2**}

¹*School of Engineering, Nazarbayev University, Nur-Sultan, Kazakhstan*

²*National Laboratory Astana, Nazarbayev University, Nur-Sultan, Kazakhstan.*

*E-mail: madina.sarsembina@nu.edu.kz

In recent years, the development of gas monitoring devices/sensors are critical for environmental protection and for humans promptly. Due to their good characteristics as fast response, low cost, and small size gas sensors have become more prevalent in different fields from healthcare industries to food processing [1].

In breath sensing, metal oxide semiconductor (MOS) sensors are commonly utilized. MOS sensors are one of the finest alternatives for breath analysis because of its compact size, ease of operation, low cost, and minimal maintenance. However, conventional gas sensors with a single metal oxide layer, detect a shift in bulk resistance in response to gas contact, resulting in limited gas

sensitivity and selectivity. For increasing gas sensitivity and selectivity, forming a p-n junction with MOS-based p-type and n-type electrodes is the best option [2].

This research purpose to investigate gas sensor based on p-n junction heterostructures of MOS (TiO/CuO) with nanoscale architecture which is ultrasensitive for acetone and work at low temperature (room temperature). It is possible to achieve by control over nanoscale architecture of the sensing material and increasing surface area.

The GLAD technique has been tested for nanorods synthesis for gas sensors. The GLAD refers to a configuration in which the material flux arrives at the surface of a substrate at an oblique angle [3].

The nanoscale array, fabricated by GLAD between top and bottom electrodes, shows p-n junction current-voltage (I–V) characteristics at room temperature and 75C.

Acknowledgement

This research was supported by the research grant 021220CRP0122 “Development of highly sensitive MOS based nano-film gas sensors” from Nazarbayev University.

Microwave-assisted synthesis of LISICON structured $\text{Li}_3\text{V}_2(\text{PO}_4)_3$ / graphene composite

Ilyas Mukushev^{1,2*}, Arailym Nurpeissova³, Gulnur Kalimuldina⁴, Zhumabay Bakenov^{1,3**}

¹*Department of Chemical and Materials Engineering, School of Engineering and Digital Sciences, Nazarbayev University, Kabanbay Batyr Ave. 53, Nur-Sultan 010000, Kazakhstan*

²*Department of Chemistry, Faculty of Natural Sciences, Eurasian National University, Satpaeva St.2, Nur-Sultan 010008, Kazakhstan*

³*National Laboratory Astana, Nazarbayev University, Kabanbay Batyr Ave. 53, Nur-Sultan 010000, Kazakhstan*

⁴*Department of Mechanical and Aerospace Engineering, School of Engineering and Digital Sciences, Nazarbayev University, Kabanbay Batyr Ave. 53, Nur-Sultan 010000, Kazakhstan*

*E-mail: ilyas.mukushev@nu.edu.kz , **E-mail: zbakenov@nu.edu.kz

One of the main challenges in cathodes at low temperatures (LT) is associated with low electronic and ionic conductivity. Graphene can be used to increase electronic conductivity, but most of the experimental methods for graphene composites require long-term high-temperature treatment and an inert atmosphere, which causes high energy consumption and cost increase. In comparison, microwave heating can simplify the reduction step of graphene oxide and provide a convenient, economical, and effective method of preparing graphene composites. LISICON structured $\text{Li}_3\text{V}_2(\text{PO}_4)_3$ (r-LVP) was reported to have enhanced LT performance due to high alkali-ion mobility and rhombohedral structure with the open framework.

In this study, r-LVP/graphene composite was successfully prepared using a microwave heating method. Microwave heating was used to simplify the reduction of graphene oxide and the synthesis of $\text{Na}_3\text{V}_2(\text{PO}_4)_3$ /graphene composite. The r-LVP/graphene composite was successfully obtained by ion exchange from the prepared $\text{Na}_3\text{V}_2(\text{PO}_4)_3$ /graphene composite. The structure, morphology and electrochemical performances of r-LVP/graphene composite were systematically studied by X-ray diffraction (XRD), transmission electron microscopy (TEM), scanning electron microscopy (SEM), Raman spectroscopy, cyclic voltammetry (CV), charge/discharge tests and electrochemical impedance spectra (EIS). The XRD analysis indicated that graphene-modified r-LVP can be successfully obtained. Both SEM and TEM images revealed small r-LVP particles embedded in thin carbon layer sheets which could provide a high ionic and electronic conductivity. Raman analysis showed that graphene has a high degree of graphitization. When used as a cathode, the r-LVP/graphene composite exhibited high-rate ability and cyclic stability at low temperatures.

Acknowledgment

This research was supported by the research grant OPFE2021001 from the Ministry of Digital Development, Innovations and Aerospace Industry of the Republic of Kazakhstan

Biomass graphene derived from date seeds as an anode material for lithium-ion battery

Kazna Tassybay^{1*}, Nurbolat Issatayev¹, Gulnur Kalimuldina², Arailym Nurpeissova³, Zhumabay Bakenov^{1,3}

¹*Department of Chemical and Materials Engineering, Nazarbayev University, Kabanbay batyr ave. 53, Nur-Sultan, RK*

²*Department of Mechanical and Aerospace Engineering, Nazarbayev University, Kabanbay batyr ave. 53, Nur-Sultan, RK*

³*National Laboratory Astana, Nazarbayev University, Kabanbay batyr ave. 53, Nur-Sultan, Kazakhstan*

*E-mail: kazna.tassybay@nu.edu.kz , **E-mail: zhumabay.bakenov@nu.edu.kz

Lithium-ion batteries (LIBs) are in great demand as energy storage systems applied in wide range of electronic devices. However, currently used commercial anodes have a limited capacity of 372 mAh g⁻¹. Therefore, development of novel carbon materials for high performance electrodes is of high interest. Recently, biomasses have attracted much attention as electrode materials for LIBs due to their low cost and environmental sustainability. In this research, a nitrogen-doped porous biomass graphene material was prepared from date seeds as an organic matter through carbonization and chemical activation. Dicyandiamide and potassium hydroxide were used as the sources of nitrogen and activating agent, respectively. The physio-chemical properties of the obtained graphene were characterized by X-ray diffraction, Raman spectroscopy and X-ray photoelectron spectroscopy. The electrochemical performance of the graphene as an anode material for lithium-ion battery was evaluated. The specific discharge capacity of the batteries with graphene synthesized at 300°C carbonization and 800°C activation temperatures was 500 mAh g⁻¹ after 100 cycles at 0.1 C. These results can provide a new direction in production of high performance and environmentally friendly energy storage materials from biomasses.

Acknowledgement

This research was supported by the research grants OPFE2021001 “New materials and devices for defense and aerospace applications” from the Ministry of Digital Development, Innovations and Aerospace Industry of the Republic of Kazakhstan.

Layer by layer arrangement of a hybrid piezo-triboelectric nanogenerator based on a biocompatible flexible PVDF composite and Al electrode for implantable cardiac pacemaker

Assem Mubarak^{1,*}, Gulnur Kalimuldina^{2,*}

¹*Department of Biomedical Sciences, School of Medicine, Nazarbayev University, Kabanbay Batyr Ave. 53, Nur-Sultan 010000, Kazakhstan*

²*Department of Mechanical and Aerospace Engineering, School of Engineering and Digital Sciences, Nazarbayev University, Kabanbay Batyr Ave. 53, Nur-Sultan 010000, Kazakhstan*

*E-mail: assem.mubarak@nu.edu.kz , **E-mail: gkalimuldina@nu.edu.kz

Bioelectronics has become an integral part of medicine over the past decade, used for diagnostic and therapeutic purposes. The development of a quality power supply unit ensures the reliable operation of bioelectronics. However, conventional power supplies cannot be used in implantable products due to their heavy weight, size and potentially harmful substances to the human body. The implantable pacemaker is one of the most currently available used bioelectronics. Despite numerous modifications and reductions in size to ensure patient comfort, the modern pacemaker has several drawbacks. The fact that the heart, like other organs of the human body, is soft and has limited space to accommodate poses new challenges to power systems to minimize

interface mismatch while still providing sufficient power for clinical applications. This study focuses on developing unconventional power options for implantable devices based on hybrid nanogenerators. The hybrid nanogenerator incorporated piezoelectric and triboelectric properties, allowing a more powerful nanogenerator for further use. The piezoelectric material was based on PVDF with several types of additives. A quenching with liquid nitrogen was used to synthesize the beta phase of PVDF.

Moreover, various concentrations of different additives to the polymer were studied to increase the power output. Subsequently, a triboelectric generator was developed from a positively charged aluminum electrode as the first layer and a negatively charged PVDF as the second layer. A hybrid nanogenerator prevails over others by combining two or more types of generators providing higher electrical output required for a miniature power supply. Eventually, the challenges and future opportunities in the applications of nanogenerators are delivered in the conclusive remarks.

Acknowledgement

This research was supported by the research grant AP08052143 “Development of wearable self-charging power unit” the Ministry of Education and Science of the Republic of Kazakhstan

Thin-film sulfur cathode for Li-S microbatteries

Arman Umirzakov^{1*}, Berik Uzakbaiuly^{1,2,3}, Aliya Mukanova^{1,2,3**}, Zhumabay Bakenov^{1,2,3}

¹*School of Engineering and Digital Science, Nazarbayev University, Z05P4X0 Nur-Sultan, Kazakhstan*

²*Institute of Batteries LLC Z05P4X0 Nur-Sultan, Kazakhstan*

³*National Laboratory Astana, Z05P4X0 Nur-Sultan, Kazakhstan*

*E-mail: arman.umirzakov@nu.edu.kz , **E-mail: aliya.mukanova@nu.edu.kz

The development of an all-solid-state Lithium-Sulfur (Li-S) microbattery is a fresh topic and considered as one of the most promising ideas because sulfur (S) is not only a widespread and cheap material but also has a high theoretical capacity, and serves as a material with extremely high reliability and safety [1]. However, several practical problems have delayed the widespread application of sulfur as a cathode material and even more on a microdimensional scale. For example, problems related to thin film formation methods like PVD (physical vapor deposition) that is primary, but due to the chamber contamination by sulfur and negative effects on the vacuum system, it is better to avoid them. Another problem is that pure S is an insulating material ($5 \cdot 10^{-30}$ S cm⁻¹ at 25°C)[2] this fact necessitates the use of conductive additives in order to build a highly conductive matrix [1].

This study presents a commonly used method for making sulfur cathodes but with modifications in order to obtain a homogeneous, conductive layer with a thickness of no more than 2 μm. The mechanical activation synthesis of sulfur and a conductive agent by ball milling under various ratios and parameters were implemented. Next, prepared slurry adding CMC (carboxymethyl cellulose) binder and dissolved in DI (deionised) water. A thin-film layer of the cathode material was coated by the spin coating method on Al foil. In the work, physical-chemical studies, electrochemical studies, and post-mortem characterization were carried out in order to develop a S cathode thin film. All these studies lead to 1320 mAh g⁻¹ after 1st cycle and capacity retention of around 750 mAh g⁻¹ after 50 cycles.

Acknowledgement

This research is supported under the state targeted program №51763/ПЦФ-МЦРОАП РК-19 "New materials and devices for defense and aerospace applications" by the MDDAI RK.

Electrochemical behavior of an electrode based on TiO₂ as a perspective anode for magnesium-ion batteries

Raigul Jumanova^{*}, Akmaral Argimbayeva, Khaisa Avchukir, Ainaz Abildina, Gulmira Rakhymbay, Yeldana Bakhytzhani¹

Center of Physical Chemical Methods of Research and Analysis, Al-Farabi Kazakh National University, Almaty, Kazakhstan

*E-mail: r.zh.shohaeva@mail.ru

Magnesium-ion batteries (MIBs) are currently the topical electrochemical system for various large-scale electronic devices. Due to the high content of magnesium in nature, its non-toxicity and high capacity, MIBs are a promising alternative to lithium-ion batteries. However, the development of MIBs is hampered by the incompatibility of the electrolyte with the Mg anode and the slow kinetics of the introduction/extraction of Mg²⁺ ions into electrode materials. To eliminate these disadvantages, alternative anode materials capable of reversibly intercalating Mg²⁺ ions can be used instead of a metal magnesium anode.

TiO₂ is considered to be a promising matrix for the reversible introduction of Mg²⁺ ions among possible MIB anode material candidates. However, when TiO₂ is used in MIB, its low electronic and ionic conductivity limits its practical capacity and performance. Nanostructured materials with various morphologies are well suited to improve the electrochemical properties of TiO₂. For this purpose, in this work, we chose an easy-to-control synthesis method and the best conditions for controlling the morphology of nanotubes by electrochemical anodization of Ti. The Ti foil was electrochemically anodized in an organic electrolyte containing 96.7 wt. % glycerol, 1.3 wt. % NH₄F and 2 wt. % water for 3 hours at 60 V followed by heat treatment at 450°C. The crystal structure of TiO₂ anatase was confirmed by XRD. SEM microimages show a uniform distribution of nanotubes (Nts). Electrochemical tests were carried out using cyclic voltammetry (CV) at different scan rates, number of cycles and concentrations of Mg(TFSI)₂-ethylene carbonate/dimethyl carbonate electrolytes in the potential range of 0.5 and 2.5 V versus Mg/Mg²⁺. On cyclic voltammograms, an increase in the currents of the cathode and anode peaks is observed with an increase in the concentration of electrolytes and the rate of potential sweep, which proves the intercalation/deintercalation of Mg²⁺ ions. In addition, a more reversible behavior of TiO₂ is noticeable in the first cycle, but starting from the second cycle, irreversibility prevails. The height of the cathodic peaks increases with subsequent cycling, which may be due to the improved incorporation of magnesium ions into the electrode. The height of the cathodic peaks increases with subsequent cycling, which may be due to the improved intercalation of magnesium ions into the electrode. However, according to the height of the anodic peaks, it can be assumed that the deintercalation of magnesium ions becomes more difficult, and with a larger amount of cycling, the peaks completely disappear. Therefore, it is necessary to improve the characteristics of TiO₂ in order to achieve the reversibility of Mg²⁺ intercalation/deintercalation.

3D printing of high-performance electrodes for all-solid-state rechargeable lithium-ion batteries

Emmanuel Chisom Nnwaogu^{1,3*}, Arailym Nurpeissova¹, Gulnur Kalimuldina², Zhumabay Bakenov^{1,3}

¹National Laboratory Astana, 53 Kabanbay Batyr Ave., Nur-Sultan, 010000, Kazakhstan

²Department of Mechanical and Aerospace Engineering, School of Engineering and Digital Sciences, Nazarbayev University, 53 Kabanbay Batyr Ave., Nur-Sultan, 010000, Kazakhstan

³Department of Chemical and Materials Engineering, School of Engineering and Digital Sciences, Nazarbayev University, 53 Kabanbay Batyr Ave., Nur-Sultan, 010000, Kazakhstan

*E-mail: emmanuel.nwaogu@nu.edu.kz

Three-Dimensional (3D) electrode architecture of lithium-ion batteries (LIBs) is a new generation energy storage system with high energy and high-power capacity to satisfy high consumer demands, especially for its application in biomedical, electrical vehicles, and portable electronics. The printing process of this 3D architecture electrode was made possible through the ink-extrusion method, which has offered a supper balance promise between high energy density and power density. Moreover, the 3D printing framework is a simple and low-cost alternative to traditional lithium-ion electrode setups, which maintains an excellent electrochemical property of higher specific capacity and cyclic stability. Here, this study investigates the high performance and optimization of 3D-printed electrodes of NMC (Cathode) and Mxene (anode) for all-solid-state lithium-ion rechargeable batteries (ASSLRB). However, different electrode inks with proportions of 80:10:10, 70:15:15, and printing pressure of 108kPa and 120kPa, respectively, were employed during slurry optimization (Figure 1). We recommend that 3D printing of electrode conductive filaments delivers stress-free and less time fabrication setups while maintaining high energy capacity for the next generation of high-performance energy storage devices.

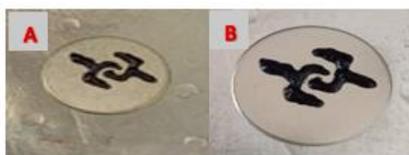


Figure 1. Illustrate different 3D printed electrodes with different proportions and printing pressure (a) 80:10:10/108kPa, (b) 70:15:15/120kPa.

Acknowledgement

This research was funded by the research grant 091019CRP2114 “Three-Dimensional All Solid State Rechargeable Batteries” from Nazarbayev University.

A flexible and wearable single electrode triboelectric nanogenerator

Y. Nurmakanov^{2*}, G. Kalimuldina¹, R. Kruchinin²

¹Nazarbayev University, Department of Mechanical and Aerospace Engineering, School of Engineering and Digital Sciences, Nazarbayev University, Kabanbay Batyr Ave. 53, Nur-Sultan 010000 Kazakhstan

²Nazarbayev University, School of Engineering and Digital Sciences, Nazarbayev University, Kabanbay Batyr Ave. 53, Nur-Sultan 010000 Kazakhstan

*E-mail: yerzhan.nurmakanov@nu.edu.kz

Harvesting abundant mechanical energy is considered one of the promising technologies for developing autonomous self-powered power units, active sensors, and Internet-of-Things (IoT) devices. The triboelectric harvesters based on contact electrification and electrostatic induction have recently attracted much attention among various energy harvesting technologies because of their advantages, such as high performance, lightweight, and simple design. However, obtaining a high-output performance is still of significant concern for many applications.

In this work, we proposed flexible and wearable triboelectric nanogenerators (TENG) where a highly conductive cotton cloth (CC) textile was utilized as an electrode and polydimethylsiloxane (PDMS) were used as an encapsulating triboelectric material to construct a single electrode mode TENGs. Moreover, to enhance the output performance of PDMS-based TENGs titanium dioxide nanoparticles (NPs) were embedded as a function of weight ratio.

As prepared, wearable single-electrode-mode TENG devices can efficiently convert the mechanical energy into electricity while making continuous contacts/separations with counter tribo-positive friction objects like human skin, nylon, and cotton fabrics. The peak-to-peak open-circuit voltage (V_{oc}) and short-circuit current (I_{sc}) of single-electrode TENG without NPs were about 40 V and 0.42 μ A, respectively. However, 5 wt.% of TiO_2 resulted in an increase in V_{oc} and I_{sc} up to 116 V and 0.83 μ A, respectively. Moreover, the influence of the concentration of NPs, external pressing force and load resistance on the electrical output performance of TENGs were investigated. Corresponding TENG could power 130 LEDs in series just by tapping by a human hand. Moreover, the ability to charge the capacitors and drive calculator was also demonstrated which showed that the TENGs can be potentially used as a self-powering source for small electronics.

Acknowledgments

This work was supported by the research grant AP08052143 “Development of wearable self-charging power unit” from the Ministry of Education and Science of the Republic of Kazakhstan.

Preparation of a piezoelectric porous mat aerogel

Aisar Abdrakhmanov^{1*}, Aruna Rakhimzhanova², Gulnur Kalimuldina¹

¹*Department of Mechanical and Aerospace Engineering, School of Engineering and Digital Sciences, Nazarbayev University, Kabanbay Batyr Ave. 53, Nur-Sultan 010000, Kazakhstan*

²*Department of Chemical and Materials Engineering, School of Engineering and Digital Sciences, Nazarbayev University, 53 Kabanbay Batyr Ave., Nur-Sultan, 010000, Kazakhstan*

*E-mail: aisar.abdrakhmanov@nu.edu.kz, aruna.rakhimzhanova@nu.edu.kz

Ever since the discovery of the piezoelectric phenomenon, piezo electronics have been generally established and attracted increasingly extensive attention. Piezoelectric materials can serve as crucial units for energy-harvesting equipment or as active parts of sensors. Research's long-term goal is to boost the output of piezoelectricity, improve the sensitivity of piezoelectric-based sensors and extend utilization scope. Piezoelectric and triboelectric nanogenerators (PENGs/TENGs) are promising components for the next generation of self-powered electronic devices. Polyvinylidene-fluoride (PVDF) has the property of high electron affinity in a triboelectric series and shows a ferroelectric performance caused by the beta-phase crystal structure. Traditionally, beta-phase PVDF exhibits the highest electrical output efficiency in the polling state because of the side-by-side arrangement of fluorine and hydrogen. The contact area influences piezoelectric and triboelectric hybrid nanogenerator (PTNG) performance; modified PVDF with a high surface area has been investigated widely for increasing the mechanical contact area. For this research, PVDF aerogel was obtained as a piezoelectric material for nanogenerators. Aerogel was obtained by mixing PVDF and carboxymethyl cellulose through the novel quenching method. X-ray diffraction and Fourier-transform infrared spectroscopy analyses investigated the beta-phase contents in aerogels.

Acknowledgment

This research was supported by the research grant 240919FD3914 “Self-Charging Rechargeable Lithium-ion Battery” from Nazarbayev University.

Functionalized polytetrahydrofuran-based solid polymer electrolytes for safe lithium-ion batteries by UV-cross-linking

Elmira Nurgazyieva^{1*}, Sandugash Kalybekkyzy^{1,2**}, Zhumabay Bakenov^{1,2}, Almagul Mentbayeva²

¹*National Laboratory Astana, Nazarbayev University, Nur-Sultan, Kazakhstan*

²*Department of Chemical and Materials Engineering, School of Engineering and Digital Sciences, Nazarbayev University, Nur-Sultan, Kazakhstan*

*E-mail: elmira.nurgazyieva@nu.edu.kz , **E-mail: sandugash.kalybekkyzy@nu.edu.kz

Lithium-ion batteries have emerged in application of all smart electronics, wearable devices and electric vehicles for last decade. Polymer based solid electrolytes (SPE) have the ability to meet the requirements such as low flammability, good flexibility, thermal stability and high safety. Among the polymer electrolytes, the poly(ethylene oxide) PEO-, polyacrylonitrile (PAN) -based solid polymer electrolytes have been explored extensively. Poly(tetrahydrofuran) (PTHF), which is structurally similar to PEO but has less oxygen heteroatoms in the backbone, is one attractive polymer candidate for a loosely coordinating SPE. PTHF remains virtually unexplored as a solid electrolyte, despite the promise of looser coordination due to less oxygen heteroatoms in the polymer backbone.

Polytetrahydrofuran was modified by introducing acrylate groups and polymer films were obtained by UV-cross-linking method. Furthermore, the synthetic approach used to introduce

carbamate groups into the polymer network, which are known to improve mechanical strength while having minimal effect on transport and electrochemical properties.

Acknowledgement

This research was supported by the research grants #AP08855889 “Development of Flexible and Safe Next - Generation Li - Ion Batteries” from MES RK.

Effect of doping with cations and anionic groups on the ionic conductivity properties of latp solid electrolytes for li-ion batteries

Yelnury Baltash^{1*}, A. Mashekova^{1,2}, M. Yegamkulov^{1,2}, I. Trussov¹, A. Mukanova^{1,2**}

¹*Institute of Batteries, Z05P4X0, Kazakhstan, Nur-Sultan,53, Kabanbay Batyr Avenue*

²*Nazarbayev University, Z05P4X0, Kazakhstan, Nur-Sultan,53, Kabanbay Batyr Avenue*

*E-mail: 97.elnura@gmail.com , **E-mail: aliya.mukanova@nu.edu.kz

The good energy capacity of lithium-ion batteries (LIBs) makes them promising electrochemical energy storage devices. Existing commercial batteries use flammable liquid electrolytes, which are unsafe, toxic and environmentally unsound, and have poor chemical stability. Recently, solid Li-ion conducting ceramic electrolytes have received considerable attention, since they combine high ionic conductivity with low electrical conductivity, chemical stability and potentially sufficient mechanical properties. Currently, Al-substituted lithium titanophosphate $\text{Li}_{1.3}\text{Al}_{0.3}\text{Ti}_{1.7}(\text{PO}_4)_3$ is the most common solid electrolyte with a NASICON structure for use in solid-state electrochemical devices due to its high ionic conductivity ($\sim 10^{-3}$ - 10^{-4} S/cm at room temperature), thermal stability, stability in air, relatively inexpensive synthesis and safety. It is known that the ionic conductivity of NASICON materials is significantly affected by the microstructure (porosity, grain size, presence of impurity phases), and the conductivity strongly depends on the sample density. However, LATP has the disadvantage that occurs at contact with lithium metal where Ti^{4+} is reduced to Ti^{3+} , leading to degradation of electrolyte surface and reduction of its ionic conductivity. This work proposes doping LATP with tetravalent, divalent cations and anionic groups as to suppress titanium reduction. The polycationic doping of LATP was carried out by adding a various amount of Zr, Hf, Ca, Mg, Sr and SiO_4^- , MoO_4^- in LATP structure. The synthesis of doped LATP with cations and anionic groups was performed by molten flux, solid-state reaction and solution-based methods. The samples were synthesized and their structural, morphological characteristics and ionic conductivity properties were studied. X-ray analysis revealed the introduction of divalent cations into the LATP structure without the formation of impurity phases. Doping of LATP with calcium, magnesium and strontium decreased the total ionic conductivity by an order of magnitude. The results of this work clearly demonstrate that there is possibility of forming a NASICON-structured material with higher Li reduction resistance due to lower Ti content, and also provides an opportunity to develop solid electrolytes with different compositions.

Acknowledgement

This research was supported by the research grants №AP08052231 “Development of solid electrolytes with high ionic conductivity for next generation lithium-ion batteries” from the MES RK for 2020-2022.

Factors affecting the design of hydrogen separators based on dense metallic membranes

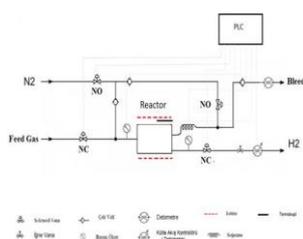
Fatih Pişkin, Hasan Akyıldız and Tayfur Öztürk

INNOVASCOPE Materials Technologies Ltd. Sti. METUTECH, Ankara, Turkey

*E-mail: innovascope@innova-scope.com

Pure hydrogen is needed for a number of applications; annealing furnaces, semiconductor processing, LED, photovoltaic manufacturing etc. Perhaps the most important in this respect is power generation via PEM fuel cells.

Dense metallic membranes in principle provide 100% pure hydrogen. This is irrespective of the purity of the gas to be processed. In fact, the fraction of hydrogen in the feed gas varies quite enormously. It may be industrial grade hydrogen with a purity of 99% or higher. Or syngas produced from steam reforming of natural gas or coal where the fraction may be in the neighbourhood of 75 % or so. Hydrogen produced from renewable sources e.g. biomass gasification, the fraction may be 40%. In gas network, currently the fraction aimed for is not more than 20 % hydrogen.



Hydrogen separator, layout



Hydrogen separator, HS-V1, 1 nl/min.
Innovascope Mat Techn Ltd Sti

Hydrogen separation in dense metallic membranes involve dissolution–diffusion mechanism. Pd is almost always present in the membrane either as alloying element or surface coating which help split hydrogen into atomic form which is then dissolved in the membrane and diffused across the thickness where, aided by Pd again, combine into molecular form. The presence of species such as H₂S and CO in the feed gas is important as it might poison the membrane. Therefore, the choice of separation membranes would depend on the species present in the feed gas. It may also be pointed out that membranes are operated under conditions where hydride formation is avoided as this, in most of the times, lead to volume changes and distortion which adversely affect the durability of the membrane.

For a given conditions, i.e. operating temperature and inlet and outlet pressure, the hydrogen flux across the membrane depends on the permeability of the membrane as well as its thickness. Currently all hydrogen separators makes use of tubings as membrane material where the wall thickness is around 100 μ m or so. Thinner tubings would be highly desirable or it may be necessary to switch to thin film membranes such as those could be deposited via magnetron sputtering.

Functional PAN carbon nanofibers decorated with nickel and nickel oxide nanoparticles for lithium-sulfur batteries

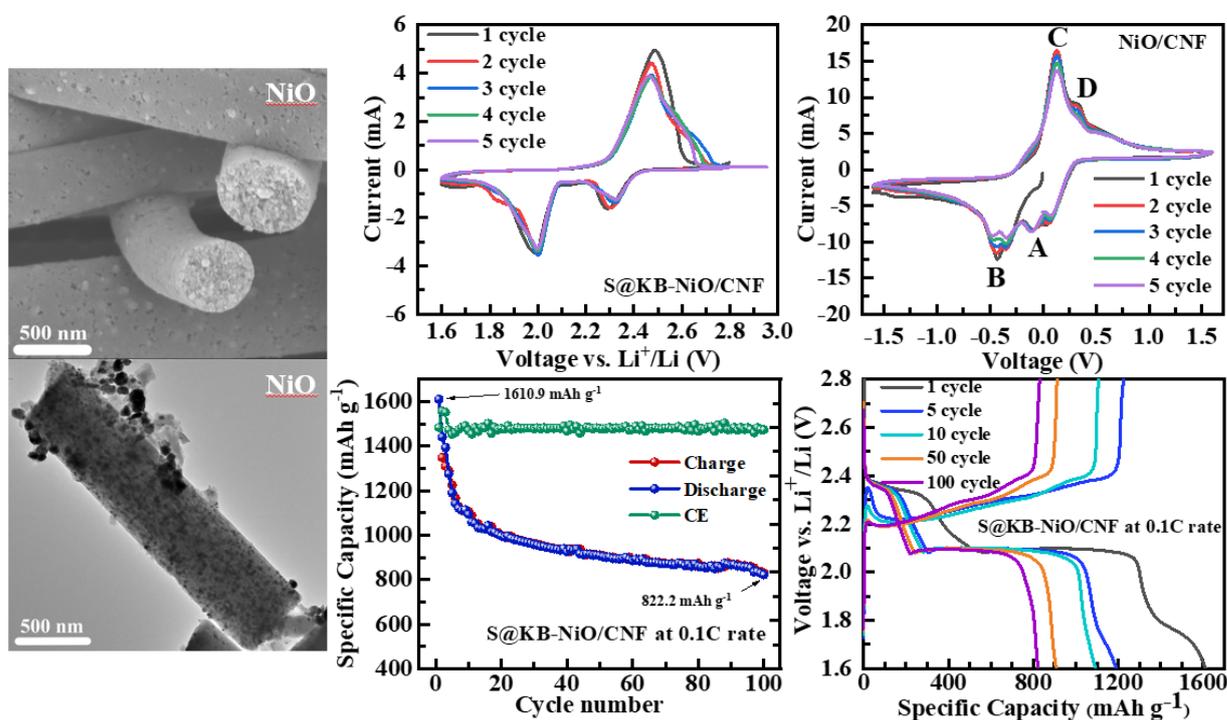
Islam Rakhimbek^{1*}, Nurzhan Baikalov^{1,2}, Almagul Mentbayeva², Aishuak Konarov², Zhumabay Bakenov^{1,2**}

¹National Laboratory Astana, Nazarbayev University, Nur-Sultan 010000, Kazakhstan

²School of Engineering and Digital Sciences, Nazarbayev University, Nur-Sultan 010000, Kazakhstan

*E-mail: islam.rakhimbek@alumni.nu.edu.kz, **E-mail: zhumabay.bakenov@nu.edu.kz

The current status of Lithium-Sulfur Batteries' (Li-S) electrochemical performance is negatively affected by the dissolution of long-chained lithium polysulfides (LiPS) in the electrolyte and shuttling in the system of the battery. This phenomenon was suggested to be minimized by an application of carbon nanofibers (CNF) functionalized with nickel oxide (NiO) and nickel nanoparticles as in-situ membranes, interlayers. The synthesis of materials was carried out via the electrospinning technique with subsequent heat treatment of collected nanofibers. The implementation of interlayers significantly improved the kinetics of LiPS RedOx reactions providing a remarkable initial capacity of 1610,9 mAh g⁻¹, improving the reversibility and stability of charge-discharge processes with low capacity decay per cycle, and reaching a meager charge transfer resistance of 7 Ω.



Acknowledgement

This research was supported by the Ministry of Education and Science of The Republic of Kazakhstan as a funding for the project “Engineering of multifunctional materials of next generation batteries”.

Ionic conductivity of LATP-based thin-film solid electrolytes prepared by magnetron sputtering

Aigul Shongalova^{1,2}, Mukagali Yegamkulov^{1,2}, Aliya Mukanova^{1,2,3*}, Zhumabay Bakenov^{1,2,3},

¹*Institute of Batteries, Nazarbayev University, Nur-Sultan, Republic of Kazakhstan*

²*Department of Chemical and Materials Engineering, School of Engineering and Digital Sciences, Nazarbayev University, Nur-Sultan, Kazakhstan*

³*National Laboratory Astana, Nazarbayev University, Nur-Sultan, Kazakhstan*

*E-mail: aliya.mukanova@nu.edu.kz

The benefits of solid electrolytes is the possibility of all-solid state microbatteries fabrication. Among the various solid electrolytes the NASICON type ceramic $\text{Li}_{1.3}\text{Al}_{0.3}\text{Ti}_{1.7}(\text{PO}_4)_3$ (LATP) has attracted high interest due to its air and water stability, high Li^+ conductivity and low cost. The ionic conductivity of crystalline bulk LATP is in the range of $\sim 10^{-3}$ - 10^{-4} S/cm. The ionic conductivity at room temperature for thin-film crystalline LATP currently does not exceed 10^{-6} S/cm (film thickness are varies from 300 nm to 1000 nm). The crystalline thin-films form via annealing during synthesis or after deposition. LATP crystallizes at temperatures above 700 °C. The high temperatures leads to the loss of lithium, which negatively affect the ionic conductivity. The lithium compensates by incorporation of additional source of lithium, by using a rapid thermal processes and reactive gases. However, the reported results of electrochemical spectroscopy (EIS) show a big discrepancy in ionic conductivity. The ionic conductivity obtained by in-plane is much higher compared to cross-plane. In the most studies EIS characterization of thin films with the crystalline structure is conducted through in-plane configuration. However, the batteries have a sandwich-like structure, i.e. during battery operation the large amount of ions pass through the plane of the electrolyte, therefore through plane should provide more realistic data of the ionic conductivities. Besides, for bulk LATP electrolytes, a protective coating such as polymer electrolytes, LiPON, etc. are used to avoid titanium reduction leading to the high resistance on the electrolyte-electrode interface.

In this study, we synthesized amorphous thin-film electrolytes based on LATP by magnetron sputtering in four series of experiments. In the first series, the effect of deposition gas (Ar, O₂, N₂) on the EIS characteristics of the LATP electrolytes was tested. The second and third series of samples were made to improve ionic conductivity of the electrolytes using cosputtering of Li₂O and Li₃PO₄ to compensate the Li lost during deposition. In the fourth series, extra layers of LiPON were examined to prevent titanium reduction in contacts with lithium metal anode. A room-temperature conductivity σ_{RT} of $\sim 10^{-6}$ S cm⁻¹ was obtained for the LATP thin film in N₂ atmosphere. The compositional dependence of Li-ion transport mechanism will be discussed at the conference.

Acknowledgement

This research was supported by research grants №AP08052231 “Development of solid electrolytes with high ionic conductivity for next generation lithium-ion batteries” from the MES of RK Kazakhstan for 2020-2022 and the research grants #51763/ПЦФ-МЦПОАИ ПК-19 “New materials and devices for defense and aerospace applications” from MDDIAI RK.

Sol-gel synthesis of LiFePO₄ for LIB based on lithium carbonate from Kazakhstani spodumene feedstocks

Assem Zhanabayeva^{1,2*}, Arailym Nalibayeva^{1*}, Dinara Zhumabayeva¹, Erlan Abdykhalykov¹, Zhumabay Bakenov³, Gaukhar Bishimbayeva^{1***}

¹*D.V. Sokolsky Institute Institute of Fuel, Catalysis, and Electrochemistry, Almaty, Kazakhstan*

²*Department of Chemical Engineering, Kazakh-British Technical University*

³*School of Engineering of Nazarbayev University, Astana, Kazakhstan*

*E-mail: a.k.zhanabaeva@mail.ru, **E-mail: aray77@mail.ru, ***E-mail: bigauhar@mail.ru

LiFePO₄ (LFP) cathode material with an olivine structure, in comparison with other cathode materials, has a number of positive properties, such as: high theoretical capacity and stability, low cost and environmental friendliness. The sol-gel method is one of the effective single-step methods for the production of LFP to control the structure of the electrode materials and provide a nanostructured homogeneous composition of the product particles. LFP was synthesized by sol-gel method from high-purity lithium carbonate obtained from spodumene raw materials of Kazakhstani deposits.

Lithium iron phosphate was synthesized by the interaction of lithium carbonate (Li₂CO₃), 9-aqueous iron (III) nitrate (Fe(NO₃)₃ · 9H₂O), ammonium dihydrogen phosphate (NH₄H₂PO₄) and citric acid, followed by drying and calcination of the resulting gel in an inert atmosphere.

The phase composition of the resulting powders (LiFePO₄) was determined by X-ray diffraction. The electrochemical properties of the synthesized electrode materials were studied by traditional research methods: cyclic voltammetry and galvanostatic charge/discharge curves. The data of cyclic voltammetry confirm the high intercalation reversibility of lithium ions in the obtained samples at the indicated potential limits.

The LIB with LFP2 cathode has an initial discharge capacity of 97 mAh/g, which is 60.6% of the theoretical capacity (1C=160 mAh/g). After 50 cycles, the discharge capacity has increased to 105 mAh/g. The width of the plateau in the battery indicates a large polarizability caused by the impurities present. The battery is stable, as indicated by the stability of the capacity of the first and fiftieth cycles.

Thus, by sol-gel method successfully synthesized and studied samples of lithium iron phosphate synthesized using lithium carbonate obtained from domestic spodumene and purified by us earlier to battery grade. The structure and morphology of the obtained cathode material correspond to the standard profile of lithium iron phosphate. The tests of the synthesized electrode materials in lithium half-cells and push-button cells showed good electrochemical properties, stable battery performance, high intercalation reversibility of lithium ions in the samples within potentials 2.5-4.3V.

Investigation of surface carbide layers of tungsten under the influence of helium plasma

Arman Miniyazov^{1,3*}, Mazhyn Skakov², Timur Tulenbergenov¹, Igor Sokolov¹, Olga Stepanova³

¹"Institute of Atomic Energy" Branch of the National Nuclear Center of the Republic of Kazakhstan, Kurchatov, Republic of Kazakhstan

²National Nuclear Center of the Republic of Kazakhstan, Kurchatov, Republic of Kazakhstan

³"Shakarim University of Semey" of the Ministry of Education and Science of the Republic of Kazakhstan

**E-mail: miniyazov@nnc.kz*

The relevance of the research is caused by development of a fusion energy, where issues of surface modification of plasma-facing materials of the first wall and divertor of a fusion reactor are of great importance. Therefore, obtaining a reliable database on the properties of materials and other elements in contact with plasma, simulation of the plasma effect on their surfaces using an imitation installation are highly relevant tasks of material research in modern physics when developing thermonuclear technology, including research at the Kazakhstani Material Testing Tokamak KTM.

The presence of structural materials and their impurities in the installation chamber will lead to the formation of mixed layers in the plasma-facing surfaces during redeposition due to erosion. In particular, carbon in the chamber of fusion reactors entails a number of problems. Carbon acting on the divertor surface can penetrate into the divertor volume and promote erosion and formation of porous layers on the tungsten surface and leads to tungsten carbidization.

Hence, the goal of the research is to study external effects at a high energy flux and plasma irradiation on the structure and physical and mechanical properties of tungsten with a carbide layer, under conditions close to a fusion installation and the Kazakhstani Material Testing Tokamak KTM.

In this research, the results of experimental studies on the effect of plasma irradiation with a carbidized tungsten surface are obtained. Data on the structure and properties of tungsten with a carbidized near-surface layer have been obtained.

The practical significance of the research lies in the fact that the research results will be used in designing of fusion reactor components, analysis of the resource and degree of erosion effect of divertor components on plasma parameters.

Acknowledgement

The work was carried out at the National Nuclear Center of the Republic of Kazakhstan within the framework of a scientific and technical program on the topic "Investigation of the interaction of plasma with a carbidized tungsten surface".

Synthesis of LiCoO₂ thin-film cathode for lithium-ion microbatteries

Akzhan Bekzhanov^{1*}, Aliya Mukanova^{1,2,3}, Berik Uzakbaiuly^{1,2,3**}, Zhumabay Bakenov^{1,2,3}

¹*School of Engineering and Digital Science, Nazarbayev University, Z05P4X0 Nur-Sultan, Kazakhstan*

²*Institute of Batteries LLC Z05P4X0 Nur-Sultan, Kazakhstan*

³*National Laboratory Astana, Z05P4X0 Nur-Sultan, Kazakhstan*

*E-mail: akzhan.bekzhanov@nu.edu.kz

LiCoO₂ thin film cathode, which has attracted considerable attention in the past decades due to its promising application in micro-batteries, is commonly produced by magnetron sputtering combined with post-annealing treatment. However, the high temperature treatment, film thickness plays crucial role for preferred orientation of crystal lattice plane. In this study, LiCoO₂ film cathode is sputtered onto the Si wafer substrate. The annealed LiCoO₂ thin film cathode is highly crystallized as hexagonal structure, exhibiting a capacity retention of 75% at 1 C after 200 cycles and excellent rate performance with least 55% with capacity retention. The excellent electrochemical performance is ascribed to highly crystallized LiCoO₂ thin film, which is triggered by high kinetic energy of the sputtered species and thin film thickness. This work provides a new option to deposit high quality LiCoO₂ thin film and changing preferred crystal plane orientation via film thickness.

Acknowledgement

This research is supported under the state targeted program №51763/ПЦФ-МЦРОАП PK-19 "New materials and devices for defense and aerospace applications" by the MDDAI RK.

Passivation of zinc dendrites by spin coating method

Dana Kurmangaliyeva^{1*}, Aishuak Konarov^{1,3*}, Nurzhan Umirov^{1,2}, Zhumabay Bakenov^{1,2,3}

¹*Nazarbayev University, Kabanbay Batyr Ave 53, Nur-Sultan, Kazakhstan*

²*Institute of Batteries LLC, Kabanbay Batyr Ave 53, S4, 511, Nur-Sultan, Kazakhstan*

³*National Laboratory Astana, Kabanbay Batyr Ave 53, S2, Nur-Sultan, Kazakhstan*

*E-mail: dana.kurmangaliyeva@nu.edu.kz, **E-mail: aishuak.konarov@nu.edu.kz

Aqueous based batteries are an attractive alternative to eliminate the LIB pre-investment deficit in large-scale energy storage, eliminate safety concerns and reduce production costs. Metal Zn is considered the most promising anode for aqueous batteries due to its high capacity, low cost and environmental friendliness. Despite the rapid progress made in the development of highly efficient cathodes and electrolytes, it has been observed that the underestimated but not neglected Zn-anode dendrites shorten battery life. To suppress adverse reactions and dendrite growth, a highly viscoelastic poly 2-vinyl pyridine film functioning as an artificial interfacial solid/electrolyte (SEI) is homogeneously deposited onto the Zn surface using a simple spin coating strategy. The main purpose of this study is the suppression of zinc dendrites to test the basic electrochemical characteristics of the battery and effectively suppress Zn dendrites and prolong the service life of the symmetrical Zn cell. The object of the study is poly 2-vinylpyridine on a zinc anode material.

This work reveals that the P2VP coated Zn electrode, which does not contain side reactions and dendrites, has high cyclic stability and increased Coulomb efficiency, which also contributes to an increase in the performance of the complete element when it is connected to V₂O₅ and LiFePO₄ cathodes.

Acknowledgement

This research is supported under the state targeted program №51763/ПЦФ-МЦРОАП PK-19 "New materials and devices for defense and aerospace applications" by the MDDAI RK.

Effect of acid etching of stainless-steel foils in rechargeable lithium-ion batteries

Kamila Maratova*, Aishuak Konarov^{1,3*}, Nurzhan Umirov^{1,2}, Zhumabay Bakenov^{1,2,3}

¹ *Nazarbayev University, Kabanbay Batyr Ave 53, Nur-Sultan, Kazakhstan*

² *Institute of Batteries LLC, Kabanbay Batyr Ave 53, S4, 511, Nur-Sultan, Kazakhstan*

³ *National Laboratory Astana, Kabanbay Batyr Ave 53, S2, Nur-Sultan, Kazakhstan*

*E-mail: kamila.maratova @nu.edu.kz, **E-mail: aishuak.konarov@nu.edu.kz

Research into rechargeable aqueous batteries is driven by the need for low-cost, high-safety batteries for large-scale energy storage applications. The effect of current collectors on battery performance is frequently disregarded, despite the fact that the majority of research efforts concentrate on creating electrolyte formulations and electrode materials.

A commonly used current collector in aqueous batteries is stainless steel foil, which has the benefits of being inexpensive, good conductivity, good flexibility, lightweight, and more. The difficulty in shedding active materials and high contact resistance that stainless steel foil encounters as a current collector, however, remain. In this work, the surface of stainless-steel foil is modified by chemical etching, and the influence of surface morphology of stainless-steel foil on battery performance is investigated.

The chemical etching technique was successfully used to modify stainless steel foil. The surface of modified stainless-steel exhibits evenly spaced defects (etching pits). The improved stainless steel foil's moderate roughness, effective contact area, and good electrical conductivity are all made possible by the formation of defects. The results show that the stainless-steel foil treated with 1M HCl etching solution for 10 min has the best electrochemical performance.

Acknowledgement

This research is supported under the state targeted program №51763/ПЦФ-МЦРОАП РК-19 "New materials and devices for defense and aerospace applications" by the MDDAI RK.

ACKNOWLEDGEMENTS

The Advanced Energy Storage Systems and Functional Nanomaterials Research Group and Prof. Zhumabay Bakenov would like to express our cordial thanks to all who helped make this conference a success.

**Our great pleasure to express sincere thanks to the organizers:
Institute of Batteries LLP, Nazarbayev University, and PI “National Laboratory Astana”.**

We would like to express our very special gratitude to the all Speakers,

Sponsors of INESS 2022, and

**Ministry of Digital Development, Innovations and Aerospace Industry of the Republic
of Kazakhstan**

for excellent contribution to our event.

**Last, but not least, we would like to thank all Chairmen and Co-Chairmen
of the respective sessions and all Members of the Scientific Advisory and Organizing
committees.**

Without their tireless efforts, the conference would not have been possible.

GOLD



SILVER



DistriTech

BRONZE

