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Abstract Book



# The 12<sup>th</sup> International Conference on Nanometrials and Advanced Energy Storage Systems

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The 12<sup>th</sup> International Conference on Nanomaterials and Advanced Energy Storage Systems (INESS - 2024)

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***We greatly appreciate your participation and valuable contribution to our Conference. We are honored and pleased to welcome you at INESS-2024!***

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***On behalf of the Organizers,***

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## Current Trends in the Korean Battery Industry Interface Analysis of the Si Anodes in the Sulfide-based Solid Electrolyte

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The Korean battery industry has rapidly emerged as a global leader, driven by groundbreaking innovations, significant investments, and a strong commitment to sustainability. This keynote will explore current trends, including advancements in lithium-ion and solidstate batteries, and the growing importance of electric vehicle (EV) batteries. Key companies like LG Energy Solution, Samsung SDI, and SK Innovation are pushing the boundaries of performance, safety, and cost-efficiency. The industry is also shifting towards ecofriendly practices with investments in recycling technologies and sustainable materials, supported by robust government policies and international collaborations.

Despite challenges such as supply chain constraints and raw material scarcity, Korea's strategic planning and innovation continue to propel the industry forward. This keynote will provide a comprehensive overview of these trends, highlighting Korea's pivotal role in the global battery market and future industry directions.

All-solid-state batteries (ASSBs) are promising for future energy storage due to higher energy densities and improved safety compared to traditional lithium-ion batteries. However, challenges at the active material-solid electrolyte interface hinder their adoption. Recent studies show that Si-based materials can be used in ASSBs, but the complex nature of composite electrodes complicates interfacial kinetics evaluation. Understanding individual anode particle interfaces is crucial. Traditional methods fall short for ASSBs, requiring new approaches. This study uses a microelectrode with a cylindrical cavity trap to examine depth-of-discharge (DOD)-dependent interfacial charge transfer kinetics between silicon (Si) anode particles and solid electrolytes. Si anode particles were immobilized in cavity traps and integrated into an argyrodite-type (Li<sub>6</sub>PS<sub>5</sub>Cl) solid electrolyte system.

We validated electrochemical stability over several cycles, applied pulsed currents after each DOD state, and measured potential peak responses to create Tafel plots. This determined DOD-dependent charge transfer resistance at the anode/solid electrolyte interface, providing insights into interfacial kinetics. This study offers an innovative method for analyzing single anode particles in a solid electrolyte matrix, enhancing understanding of interfacial challenges and advancing the development of high-performance ASSBs with silicon anodes.

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### References

- [1] A. Banerjee, X. Wang, Ch. Fang, E.A. Wu, Y.-Sh. Meng, ACS Chemical Reviews, 14 (2020) 6878-6933.
- [2] D.H.S. Tan, Y.-T. Chen, H. Yang, W. Bao, B. Sreenarayanan, J.-M. Doux, W. Li, B. Lu, S.-Y. Ham, B. Sayahpour, J. Scharf, E.A. Wu, G. Deysher, H.E. Han, H.J. Hah, H. Jeong, J.B. Lee, Zh. Chen, Y.Sh. Meng, Science, 373 (2021) 1494-1499.
- [3] A. Song, W. Zhang, H. Guo, L. Dong, T. Jin, Ch. Shen, K. Xie, Advanced Energy Materials, 13 (2023) 2301464.
- [4] C. Heubner, U. Langklotz, C. Lämmel, M. Schneider, A. Michaelis, Electrochimica Acta, 330 (2020) 1351602.



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## Digital Twin Battery Modeling and Simulations

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The adoption of digital twin technology has witnessed a paradigm shift, extending from its traditional use in replicating and simulating large-scale systems to new application in micro- and nano-sized electrochemical devices such as lithium-ion batteries (LIBs). This evolution is propelled by the significance of understanding and evaluating the microstructures of composite electrodes, rendering digital twin battery modeling a focal point of extensive research endeavors in recent years. This presentation offers a concise overview of digital twin battery modeling for LIBs and next-generation batteries. Particularly, as more precise tomographical images can be gathered with the improvement of 3D reconstruction or x-ray microscope technology, digital twin battery modeling becomes more powerful and essential to fill the gap between materials and systems. Moreover, well-created microstructures enable the extraction of latent parameters with high precision. Hence, the integration of digital twin battery modeling and simulations emerges not as optional analysis but as mandatory research item for the innovative research and development of next-generation batteries.

### References

1. Energy Storage Materials, 19 (2019) 124-129
2. Nano Energy, 62 (2019) 810-817
3. Chemical Engineering Journal, 391 (2020) 1235282
4. Advanced Energy Materials, 10(35) (2020) 2001563
5. ACS Energy Letters, 5(9) (2020) 2995-3004
6. Nano Energy, 79 (2021) 105456
7. Energy Storage Materials, 41 (2021) 289-296
8. Advanced Energy Materials, 12 (2022) 2103108
9. Energy Storage Materials, 49 (2022) 481-492
10. Nano Energy, 102 (2022) 107679
11. Energy Storage Materials, 55 (2023) 193-204
12. Advanced Energy Materials, 13 (2023) 2204328
13. Advanced Energy Materials, 13 (2023) 2300172

## Na-O-A Configuration for Oxygen Redox of Sodium Cathode

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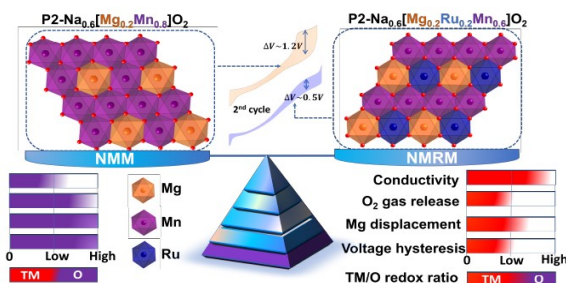
Mn-based P2-Na<sub>x</sub>[Li<sub>y</sub>TM<sub>1-y</sub>]O<sub>2</sub> cathode materials are available to reach high capacity through the combination of cationic and anionic redox in Na cells.<sup>1-11</sup> The Na-O-Li configuration induces the delivery of additional capacity assisted by the oxidation of oxygen when lone-pair electrons are formed in the O 2p orbital, provided that at least one of the following conditions is satisfied: 1) lattice oxygen evolution<sup>1</sup> or 2) migration of the Li element to Na layers although the corresponding charge transfer is kinetically sluggish.<sup>2</sup> The reaction is not limited to compounds that have alkali ions in the TM layer but is also available with divalent ions; namely, the presence of Mg in the TM layer, P2-Na<sub>x</sub>[Mg<sub>y</sub>Mn<sub>1-y</sub>]O<sub>2</sub> (x = ~2/3, y = ~0.28).

The effect of the 4d Ru element in P2-Na<sub>0.6</sub>[Mg<sub>0.2</sub>Ru<sub>0.2</sub>Mn<sub>0.6</sub>]O<sub>2</sub> is investigated. Ru-free Na<sub>0.6</sub>[Mg<sub>0.2</sub>Mn<sub>0.8</sub>]O<sub>2</sub> is activated with the Mn<sup>3+</sup>/Mn<sup>4+</sup> redox, after which the charge is compensated by the sluggish oxidation of lattice oxygen (O<sup>2-</sup>) to O<sub>2</sub><sup>n-</sup> triggered by O<sub>2</sub> evolution from the oxide lattice. These effects are generally unfavorable and result in poor



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long-term cycle stability induced by the irreversible migration of  $\text{Mg}^{2+}$  from the transition metal (TM) to Na layers in the P2 structural framework. Benefiting from the covalent Ru bonded with O in the TM layers, the Mg migration reversibly progresses from the TM to sodium slabs without  $\text{O}_2$  evolution in the structure. The associated reaction progresses via the active  $\text{Mn}^{4+}/\text{Mn}^{3+}$  and  $\text{O}^{2-}/(\text{O}_2)^{n-}$  reaction in addition to the  $\text{Ru}^{5+}/\text{Ru}^{4+}/\text{Ru}^{3+}$  redox pairs, endorsing the capacity increase ( $\sim 210 \text{ mAh g}^{-1}$ ), with  $\sim 72.1\%$  retention for 300 cycles.



**Figure 1.** The presence of the higher-covalency Ru–O bond minimizes Mg migration from the TM to Na layers.

### References

- [1]. House, R. A.; Maitra, U.; Pérez-Osorio, M. A.; Lozano, J. G.; Jin, L.; Somerville, J. W.; Duda, L. C.; Nag, A.; Walters, A.; Zhou, K. J.; Roberts, M. R.; Bruce, P. G. *Nature* **2020**, *577* (7791), 502–508.
- [2]. Voronina, N.; Shin, M. Y.; Kim, H. J.; Yaqoob, N.; Guillon, O.; Song, S. H.; Kim, H.; Lim, H. D.; Jung, H. G.; Kim, Y.; Lee, H. K.; Lee, K. S.; Yazawa, K.; Gotoh, K.; Kaghazchi, P.; Myung, S. T. *Adv Energy Mater* **2022**, *12*, 2103939.

## Advances in Carbon Nanotube Engineering: Chirality and Beyond

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Carbon nanotubes (CNTs) have become a cornerstone material in the energy sector, owing to their remarkable electrical conductivity, mechanical strength, and thermal stability. These exceptional properties make CNTs highly suitable for a variety of applications, including energy storage in batteries and supercapacitors, efficient energy conversion in fuel cells, and as conductive additives in composite materials. The ability to tailor the structural and electronic properties of CNTs further enhances their potential in developing advanced energy devices.

In this context, our research emphasizes the controlled manipulation of the chirality of carbon nanotubes, which directly affects their electromechanical properties. We analyzed the detailed chiral transition processes in CNTs exposed to high temperatures from Joule heating, accompanied by a slow elongation in a quasi-static process. Our experiments revealed a trend towards increased chiral angles. Theoretical analysis considered the orientation-dependent formation energy of dislocations generated from the evaporation of carbon dimers and the associated formation of 5|8|5 defects. The calculated formation energy indicated that at low chiral angles, the specific dislocation was energetically favored. Therefore, nanotubes with initially small chiral angles tend to increase their chiral angle during transitions. This study highlights the potential for mechanical manipulation of CNTs to control their electronic properties and construct electronic devices approaching the size scaling limit [1].

Additionally, we report a straightforward one-step method for the selective etching of metallic single-walled carbon nanotubes in the aerosol phase using nitrous oxide. To understand the mechanism behind the selective etching of CNTs, it is crucial to examine the individual stages of the oxidation process. The initial stage—active oxygen atom adsorption—plays a key role in the etching process. As gas phase decomposition of nitrous oxide is inhibited under the studied conditions, we consider the process to proceed on the CNT surface. The subsequent addition of oxygen reduces the electron density within the carbon network, weakening the C-C bonds and ultimately leading to the deterioration of the nanotube [2].



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Finally, we explored a novel approach for altering the chirality of nanotubes through a single-step enrichment process of CNTs with small diameters using riboflavin. Solubilization of CNTs in a riboflavin aqueous solution occurs due to the  $\pi$ -conjugated isoalloxazine assembly on the surface of the nanotubes and the formation of hydrogen bonds between the hydrophilic ribityl chain and the aqueous media. Specific adsorption of riboflavin to CNTs minimizes interactions between the CNTs and gel separation media, resulting in the selective extraction of (6,5)-CNTs.

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### References

[1] D.-M. Tang, S.V. Erohin, D.G. Kvashnin, V.A. Demin, O. Cretu, S. Jiang, L. Zhang, P.-X. Hou, G. Chen, D.N. Futaba, Y. Zheng, R. Xiang, X. Zhou, F.-C. Hsia, N. Kawamoto, M. Mitome, Y. Nemoto, F. Uesugi, M. Takeguchi, S. Maruyama, H.-M. Cheng, Y. Bando, C. Liu, P.B. Sorokin, D. Golberg, *Science* 374 (2021) 1616–1620.

[2] A.A. Alekseeva, D.V. Krasnikov, G.B. Livshits, S.A. Romanov, Z.I. Popov, L.A. Varlamova, E.V. Sukhanova, A.S. Klimovich, P.B. Sorokin, S.V. Savilov, A.G. Nasibulin, *Carbon* 212 (2023) 118094.

## Thermoresponsive Solid-state Electrolytes for Safe Lithium Metal Batteries

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Exploring advanced strategies in alleviating the thermal runaway of lithium metal batteries (LMBs) is critically essential. Herein, a novel electrolyte system with thermoresponsive characteristics is designed to largely enhance the thermal safety of 1.0 Ah LMBs (Figure 1). Specifically, vinyl carbonate (VC) with azodiisobutyronitrile is introduced as a thermoresponsive solvent to boost the thermal stability of both the solid electrolyte interphase (SEI) and electrolyte. Firstly, abundant poly(VC) is formed in SEA with thermoresponsive electrolyte, which is more thermally stable against lithium hexafluorophosphate compared to the inorganic components widely acquired in routine electrolyte. This increases the critical temperature for thermal safety (the beginning temperature of obvious self-heating) from 71.5 to 137.4°C. The remained VC solvents can be polymerized into poly(VC) as the battery temperature abnormally increases. The poly(VC) can not only afford as a barrier to prevent the direct contact between electrodes, but also immobilize the free liquid solvents, thereby reducing the exothermic reactions between electrodes and electrolytes. Consequently, the internal-short-circuit temperature and “ignition point” temperature (the starting temperature of thermal runaway) of LMBs are largely increased from 126.3 and 100.3°C to 176.5 and 203.6°C. This work provides novel insights for pursuing thermally stable LMBs with the addition of various thermoresponsive solvents in commercial electrolytes.

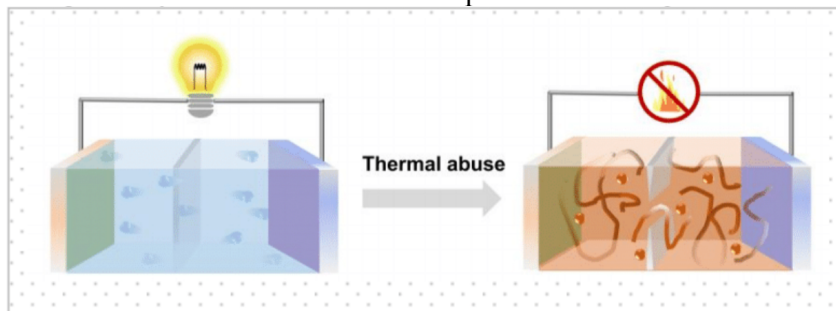


Figure 1. The schematic diagram for the working mechanism of thermoresponsive solid-state electrolyte.



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### References

- [1] Cheng XB, Yang SJ, Liu Z, Guo JX, Jiang FN, Jiang F, Xiong X, Tang WB, Yuan H, Huang JQ, Zhang Q.\* Electro Chemically And Thermally Stable Inorganics-rich Solid Electrolyte Interphase for Robust Lithium Metal Batteries. *Advanced Materials*, 2023, 35,2307370.
- [2] Jiang FN, Cheng XB,\* Yang SJ, Xie J, Yuan H, Liu L, Huang JQ, Zhang Q.\* Thermoresponsive Electrolytes for Safe Lithium Metal Batteries. *Advanced Materials*, 2023, 35, 2209114.
- [3] Yang S-J, Yao N, Jiang F-N, Xie J, Sun S-Y, Chen X, Yuan H, Cheng X-B,\* Huang J-Q,\* Zhang Q.\* Thermally Stable Polymer-Rich Solid Electrolyte Interphase for Safe Lithium Metal Pouch Cells, *Angewandte Chemie International Edition*, 2022, 134,2214545.
- [4] Cheng X-B, Zhang R, Zhao C-Z, Zhang Q.\* Toward Safe Lithium Metal Anode in Rechargeable Batteries: A Review, *Chemical Reviews*, 2017, 117, 10403.

## Development of Reel-to-Reel Production of 2G HTS Wires for Compact Fusion Application and its Possible Utilization for Manufacturing of Energy Storage Materials

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Since its establishment in 2011 Faraday Factory Japan (FFJ) has been developing the technology for long-length fabrication of high-temperature superconducting wires of second generation (2G HTS). Our process based on reel-to-reel deposition of multilayer thin films (including epitaxial films) on flexible metal substrates by combination of various techniques including magnetron sputtering, e-beam evaporation, ion beam assisted deposition (IBAD), pulsed laser deposition (PLD), electroplating etc. [1-2]. Since 2019 the main driver for scaling up the production was compact fusion projects where 2G-HTS based magnets, generating magnetic field of 20 T at 20 K, is the key component of fusion reactor [3-5]. Rapid growth of FFJ production is shown in Fig.1 with the annual capacity exceeded 2000 km in 2023 and average critical current ( $I_c$ ) approaching 200 A/4mm, which imply engineering critical current density ( $J_e$ ) at 20K-20T of about 1000A/mm<sup>2</sup>. In 2024 FFJ has established the world's largest facility for manufacturing of 2G HTS tapes with the projected capacity of 1.0 GAm/year and ready to further expand production capacity with anticipated demand growth.

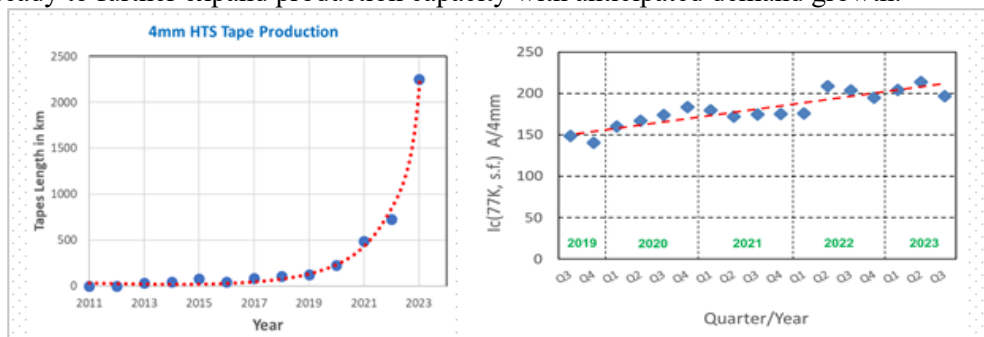


Figure 1. Progress in annual production and average critical current of superconducting wires by Faraday Factory Japan.

The progress in the development of high-speed reel-to-reel fabrication of multilayers and its proven efficiency in manufacturing long-length superconducting tapes paves the way for the potential utilization of this technology in the production of advanced functional materials in other critical industries. Among these, thin-film solid-state batteries stand out as a highly attractive candidate for adapting our technology for mass production [6,7]. The initial experiments conducted with our reel-to-reel equipment demonstrated that the multilayered structure of battery materials and a thin film/solid state full battery can be fabricated with minor modifications to the deposition area of the equipment. The methodology for optimizing deposition conditions



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based on the linear combinatorial approach is well-suited for multilayered battery fabrication, making the developed technology an ideal solution for manufacturing thin film batteries.

### References

- [1] S. Lee et al., Superconductor Science and Technology 27 (2014) 044022.
- [2] S. Samoilenkov et al., Superconductor Science and Technology 29 (2016) 024001.
- [3] A. Molodyk et. al., Scientific Reports 11 (2021) 2084.
- [4] A. Molodyk and D.C. Larbalestier, Science 380 (2023) 1220.
- [5] R.F. Vieira et al., IEEE Transactions on Applied Superconductivity, 34, (2024) 1.
- [6] A. Jetybayeva et al. Journal of Materials Chemistry A, 9 (2021) 15140.
- [7] A. Jetybayeva et al. , ACS symposium series, 1414 (2022) 201.

## Buckybowl Meets Carbons

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Since the remarkable discovery of the two-dimensional electron system in graphene, it has found widespread use in various applications due to its extremely high carrier mobility. However, graphene lacks bandgap, limiting its application as a semiconductor. To overcome this limitation, several methods have been explored, including the formation of graphene nanoribbons (GNRs), graphite intercalation compounds (GICs), and the doping of carbon atoms in graphene with other elements. [1] However, there is still a need for a simple and easy-to-manufacturing method to generate band gaps in graphene. In this study, we focused on forming a bandgap in graphene by investigating its electronic structure upon the physisorption of aromatic compounds [2] using density functional theory. By employing this theoretical approach, we aimed to gain insights into the electronic properties of graphene and understand the potential for bandgap modulation through the interaction with aromatic molecules.

As our initial model compound, we selected trioxosumanene (**1**) [3]. This compound exhibits a three-fold symmetric curved aromatic structure characterized by three carbonyl groups (Fig.1). We placed **1** on a monolayer graphene and performed electronic structure calculations to analyze its properties. When the bowl of **1** faced upwards (bowl-up), we observed a downward shift of the Dirac point, but the bandgap formation was not evident. In contrast, when the bowl of **1** faced downwards (bowl-down), we observed the formation of a bandgap of 0.18 eV around the K point. The wave function analysis indicated that the oxygen's *p*-orbital hybridized with the *p<sub>z</sub>*-orbital of the carbon atoms in graphene. Electron density analysis revealed localized electron holes in graphene, specifically beneath the oxygen atoms.

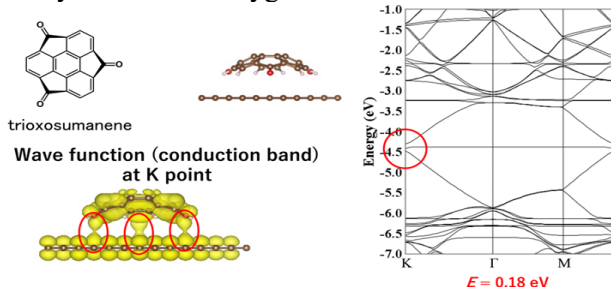


Figure 1. Trioxosumanene on monolayer graphene (5×5)



## References

- [1] M. S. Dresselhaus, G. Dresselhaus, *Adv. Phys.* **1981**, *30*, 139.  
 [2] H. Tanaka, R. Arima, M. Fukumori, D. Tanaka, R. Negishi, Y. Kobayashi, S. Kasei, T.K. Yamada, T. Ogawa, *Sci Rep.* **2015**, *5*, 12341.  
 [3] T. Amaya, M. Hifumi, M. Okada, Y. Shimizu, T. Moriuchi, K. Segawa, Y. Ando, T. Hirao, *J. Org. Chem.* **2011**, *76*, 8049.

## Electrolyte solvation chemistry for low temperature lithium batteries

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Low temperature batteries require high dissociation lithium salts to increase charge carriers and achieve favorable transport kinetics under harsh operating conditions<sup>[1]</sup>. However, this type of electrolyte is prone to corrosion of aluminum foil and leads to the disconnection of the electronic path between the active material and the aluminum current collector, reducing the stability of the battery under high voltage. This report proposes universal strategies to improve interface stability from two aspects: negative electrode fluorination interface and positive electrode aluminum foil protection strategy, and provides the special role of solid electrolyte in low-temperature lithium batteries to achieve efficient operation of low-temperature lithium batteries.

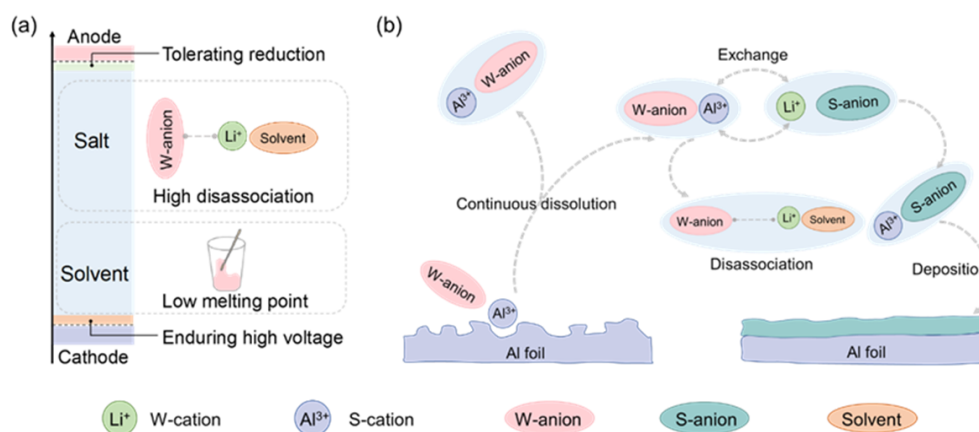


Figure 1. Electrolyte requirements for the stable operation of Li metal batteries at low temperature. S/W-cation/anion represents strongly/weakly coordinated cation/anion. (a) Design principles for low-temperature electrolytes. Li salts with weakly coordinated anions are expected to facilitate dissociation. Solvents with low melting point promise better rheology. (b) Schematic illustration of NO<sub>3</sub><sup>-</sup> inhibiting Al foil corrosion. According to Hard-Soft-Acid-Base principle, Al<sup>3+</sup> has smaller radius and higher charge density than Li<sup>+</sup>, leading to the favorable interaction with NO<sub>3</sub><sup>-</sup> (e.g., S-anion) and promoting the formation of Al-NO<sub>3</sub><sup>-</sup> precipitation. The donor number of NO<sub>3</sub><sup>-</sup> and FSI<sup>-</sup> is 22.2 and 16.9, respectively.

## References

- [1] Duan, J. Y, Chen, J x. et al. *J Energy Chemistry*, **87** (2023) 473–478





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## Appearance of the highest mobility holes in a 2D system epitaxially grown on a silicon wafer

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A new technological breakthrough in epitaxial growth of the highest quality group IV semiconductor material 2D system, attractive for new fundamental research and also suitable for large-scale practical applications, will be presented. Mobility of free carriers in conduction (electrons) or valence (holes) bands, along with a reasonably large energy band gap, is one of important quality figures of any semiconductor material, which determines its suitability for advanced applications in a large variety of classical electronic and sensor devices, as well as for novel applications in emerging quantum electronics.

Recently, a record-high mobility of holes, reaching  $4.3 \times 10^6 \text{ cm}^2 \text{V}^{-1} \text{s}^{-1}$  in an epitaxial compressively strained germanium (cs-Ge) quantum well semiconductor 2D system, grown on a standard silicon (Si) wafer, with (001) crystallographic orientation, was reported.[1] This significant increase of the mobility by over four times, compared to the previous state of the art, allows for the first time hole devices to outperform electronics in the group I semiconductor materials.

In order to appreciate the archived breakthrough, the historic evolution of hole mobility in the group IV semiconductors at low temperatures shown in Fig. 1. For comparison, the highest mobility electrons in tensile strained Si (ts-Si) quantum wells shown.[2] The demonstrated hole mobility in cs-Ge on Si (cs-GoS) material systems twice larger of the best mobility of electrons reported to date in the state of the arts-Si.

Furthermore, this achievement reduces the gap between the highest hole mobility in gallium arsenide (GaAs) 2D system modulation doped heterostructures grown on the same material substrate, i.e. GaAs, which was recently increased from  $2.3 \times 10^6 \text{ cm}^2 \text{V}^{-1} \text{s}^{-1}$  to  $5.8 \text{ cm}^2 \text{V}^{-1} \text{s}^{-1}$ . [3,4] It should be noted, III-V materials are more complicated to process, are much more expensive, not widely abundant in the Earth's crust, compared to Si and Ge. In addition, unfortunately III-V do not exist in isotopically pure forms, and are not compatible with the advanced Si technologies for mass production opportunities. All other known semiconductors, including III-V, II-VI, perovskites, 2d Materials, etc. show substantially lower carrier mobility than in the cs-GoS and GaAs hetero structures.

This reported breakthrough in the enhancement of hole mobility in cs-GoS was achieved due to the development of state-of-the-art epitaxial growth technology culminating in superior monocrystalline quality of the material system with very low density of background impurities and other imperfections. This superior material system with the combination of unique properties opens new opportunities for innovative quantum device technologies and applications in quantum as well as in classical electronics, and sensors.

### References

- [1] M. Myronov, J. Kycia, P. Waldron, W. H. Jiang, P. Barrios, A. Bogan, P. Coleridge, and S. Studenikin, *Small Science* 3(2023).
- [2] M. Y. Melnikov, A. A. Shashkin, V. T. Dolgoplov, S.-H. Huang, C. W. Liu, and S. V. Kravchenko, *Appl. Phys. Lett.* 106, 092102 (2015).
- [3] J. D. Watson, S. Mondal, G. Gardner, G. A. Csáthy, and M. J. Manfra, *Phys. Rev. B* 85, 165301 (2012).
- [4] Y. J. Chung, C. Wang, S. K. Singh, A. Gupta, K. W. Baldwin, K. W. West, M. Shayegan, L. N. Pfeiffer, and R. Winkler, *Physical Review Materials* 6, 034005 (2022).



## What boron is doing in NMC cathode materials for Li-ion batteries?

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A competition between the electric and internal combustion engines requires overcoming the technological barrier in specific energy of Li-ion battery cells of 300 Wh/kg by 2025, and 350 Wh/kg - by 2030 that calls for advanced cathode materials, such as Ni-rich layered transition metal oxides providing electrochemical capacity up to ~220 mAh/g. NMC ( $\text{LiNi}_x\text{Mn}_y\text{Co}_z\text{O}_2$ , where  $x+y+z = 1$ ) cathode materials are still the subject of intense research aimed at increasing mass and volumetric energy density, cycle life, and performance at elevated charge/discharge rates. Almost all elements of the Periodic Table were used to dope and/or create protective coatings for NMC materials, with the exception of highly toxic, radioactive and chemically inert ones [1]. Among other elements, boron is the most elusive one because its low atomic number makes it difficult to detect it with the common diffraction and imaging techniques, particularly at local scale (surfaces, grain boundaries). In this work we resolve the long-standing mystery of the role of boron in "doping" or "coating" the Ni-rich NMC cathode materials [2]. Combining the experimental and computational approaches we demonstrate that boron does not enter the NMC crystal lattice even in minor amount, but instead forms tiny lithium borate coating layer around the NMC811 crystallites. Through changing the lithium chemical potential, boron promotes growth of elongated platelike NMC811 crystals radially arranged into spherical agglomerates, in contrast to common misconception of needle-like crystallites that contradicts the DFT-calculated relative surface energies. Improvement of capacity retention in the boron-modified NMC811 comes from a combined effect of protective lithium borate coating, increasing reversibility of the H2-H3 phase transition (Figure 1) and improved mechanical stability due to radial microstructure.

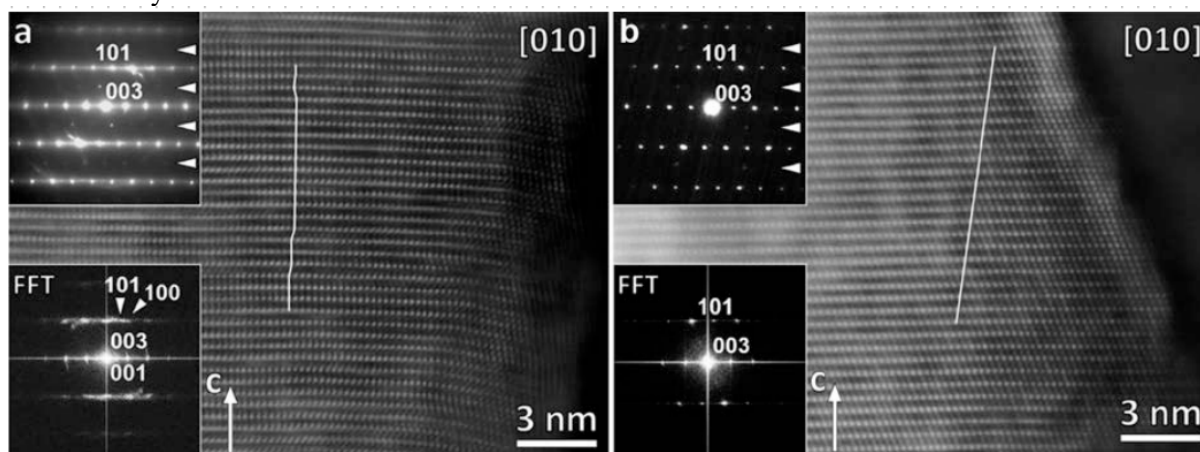


Figure 1. HAADF-STEM images along with the corresponding SAED/FFT patterns of the pristine (a) and boron-modified (b) NMC811 samples after 30 galvanostatic charge-discharge cycles.

**Acknowledgement:** the work has been supported by the Russian Science Foundation, grant 23-73-30003.

### References

- [1] A.A. Savina, A.M. Abakumov, *Heliyon*, 9 (2023) e21881.
- [2] I.A. Skvortsova, E.D. Orlova, A.O. Boev, D.A. Akseyonov, I. Moiseev, E.M. Pazhetnov, A.A. Savina, A.M. Abakumov, *J. Power Sources*, 583 (2023) 233571.



## Data-mining approach subgroup discovery for novel energy materials design

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Despite the accelerating progress in technology in recent years, only a small fraction of possible functional materials for various applications have been explored so far. One of the reasons for the slow exploration of materials space is the extreme complexity of the relation between the atomic composition of a material and its functional properties. Moreover, traditional computational approaches with high predictive power, such as density-functional theory and other first-principles methods, remain too demanding to directly explore the vast materials space. In particular, important properties of energy materials, such as activity and selectivity of a catalyst for chemicals conversion, batteries, and fuel cells, are in general difficult to predict. We demonstrate how to bridge the materials-space complexity with an artificial-intelligence (AI) approach called subgroup discovery (SGD) for two examples from heterogeneous catalysis and electrocatalysis.

SGD belongs to the class of data-mining methods that allow for identification of statistically significant subsets with unique properties in data. We have developed this approach to identify combinations of a catalytic material's features (catalyst's genes) that result in optimal catalytic properties. The approach is applied to the challenging problem of converting CO<sub>2</sub> to fuels and other useful chemicals [1]. Using this example, we show how SGD helps to uncover competing mechanisms of reactant activation.

In the second example, SGD is applied to understand and design novel catalysts for oxygen evolution reaction (OER) based on transition-metal-organic frameworks (Figure 1) [2]. Based on physical understanding of SGD subgroups, we demonstrate why only a combination of material's features can result in good catalytic performance in case of complex reactions with several intermediates. The design strategy discovered by AI allowed us to find an exceptionally efficient catalyst whose performance and stability were confirmed experimentally.

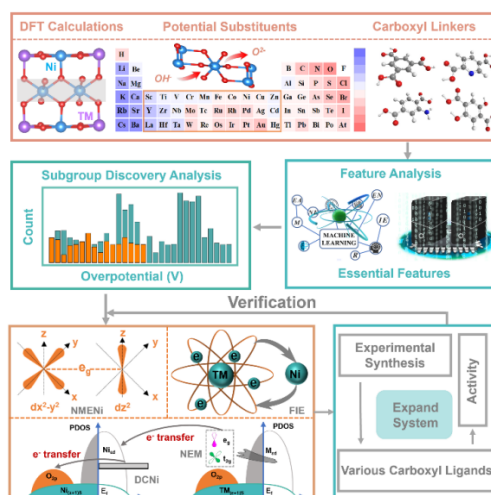


Figure 1. The data-driven approach to the design of novel OER catalysts based on transition-metal-organic frameworks.

### References

[1] A. Mazheika et al., Nature Comm., 13 (2022) 419. [2] J. Zhou et al., Angewandte Chemie International Edition, e202409449



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## Designing high-voltage and high-power cathode materials for Na-ion batteries

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The targeted design of new high-energy, high-power and long-life cathode materials is critical for forthcoming widespread commercialization of the sodium-ion battery (SIB) technology. Various polyanion families of positive electrode materials including the benchmark fluoride-phosphate  $\text{Na}_3\text{V}_2(\text{PO}_4)_2\text{F}_3$  are considered in competition with oxides, with both classes still have room for improvement.

We have contributed to the development of polyanion electrodes by offering promising positive electrode materials designed via combining a beneficial  $\text{NaVPO}_4\text{X}$  ( $\text{X} = \text{O}, \text{F}$ ) chemical composition and a unique  $\text{KTiOPO}_4$ -type structural framework [1] which was realized by a facile low-temperature hydrothermally-assisted solid-state ion exchange approach. The fluorine-containing representative,  $\text{NaVPO}_4\text{F}$ , outperforms many renowned Na-based cathodes revealing high-energy and high-power electrochemical behavior with  $136 \text{ mAh g}^{-1}$  (95% of the theoretical capacity, at C/10) at  $\sim 4.0 \text{ V}$  vs.  $\text{Na}^+/\text{Na}$  and  $123 \text{ mAh g}^{-1}$  at 40C (Figure 1a,b), and unlocking the practical specific energy of  $540 \text{ Wh kg}^{-1}$  setting a benchmark for polyanion Na-ion battery positive electrodes [2].

The oxygen-based counterpart, a new  $\text{NaVOPO}_4$  polymorph adopting a  $\text{KTiOPO}_4$ -type framework, presents as a promising high-rate, low-strain and long-life positive electrode material for SIBs. The electrochemical performance of  $\text{NaVOPO}_4$  is evaluated through galvanostatic charge/discharge tests, cyclic voltammetry, potentiostatic intermittent titration and electrochemical impedance spectroscopy. Carbon-coated  $\text{NaVOPO}_4$  demonstrates a specific capacity of  $\sim 110 \text{ mAh g}^{-1}$  at a C/10 rate and an average potential of  $\sim 3.93 \text{ V}$  vs.  $\text{Na}^+/\text{Na}$  (Figure 1c). The material exhibits decent capacity retention and rate capability, retaining over 74% of the initial capacity after 1000 cycles at C/2 and around 87% at a 2C charge/discharge rate [3].

The crystal structure of both materials is refined based on synchrotron X-ray powder diffraction data and validated by X-ray absorption spectroscopy, transmission electron microscopy and density functional theory (DFT) calculations. Diffusion coefficients of  $10^{-11} \text{ cm}^2 \text{ s}^{-1}$  and DFT-calculated energy barriers of  $\sim 0.15\text{-}0.35 \text{ eV}$  indicate fast  $\text{Na}^+$  ion diffusion within the  $\text{NaVPO}_4\text{X}$  framework. The vanadium oxidation state and charge compensation mechanism are studied by X-ray absorption spectroscopy and DFT. Moreover, the *operando* X-ray powder diffraction analysis coupled with DFT elucidated different de/intercalation mechanisms depending on X. Overall,  $\text{NaVPO}_4\text{X}$  exhibit attractive electrochemical performance and stability as potential candidates for sodium-ion battery cathode materials.

In the talk, the peculiarities of synthesis, structure, composition and electrochemical performance will be highlighted in detail with a special attention to synthesis-structure-properties relationships.

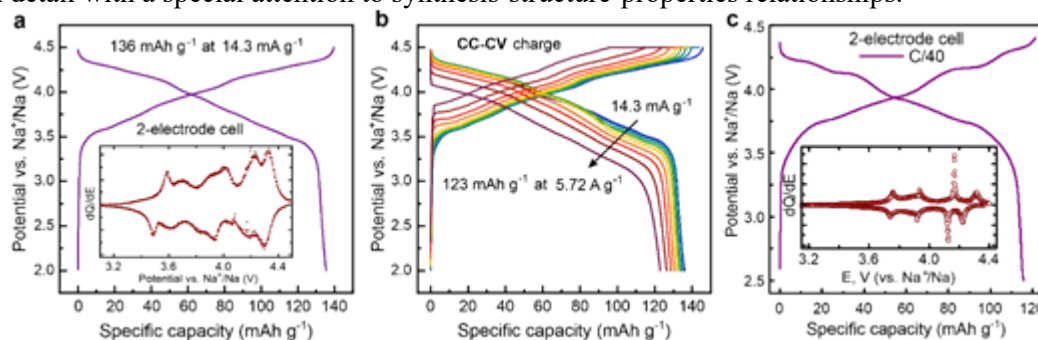


Figure 1.  $\text{NaVPO}_4\text{X}$  electrochemical performance: galvanostatic curves for  $\text{X} = \text{F}$  (a) and  $\text{X} = \text{O}$  (c), C-rate capabilities for  $\text{X} = \text{F}$  (b).



The 12<sup>th</sup> International Conference on Nanomaterials and Advanced Energy Storage Systems (INESS - 2024)

### References

- [1] S. S. Fedotov, A. Sh. Samarin, E. V. Antipov. *J. Power Sources* 480 (2020) 228840
- [2] S. D. Shraer, N. D. Luchinin et al. *Nat. Commun.* 13 (2022) 4097.
- [3] S. D. Shraer, A. D. Dembitskiy et al. *Energy Storage Mater.* 68 (2024) 103358

## **Toward Initially Chargeable Aqueous Zn Ion Batteries with High Energy Density and Long Cycle Life**

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As renewable energy is expected to expand under the 2050 carbon neutral roadmap policy, the importance of energy storage systems(ESS) is being highlighted to stabilize the power grid. Especially as an alternative for electrochemical ESS technology with MWh scale and long-term applications, aqueous Zn-based rechargeable batteries have become the most promising energy storage system due to their ultimate safety and low cost. Early endeavors involved promising materials for initially dischargeable aqueous batteries. Despite these efforts, these materials encounter significant challenges, primarily in terms of energy density and cost, due to their intrinsic cell configuration including the limited cell voltage, the use of excessive Zn anode and thick separator.

Recognizing these limitations, new concepts of initially chargeable battery technology that can break through these fundamental limitations are proposed . To address these practical limits of current aqueous rechargeable batteries, we have been coming up with conceptual designs for Zn-containing cathode with multiple reactions, anode-free or thin Zn anode, aqueous electrolytes with high potential window and cellulose-based separator with ultra-low cost, by forming a consortium with nine organizations under the support of KEPCO in early 2023.

In this talk, recent research progresses of the consortium including the exploration of new Zn-containing cathode materials through simulation-based screening, synthesis, and verification of properties, plasma-based high-speed synthesis of metal oxide nanomaterials, anode-free or thin Zn anode technology with surface stabilization for the zinc anode, design of a protective film with low-dimensional piezoelectric materials, ultra-thin Zn alloys seed layer on current collector and analysis of large area zinc metal anode will be presented. Additionally, aqueous electrolyte composition with high potential windows through screening additive/co-solvent, low-cost polymer-based hydrogel electrolytes using inorganic salts and natural cellulose-based separators will also be provided.



The 12<sup>th</sup> International Conference on Nanomaterials and Advanced Energy Storage Systems (INESS - 2024)

## Recent Achievements In Nanoscience & Nanotechnology

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Nanotechnology is an interdisciplinary field that has emerged in the global science and technology arena over the past 30 years. It focuses on the study of objects ranging in size from 0.1 to 100 nanometers, encompassing a wide range of interdisciplinary connections across physics, chemistry, and biology. Nanotechnology enables the creation, study, and manipulation of objects at the nanometer level, offering new opportunities for developing materials with unique properties and improving fields such as electronics, medicine, energy production, and the environment. Its development is contributing significantly to human progress by providing new tools to address global challenges.

An analysis of the current state and trends of development in the field of nanotechnology leads to the conclusion that the most promising area of research is the synthesis, study, and application of carbon-based nanomaterials. Carbon nanomaterials are particularly intriguing due to their exceptional physicochemical and mechanical properties, as well as their potential for a wide range of applications. The unique properties of carbon-based nanomaterials make them highly desirable for advancements in various technological fields.

In Kazakhstan, the research in the field of nanotechnologies and nanomaterials have been conducted for more than 30 years at al-Farabi Kazakh national University as well as at the Institute of Combustion Problems, Institute of Physics and Technology, and Nazarbayev University.

The original results on development of carbon nanomaterials of different functional application which were obtained. This paper presents original results on the development of a technology for producing carbon nanomaterials for various applications:

- 1) Preparation of aerogels based on nanostructured materials (CNTs, graphene oxide, MWCNTs);
- 2) Supercapacitors based on carbon nanomaterials;
- 3) Synthesis and application of membrane technology for desalination of seawater;
- 4) Synthesis and application of carbon nanofibers obtained by electrospinning;
- 5) Nanostructured carbon materials for biomedical use.
- 6) Formation of soot and synthesis of fullerenes and carbon nanotubes in flame;

This thesis is intended to present the latest and most cutting-edge developments achieved by the Institute of Combustion Problems in the fields of combustion and the production of nanomaterials designed for diverse applications. Through a comprehensive exploration of the innovative research and advancements made, this thesis aims to shed light on the Institute's contributions to the advancement of combustion science and the utilization of nanomaterials in several practical and technological domains.



## Sustainable fuel components production from waste cooking oils using Ni-Mo bimetallic ZSM-23 supported catalysts

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Currently, a significant problem attracting the attention of the scientific community is climate change caused by anthropogenic emissions of greenhouse gases, in particular CO<sub>2</sub>. A significant share of CO<sub>2</sub> emissions falls on the transport sector, where the aviation industry demonstrates the highest growth rate of this indicator, which necessitates the development of sustainable energy in this area. A promising option is sustainable aviation fuel (SAF) obtained from alternative feedstocks, which has a neutral carbon footprint and satisfy the standards for traditional aviation fuels, which in the future will reduce the dependence of the transport sector on fossil raw materials [1]. Vegetable oils and animal fats can act as alternative feedstocks; a promising option is using waste cooking oil (WCO) obtained during the heat treatment of food, due to its low cost and high availability. SAF can be obtained from WCO by its catalytic deoxygenation (DO) and subsequent isomerization [2, 3]. Thus, an important task is to develop appropriate catalytic systems that allow obtaining high-quality components of SAF. It is known that activation of oxygen-containing molecules occurs on metal centers, and isomerization occurs on acid centers. The catalysts in the DO process can be transition metals or their sulfides, and noble metals deposited on various acidic carriers [4]. However, sulfide catalysts tend to lose sulfur due to its oxidation in the process and, as a result, contamination of products with sulfur-containing substances, which is unacceptable in the case of aviation fuel. The use of noble metal-based catalysts, in turn, is difficult due to their high cost [2]. Thus, catalysts based on transition metals, in particular nickel and/or molybdenum, are of increasing interest. Zeolites are widely used as carriers due to their developed surface, thermal stability, and shape selectivity due to the molecular sieve effect.

In this study, a series of Ni-Mo catalysts supported on ZSM-23 were investigated. The catalysts were prepared using a sequential impregnation method, where Ni and Mo were added separately, or by impregnating the support with aqueous, citrate, and ammonia solutions containing both Ni and Mo salt precursors simultaneously. After impregnation, the samples were dried at 120°C (1 hour) and then calcined at 550 °C for 2 hours before being tested for activity in a hydrogen flow at 550 °C for one hour. The prepared samples were studied by plenty technique: XRD, XPS, FTIR, UV-Vis, Raman spectroscopy etc. in oxide and reduced form. The activity of these catalysts was evaluated in the hydrotreating of a mixture of fatty acids (from C16 to C18) in a flow type reactor with a fixed bed catalyst layer at 300 °C, pressure of 25 atmospheres, and WHSV = 8.5 h<sup>-1</sup>. The main products resulting from the conversion of the fatty acid mixture were normal and isoparaffins, including components of diesel and jet fuel. The Ni-Mo/ZSM-23 catalyst, prepared by impregnating ZSM-23 with a joint solution of ammonia Ni and Mo salts, demonstrated excellent activity and stability during the hydrotreating process of a fatty acid mixture. The increased activity of this catalyst may be attributed to the formation of the active Ni-Mo component. Thus, in the case of an ammonia impregnation solution, the formation of monomolybdate forms [MoO<sub>4</sub>]<sup>2-</sup> was observed in the solution, while in the case of other impregnation solutions, the formation of polymolybdates [Mo<sub>7</sub>O<sub>24</sub>]<sup>6-</sup>, [Mo<sub>8</sub>O<sub>26</sub>]<sup>6-</sup> (or in case of citrate solution it could be Mo<sub>4</sub>(cit)<sub>2</sub>O<sub>11</sub><sup>4-</sup>) were observed by Raman spectroscopy. That could be the reason of different Ni-Mo phases formation in oxide and reduced form. The NiO and NiMoO<sub>4</sub> phases were detected in the case of the samples in oxide form by XRD technique. For the next step, the Mo/(Ni+Mo) ratio of catalysts prepared using an ammonia solution of metal precursors was studied. The most promising catalysts for isomerizing alkanes production were those with a ratio of 0.25 and 0.4. The influence of process parameters on product yield was also studied (temperature, H<sub>2</sub>/raw material ratio, WHSV etc.). Interestingly that changing of the H<sub>2</sub>/raw material ratio from 2000 m<sup>3</sup>/m<sup>3</sup> to 3150 m<sup>3</sup>/m<sup>3</sup> increased the yield of isoalkanes for both catalysts by 11-35 mwt.% for the catalyst with a 0.25 Mo/(Ni+Mo) ratio and 3.5–56% for catalysts with a 0.4 Mo/(Ni+Mo). A catalyst with a Mo/(Ni+Mo) ratio of 0.4 was also studied in a long-term experiment to assess its stability and the yield of isoalkanes over time.



### Acknowledgements

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### References

- [1] J. I. C. Lau, Y. S. Wang, T. Ang, J. C. F. Seo, S. N. B. A. Khadaroo, J. J. Chew, A. N. K. Lup, J. Sunarso, Biomass and Bioenergy, 186 (2024) 107277.
- [2] A. A. Hebish, N. W. M. Zulkifli, N. M. Julkapli, M. Fazly, A. Patah, Applied Catalysis O: Open, 190 (2024) 206926.
- [3] M. Głównka, J. Wójcik, P. Boberski, T. Bialecki, B. Gawron, M. Skolniak, T. Suchocki, Renewable Energy, 220 (2024) 119696.
- [4] M. R. Khodadadi, I. Malpartida, C. W. Tsang, C. S. K. Lin, C. Len, Molecular Catalysis, 494 (2020) 111128.

## AI-driven self-powered triboelectric sensors for healthcare and robotics applications

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Highly accurate sensors have become increasingly important in robotics, AI, digital health, and IoTs. Portable health devices, smart homes, gas sensors, and autonomous robotics vehicles are only part of applications that heavily rely on sensors. Thus, sensors are essential transformers of surrounding data in modern digital life [1]. The triboelectric effect is the phenomenon in which a material becomes electrically charged as it contacts a different material through friction, and it has been known for thousands of years. Although this is one of the most frequently experienced effects we inevitably see daily, the mechanism behind triboelectrification is still being studied, possibly with debate. The application of this effect in energy harvesting was invented in 2012 by Wang et al. [2]. It is generally believed that when two different materials come into contact, a chemical bond is formed between some parts of the two surfaces, called adhesion, and charges move from one material to the other to equalize their electrochemical potential. The transferred charges can be electrons or may be ions/molecules. When separated, some of the bonded atoms keep extra electrons, and some tend to give them away, possibly producing triboelectric charges on the surfaces. The presence of triboelectric charges on dielectric surfaces can be a force for driving electrons in the electrode to work to balance the electric potential drop created. Examples of materials that are used as triboelectric sensors and powered by their triboelectric properties include Kapton, silicone rubber, polytetrafluoroethylene (PTFE) films, chitosan, polyaniline (PANI) and polydimethylsiloxane (PDMS).

In this study, we will discuss the application of self-powered TENG sensors in robotics and healthcare applications with AI integration to make them smart sensing systems.

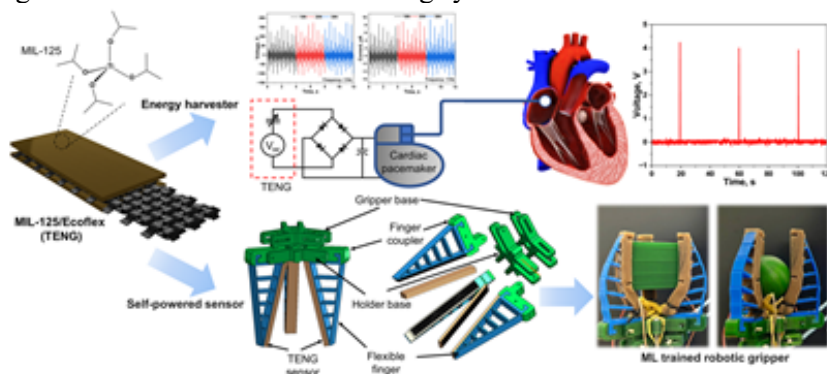


Figure 1. TENG sensor for robotic grippers.





### Acknowledgments

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### References

- [1] A. Kakim, A. Nurkesh, B. Sarsembayev, D. Dauletiya, A. Balapan, Z. Bakenov, A. Yeshmukhametov, G. Kalimuldina, *Adv. Sensor Research*, (2024).  
[2] Song et al., *Nano Energy* 84, 105919 (2021).

## Enhancing gas-sensing performance of TZO sensors through Intensely Pulsed Ion Beam (IPIB) technique

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In this study, the application of the Intensely Pulsed Ion Beam (IPIB) technique [1] has been shown to effectively enhance the gas-sensing properties of TZO-based sensors. The research reveals that IPIB irradiation significantly alters the surface morphology and crystalline structure of TZO nanostructures, resulting in improved sensitivity and selectivity to NO gas compared to other gases such as CO, CO<sub>2</sub>, NO<sub>2</sub>, ethanol, methane, and acetone. A comparative analysis of TZO, *a*TZO, and *i*TZO samples demonstrates that IPIB treatment increases the roughness and porosity of TZO films and induces beneficial lattice defects and oxygen vacancies. These modifications contribute to a substantial increase in gas response, particularly for NO gas, where the *i*TZO sensor shows an approximate 1300% increase in response at an optimal temperature of 200 °C. This significant enhancement highlights the potential of IPIB as a powerful tool for improving the performance of MOS-based gas sensors [2,3]. Additionally, stability tests conducted over a year indicate that *i*TZO sensors maintain their enhanced sensitivity with minimal degradation, suggesting that the improvements from IPIB irradiation are durable and effective for long-term applications. This durability is essential for developing reliable and efficient gas sensors for environmental monitoring and industrial applications. Our research underscores the significant benefits of using ion beam techniques like IPIB for targeted modification of gas sensor materials. The precise control over ion dose and energy allows for optimization of sensor characteristics, paving the way for the next generation of highly sensitive and selective gas sensors. The findings of this study provide valuable insights into the material science of gas sensors and open new possibilities for further research in sensor technology enhancement.

### Acknowledgements

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### References

- [1] Kaikanov, Marat, et al. "Investigation of intense pulsed ion beam generation by a magnetically insulated ion diode at a reduced impedance." *Vacuum* 217 (2023): 112496.  
[2] Yergaliuly, G., Soltabayev, B., Kalybekkyzy, S., Bakenov, Z., & Mentbayeva, A. (2022). Effect of thickness and reaction media on properties of ZnO thin films by SILAR. *Scientific reports*, 12(1), 851.  
[3] Soltabayev, B., Yergaliuly, G., Ajjaq, A., Beldeubayev, A., Acar, S., Bakenov, Z., & Mentbayeva, A. (2022). Quick NO gas sensing by Ti-doped flower-rod-like ZnO structures synthesized by the SILAR method. *ACS applied materials & interfaces*, 14(36), 41555-41570.



The 12<sup>th</sup> International Conference on Nanomaterials and Advanced Energy Storage Systems (INESS - 2024)

## Deep eutectic solvent supported quaternized chitosan head groups for anion exchange membranes: insight from atomistic modeling

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The instability of quaternized chitosan (QCS) head groups and the limited diffusion of hydroxide (OH<sup>-</sup>) ions under alkaline pH and high temperatures present significant challenges in alkaline anion exchange membrane (AEM) technology. To tackle this challenge, we study how QCS head groups interact with OH<sup>-</sup> ions in the presence of water and Deep Eutectic Solvents (DES) to enhance chemical stability and improve OH<sup>-</sup> ion diffusion in AEMs [1-3]. Our study utilized Density Functional Theory (DFT) calculations and ab initio Molecular Dynamics (MD) simulations to explore the chemical instability of QCS head groups and OH<sup>-</sup> ion diffusion with choline chloride and ethylene glycol-based DES.

According to DFT, the degradation of head groups begins with ylide formation (YF) and is followed by nucleophilic substitution (S<sub>N</sub>2) in the absence of DES. Ab initio MD simulations showed that without DES, YF was the primary degradation pathway at different hydration levels (HLs) like 1 and 3, at 298 K, while S<sub>N</sub>2 prevailed at HL 3 and temperatures of 320 K and 350 K. Nevertheless, DFT and ab initio MD studies showed that the addition of DES improved the chemical stability of head groups. Afterward, it was discovered that incorporating DES resulted in comparable diffusion behavior of OH<sup>-</sup> ions through QCS head groups at various HLs and temperatures, when compared to scenarios without DES.

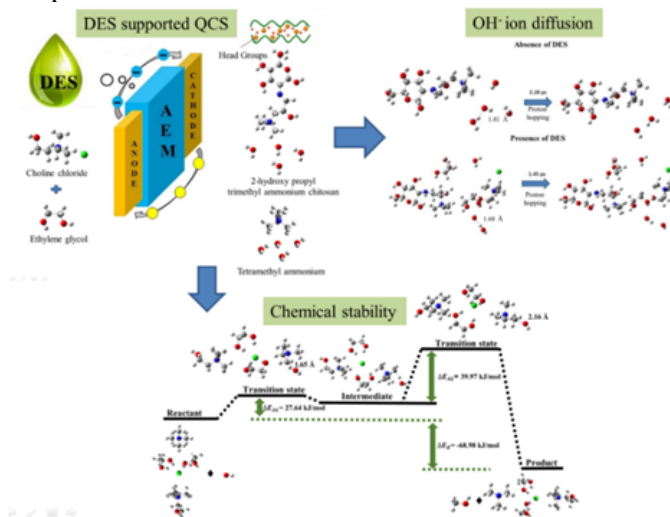


Figure 1. Degradation mechanism and OH<sup>-</sup> ion diffusion for DES supported QCS head groups in AEM.

### Acknowledgments

This work was supported by the research grant AP14869880 titled “Deep eutectic solvent supported polymer-based high performance anion exchange membrane for alkaline fuel cells”, which has been sponsored by MES RK (2022-2024).

### References:

- [1] E. L. Smith, A. P. Abbott, K. S. Ryder, *Chemical Reviews*, 12 (2014) 11060-11082.
- [2] S. Castaneda, R. Ribadeneira, *The Journal of Physical Chemistry C*, 119 (2015), 28235-28246.
- [3] T. Zelovich, L. Vogt-Maranto, M. A. Hickner, S. J. Paddison, C. Bae, D. R. Dekel, M. E. Tuckerman, *Chemistry of Materials*, 31 (2019) 5778-5787.





## Structural effects in cathodic electrocatalysts with complex nanoscale morphology

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Increasing complexity of nanosynthesis has produced a variety of intricate nanoparticle shapes which have attracted significant attention for applications in electrocatalysis. These complex nanoelectrocatalyst shapes not only introduce high surface areas and high energy active sites, but also improve electrocatalytic performance by altering electric field at the surface thereby concentrating reagents and accelerating electrocatalysis. Some aspects of nanoelectrocatalyst structural complexity remain poorly understood and difficult to predict, such as confinement effects and long-term structural stability necessary for industrial implementation. Here, we study structural performance and stability in cathodic reactions (hydrogen evolution reaction and carbon dioxide reduction to syngas) of noble metal nanoparticles with star- and core-cage structures that collectively cover major structural nanoscale features including extrusions, holes, voids, and nanogaps. In addition to the structural and surface analysis, we employ density functional theory and finite element method calculations to demonstrate that uneven electric field and current density distributions in these morphologies influence metal mobility resulting in their structural degradation (Figure 1) [1]. Our results revealed that extrusions and holes facing the anode form electric field hot spots for electrolysis, that can also facilitate surface reconstruction. The holes and voids perpendicular to the direction facing the anode form current crowding spots within the metal that facilitate electromigration, while being blind spots for electrolysis due to low local electric field in these areas. The material of the catalytic particles strongly influences the extend of structural degradation, e.g., gold structures was found to noticeably reconstruct over time while palladium structures were stable for extended time. Finally, our more recent findings show that structural features within nanocages could be electrically shielded by tuning their dimensions and the surrounding electrolyte composition resulting in them being blind spots for both electrolysis and electromigration. This work provides guidelines for the structural design of electrocatalysts, highlighting that it should not only be dictated by the surface atomic organization and the generation of electric field hotspots, but also by current distribution within the electrode itself, to ensure high material performance and improved stability.

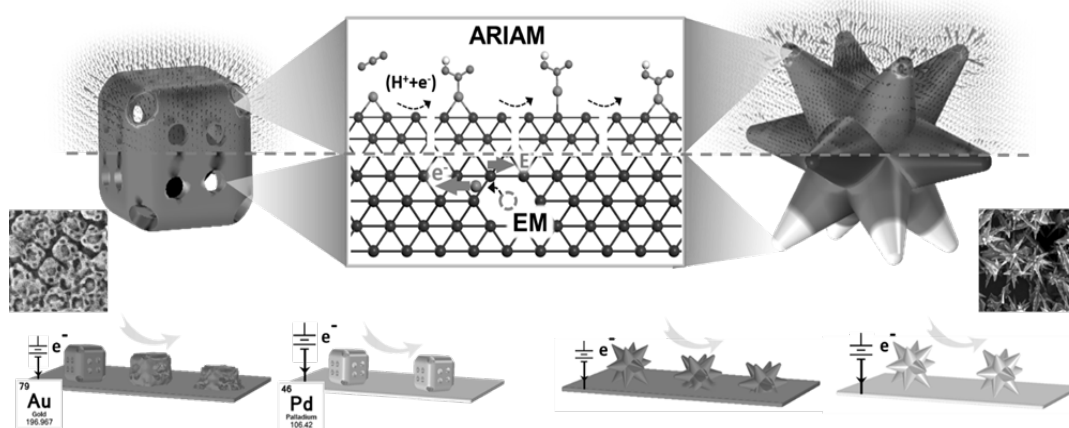


Figure 1. Complex shape transformations during electrocatalysis and associated atomic mechanisms: adsorbed reaction intermediates-facilitated atomic mobility through local electric field (ARIAM) and electromigration due to current crowding (EM).

### References

[1] F. Li, X. V. Medvedeva, J. J. Medvedev, E. Khairullina, H. Engelhardt, S. Chandrasekar, Y. Guo, J. Jin, A. Lee, H. Thérien-Aubin, A. Ahmed, Y. Pang, A. Klinkova *Nature Catalysis* 4 (2021), 479–487.



## Boosting Energy Density with Novel Fluorinated Electrolyte Formulations

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The exceptional stability of fluorinated compounds, arising from the high bond dissociation energy of the C–F bond (the strongest in organic chemistry), makes them inherently non-flammable and highly resistant to degradation, including oxidation.<sup>1</sup> These properties are particularly advantageous for electrolyte components in demanding applications like high-voltage lithium-ion and lithium-metal batteries, where they can contribute to increased energy density.<sup>2,3</sup>

We have developed novel electrolyte systems based on fluorinated ethers and esters. These electrolytes exhibit remarkable stability, enabling lithium-ion and lithium-metal batteries to operate at voltages up to 4.5 V for hundreds of cycles. This represents a significant advancement over conventional carbonate electrolytes, which are limited to operating voltages of 4.3 V (Fig. 1).

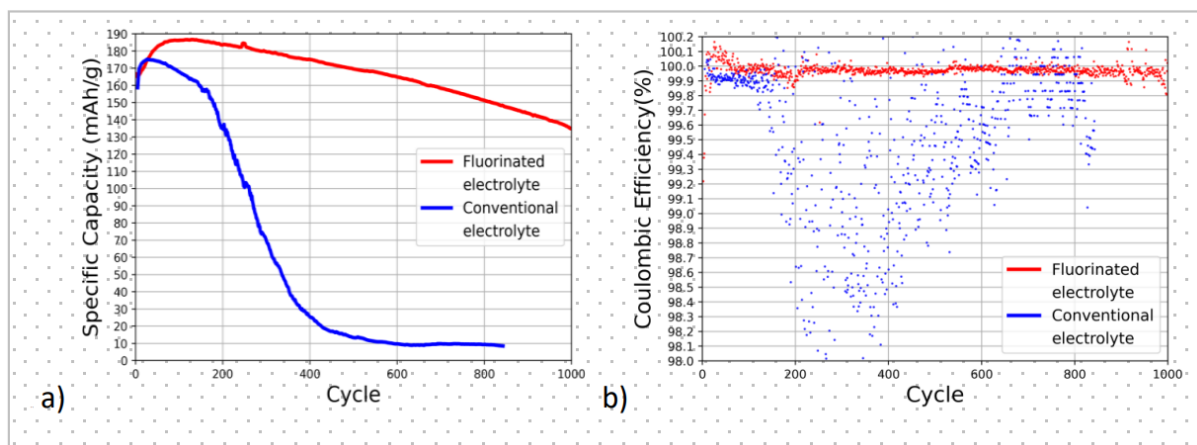


Figure 1. Comparison of electrochemical performances of full-cell NMC811||Graphite with conventional carbonate-base electrolyte (up to 4.5V) and with fluorinated electrolyte (up to 4.5V), 1000 cycles 1C rate: a)–Specific Capacity/Cycle; b)–Coulombic Efficiency/Cycle.

To evaluate their practical application, we incorporated these fluorinated electrolytes into pouch cells with a graphite||NMC811 configuration. By raising the cut-off voltage, we observed a 10-15% increase in specific capacity and energy density of the cathode material without compromising battery performance.

### References

[1] D. O'Hagan *Chem. Soc. Rev.*, 37 (2008), 308–319. [2] N. von Aspern, G.-V. Ręschenthaler, M. Winter, I. Cekic-Laskovic *Angew. Chem. Int. Ed.*, 58 (2019), 15978–160



## Electrolytes for sodium-ion batteries with metal anode

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Lithium-ion batteries (LIBs) are widely used for energy storage, but the increasing demand for portable electronics necessitates the development of more affordable and sustainable battery technologies. Sodium-ion batteries (NIBs) emerge as a promising alternative due to their lower cost and comparable performance to LIBs.

While metal anodes offer higher specific capacity in SIBs, conventional carbonate electrolytes fail to provide stable cycling performance. This research focuses on developing electrolyte systems compatible with p-metal binder-free anodes (lead, tin, and bismuth) for NIBs. A comprehensive screening of ethers (Fig. 1) was conducted to identify suitable electrolyte components for NIBs.

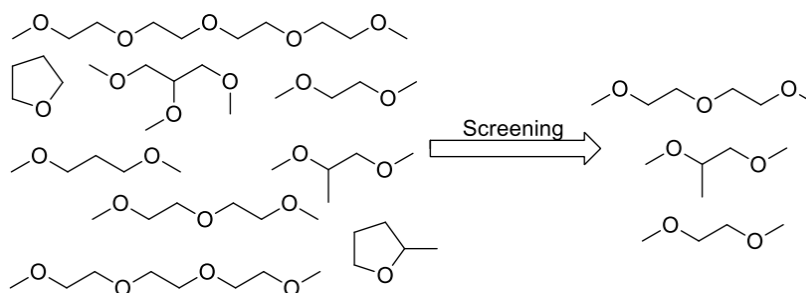


Figure 1. Structural formulas of the studied organic solvents.

The newly developed electrolyte systems demonstrated exceptional performance in Na||Metal half-cells and full cells with the configuration Metal||Na<sub>3</sub>V<sub>2</sub>(PO<sub>4</sub>)<sub>3</sub>. The proposed electrolytes achieved up to The batteries exhibited remarkable capacity retention (up to 91.5% capacity retention after 1000 cycles), Coulombic efficiency (99.95%), indicating long-term stability and efficient charge storage. Also, it is worth to note that such electrochemical systems can be used at subzero temperatures.

### References

- [1] Y. Li, F. Wu, Y. Li, M. Liu, X. Feng, Y. Bai, C. Wu Chem. Soc. Rev. 51 (2022) 4484-4536.

## Defect regulation and mechanism elucidation of lignin based carbon anode materials for K-ion batteries

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Due to their abundant potassium resources, potassium ion batteries are potential next-generation rechargeable alkali metal ion batteries. Carbon-based materials are the most promising negative electrode materials for potassium ion batteries due to their low embedding/deintercalation potentials, high capacity and stability. The conventional graphite electrode has a low theoretical capacity (KC<sub>8</sub>, 278 mAh/g) and a large volume change (61%) during the K-intercalation process, so its application is limited.

Amorphous carbon materials have large layer spacing and abundant defect structure, which can break through the theoretical capacity limit of graphite (>300 mAh/g), and are potential carbon anode materials for



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potassium ion batteries [1]. Pyrrolic nitrogen and pyridinic nitrogen exist at the edge defects of carbon materials and are considered to be effective K-storage active sites. We have previously developed a series of methods for constructing edge nitrogen structured carbon materials and prepared ultra-high nitrogen doped carbon materials. However, the aggregation structure of lignin is difficult to achieve high nitrogen doping. We proposed a supermolecule-regulated strategy for the aggregation state of biomolecules [2,3]. The aggregation of lignin molecules is disrupted and dispersed in supramolecules through intermolecular interactions between lignin and supramolecules. High nitrogen doping (21 at.%) is achieved at the molecular level, and the capacity of potassium storage is improved (420 mAh/g).

The turbostratic and distorted graphene layers of amorphous carbon hinders the diffusion of  $K^+$ . Lignin is difficult to achieve graphitization by regulating temperature. We proposed a general strategy for fabricating hard carbon materials with local graphitic nanodomains by using graphene oxide [4]. Aminated lignin and graphene oxide are uniformly assembled through electrostatic attraction. During pyrolysis and carbonization, the graphite structure induces the growth of local graphite nanodomains in lignin based carbon. This strategy obtains hard carbon with local graphite domains and large interlayer spacing, achieving a lower voltage platform and voltage hysteresis for potassium storage. Further, we studied the reasons for the failure of hard carbon anode during potassium storage [5]. The potassium ion storage process and interface properties of hard carbon in ether- and ester-based electrolytes were demonstrated using a series of ex-situ testing techniques. That clarifies the failure mechanism of hard carbon caused by solvent co-intercalation. The above research opens a new avenue for the development of carbon based negative materials for potassium ion batteries.

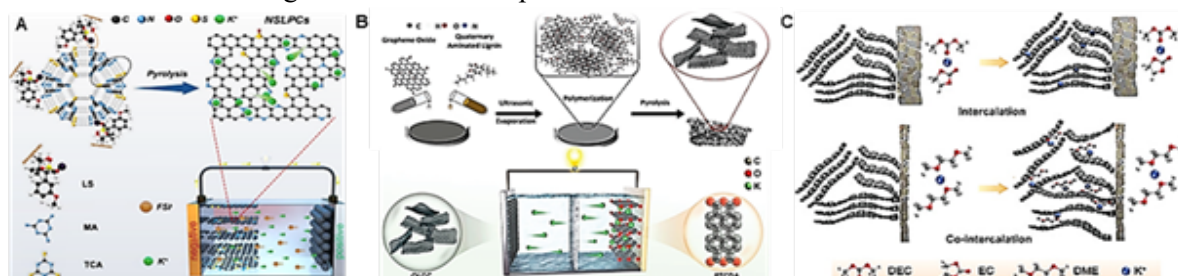


Figure 1. (A) Schematic illustrating the synthesis process of the ultra-high nitrogen doped carbon, (B) Schematic illustration of the synthesis process for hard carbon with local graphitic lattice, (C) Schematic illustration of  $K^+$  intercalation and co-intercalation of  $K^+$  ions and solvents of HC in ester and ether-based electrolytes.

### References

- [1] Yin, J.; Alshareef, H.; Zhang, W. *Angew. Chem. Int. Ed.* **2023**, *62*(17), e202301396.
- [2] Zhao, L.; Alshareef, H.; Qiu, X.; Zhang, W. *Nano-Micro Lett.* **2023**, *15*, 41.
- [3] Zhong, L.; Qiu, X.; Yang, S.; Sun, S.; Chen, L.; Zhang, W. *Energy Storage Mater.* **2023**, *61*, 102887.
- [4] Zhong, L.; Zhang, W. Alshareef, H.; Qiu, X. *Adv. Funct. Mater.* **2022**, *33*(8), 2211872.
- [5] Jian, W.; Qiu, X.; Zhang, W. *Adv. Energy Mater.* **2023**, *13*(43), 2301303.

## ZnO-based composite material for gas sensor application

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The matter of air pollution has dramatically raised worldwide concern about detecting hazardous gases in the atmosphere. Additionally, the detection and monitoring of such gases is necessary for process control in the industry as well as the general safety of the environment. ZnO is an n-type semiconductor with a wide direct bandgap width (3.37 eV), high excitation binding energy (60 meV), high electron mobility, thermal stability, and excellent electrical properties



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[1]. The materials that are of intense research interest are conducting polymers such as polyaniline (PANI), polypyrrole (PPy), and poly(3,4-ethylenedioxythiophene) (PEDOT) used in the fabrication of polymer-based gas sensors [2]. polymers in combination with metal oxides capable of working at low temperatures maintaining high sensitivity gases. Therefore, composite materials attract in terms of energy saving as they do not need an additional source of heat, consequently reducing the operating cost, simplifying the fabrication process, and extending the lifetime of the device. In this work, ZnO intercalated PVA-PEDOT:PSS composite fiber as a sensing material was electrospun. The material was characterized both morphologically and structurally by X-ray diffraction analysis, scanning electron microscopy, transmission electron microscopy, Fourier-transform infrared spectroscopy, and thermogravimetric analysis. The results from TEM and SEM show the well distribution of ZnO particles in the polymer matrix. The gas sensing results reveal that the fabricated ZnO-based composite materials exhibit a high response to 100 ppm NH<sub>3</sub> gas at 120°C. The characterization and evaluation of the fabricated composite material presented in this study provide valuable information for the design and development of high-performance gas sensors. The synergistic effects observed between different materials in the composite matrix open up new opportunities to improve sensor performance and reliability, paving the way for future advances in sensor technology.

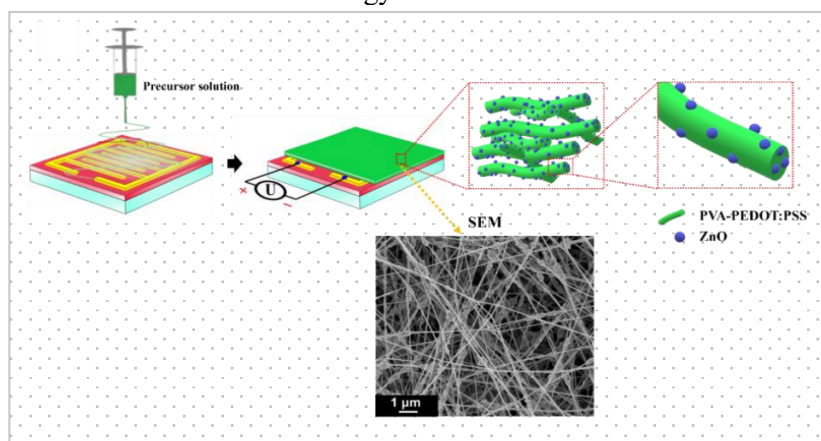


Figure 1. Graphical abstract

### References

- [1] V. S. Bhati, M. Hojamberdiev, and M. Kumar, "Enhanced sensing performance of ZnO nanostructures-based gas sensors: A Review," *Energy Reports*, vol. 6, pp. 46–62, 2020.
- [2] Conducting polymer-inorganic nanocomposite-based gas sensors: a review, Yan Yan, 2021.

## Application of graphene oxide-like activated carbon material as a sensing element for humidity sensors

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Currently, the prerequisite for developing a humidity sensor is that, despite the wide range of graphene-like materials available as raw materials, not all potentially applicable materials exhibit highly sensitive characteristics for sensing humidity over a wide range, as well as symmetrical response and recovery times [1-5]. Graphene oxide (GO) derived from activated carbon (AC) is particularly interesting due to its large specific surface area, high adsorption capacity, and the ability to produce structured free-standing membranes that are low-cost and do not require advanced technology for production. Therefore, these properties of the source material will meet the needs of consumers in various industries. The primary reason for creating a humidity sensor based on GO-AC is that the membrane has a smooth surface and a compact plate-like structure compared to the initial GO membrane, and the presence of a large number of functional oxygen-containing groups enhances its sensitivity to humidity. Additionally, the humidity sensor based on GO-AC has improved





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mechanical properties, and the synthesis of GO from AC provides a higher yield than synthetic graphite. This results in an economically efficient, profitable, and high-quality membrane for humidity sensor production.

In this work, we have developed a method for manufacturing an ultra-sensitive, simple, and low-cost humidity sensor from GO-AC. This sensor operates in a wide range of relative humidity (5-95%), has symmetrical signal response times, and maintains a high degree of stability (+/- 2%). The results of testing the sensor for the stability of electrical resistance at various humidity levels (20-95%) over 10 hours of constant humidity showed that with increasing relative humidity, the electrical resistance of the humidity sensor decreases by approximately 3-4 orders of magnitude. This confirms the sensitivity of the GO-BAU membrane to relative humidity. The physicochemical properties of this material were studied using IR spectroscopy, SEM, sorption properties, XRD, BET, XPS and moisture resistance.

### References

- [1] F. Schedin, A. K. Geim, S. V. Morozov, E. W. Hill, P. Blake, N. I. Katsnelson and K. S. Novoselov (2007) Detection of Individual Gas Molecules Adsorbed on Graphene. *Nature Materials*, 6, 652-655.
- [2] Tilek Kuanyshbekov,\* Nazim Guseinov, Zhandos Tolepov, Bayan Kurbanova, Malika Tulegenova, Kydyrmolla Akatan, Nurgamit Kantay, and Elzhas Zhasasynov., Thermally Reduced Graphene Oxide Membranes From Local Kazakhstan Graphite “Ognevsky”, *ChemistrySelect*, 2023, 8, e202301746, 1 – 13, <https://doi.org/10.1002/slct.202301746>.
- [3]. T. Kuanyshbekov, Z. Sagdollin, E. Zhasasynov, K. Akatan, B. Kurbanova, N. Guseinov, Z. Tolepov, N. Kantay, M. Beisebekov, Composite membrane based on graphene oxide and carboxymethylcellulose from local Kazakh raw materials for possible applications in electronic devices, *Journal of Composites Science*, 2023, 7, 342, doi: 10.3390/jcs7080342.
- [4]. Tilek Kuanyshbekov\*, Nazim Guseinov, Bayan Kurbanova, Renata Nemkaeva, Kydyrmolla Akatan, Zhandos Tolepov, Malika Tulegenova, Madi Aitzhanov, Elzhas Zhasasynov, Sabu Thomas. Local Natural Graphite as a Promising Raw Material for the Production of Thermally Reduced Graphene-Like Films. *Engineered Science*. 2024, 23, 1000, DOI:10.30919/esmm1000
- [5] T.K. Kuanyshbekov, K. Akatan, S.K. Kabdrakhmanova, R. Nemkaeva, M. Aitzhanov, A. Imasheva, E. Kairatuly (2021) Synthesis of Graphene Oxide from Graphite by the Hummers' Method. *J Oxidation Communications* 44(2):356–365

## Developing Nickel-Rich NCM Cathode Materials with One-Dimensional Structure for Lithium-Ion Batteries: Synthesis and Improving Cyclic Stability

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Lithium-ion batteries (LIBs) have become known as the most promising energy system because of their many applications in consumer electronics, including electric vehicles, computers, cell phones, and cameras, as well as their low cost, high energy density, and good performance [1]. From the perspective of cathode materials, layered LiMO<sub>2</sub> oxides, in which M is a combination of Ni, Mn, and Co – the so-called NCM – are gaining more and more attention and are thought to be a potential next-generation cathode material for LIBs because of their increased specific capacity (more than 150 mAh g<sup>-1</sup>) and thermal stability. In general, the chemical properties of LIBs are constantly changing. [2]. Furthermore, NCM-based cathodes have superior performance compared to the widely used lithium-iron-phosphate LiFePO<sub>4</sub> (LFP) cathodes in various domains, particularly concerning operating voltage. LFP-based LIBs are prone to producing voltages lower than 3.4 V and are associated with elevated rates of self-discharge. The composition of Ni, Mn, and Co can be significantly changed to optimize the capacity, performance, structural stability, and cost of lithium-ion batteries [3]. According to the findings,



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the B-doped NCM811 cathodes have a number of advantageous properties, such as better rate capability, greater capacity retention, and less mechanical strain when charged [4].

In this work, we primarily concentrate on the electrospinning method of producing 1D  $\text{LiNi}_{0.8}\text{Co}_{0.1}\text{Mn}_{0.1}\text{O}_2$  (NCM811) material and its improvement upon boron doping and morphological modifications. The electrospinning technique has already been used to obtain NCM material [5]. B-doped and undoped NCM811 nanofibers with the 1D structure were obtained by electrospinning method and characterized. The morphology and nanofiber structure of the resulting NCM811 samples (doped, un-doped) were studied using scanning electron microscope (SEM) and transmission electron microscope (TEM). X-ray phase analysis (XRD) studied the samples, and a series of peaks that entirely corresponded to the diffraction pattern of NCM811 were recorded. It is highly expected that the results may introduce some new ideas in the field of morphology modification and doping, which will be helpful for the rational design and manufacture of highly efficient cathode materials.

### Acknowledgments

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### References

- [1] J. Kim, H. Lee, H. Cha, M. Yoon, M. Park, and J. Cho, "Prospect and Reality of Ni-Rich Cathode for Commercialization," *Adv. Energy Mater.*, vol. 8, no. 6, 2018, doi: 10.1002/aenm.201702028.
- [2] H. Sun and K. Zhao, "Electronic Structure and Comparative Properties of  $\text{LiNi}_x\text{Mn}_y\text{Co}_z\text{O}_2$  Cathode Materials," *J. Phys. Chem. C*, vol. 121, no. 11, pp. 6002–6010, 2017, doi: 10.1021/acs.jpcc.7b00810.
- [3] Y. Xia, J. Zheng, C. Wang, and M. Gu, "Designing principle for Ni-rich cathode materials with high energy density for practical applications," *Nano Energy*, vol. 49, no. December 2017, pp. 434–452, 2018, doi: 10.1016/j.nanoen.2018.04.062.
- [4] C. H. Jung, D. H. Kim, D. Eum, K. H. Kim, J. Choi, J. Lee, ... & S. H. Hong, "New Insight into microstructure engineering of Ni-Rich layered oxide cathode for high performance lithium ion batteries," *Advanced Functional Materials*, vol. 31, no. 18, 2021, doi: 10.1002/adfm.202010095 2010095.
- [5] C. Lv, Y. Peng, J. Yang, X. Duan, J. Ma, and T. Wang, "Electrospun Nb-doped  $\text{LiNi}_{0.4}\text{Co}_{0.2}\text{Mn}_{0.4}\text{O}_2$  nanobelts for lithium-ion batteries," *Inorg. Chem. Front.*, vol. 5, no. 5, pp. 1126–1132, 2018, doi: 10.1039/c7qi00811b.

## Thermo Fisher Scientific STEM electron dose mitigation workflow for atomistic investigations of cathode materials

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$\text{LiCoPO}_4$  is a promising cathode material for the high voltage lithium-ion batteries. However, the moderate cycling stability of the material heavily limits its practical applications. The opportunity to stabilize the atomic structure of the material and improve the battery lifetime directly depends on the capability to gain knowledge on the degradation mechanisms through advanced characterization.

Cathode materials are obstinate candidates for TEM investigations due to their poor stability under the electron beam. Low electron dose should be applied in order to minimize radiolysis while imaging  $\text{LiCoPO}_4$ .

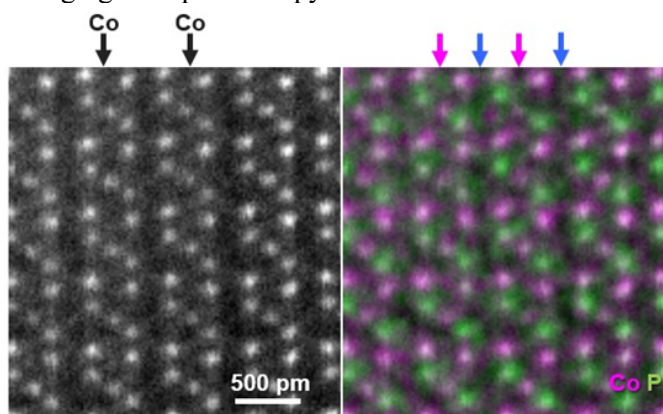
Here, we exploit simultaneous ADF-STEM and iDPC-STEM imaging to investigate the  $\text{LiCoPO}_4$  cathode material down to atomic scale, as iDPC-STEM allows for extremely low dose imaging of beam sensitive materials. By combining the experimental and simulation results a superstructure at the surface of the  $\text{LiCoPO}_4$  nanoparticle is revealed: every second Li site is partially occupied by higher Z-number atoms as periodic bright contrast is observed.



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To confirm the proposed superstructure, EDX spectroscopy at atomic resolution is performed. Figure 2 contains high resolution ADF-STEM image of the superstructure formed at the surface of the LiCoPO<sub>4</sub> nanoparticle viewed along the [001] zone axis and corresponding atomic resolution EDX elemental map showing Co in purple and P in green. It is clearly visible that indeed every other Li site (also highlighted by the arrows in Figure 2) is partially occupied by Co atoms.

To sum up, in this work we exploited atomic resolution low dose techniques to investigate beam-sensitive cathode battery material. A combination of both HR imaging and spectroscopy opens the doors to precise and trustful investigation of the cathode materials degradation at atomic scale. An example of LiCoPO<sub>4</sub> cathode material with the so-called antisite defects formation as one of the major degradation reasons helps to highlight the power of atomic resolution imaging and spectroscopy.



**Figure 2.** HR ADF-STEM image of the superstructure at the surface of the LiCoPO<sub>4</sub> nanoparticle, viewed along the [001] zone axis together with the corresponding overlaid EDX elemental map for Co (shown in purple) and P (shown in green). The black and the purple arrows point to the regions where Co occupies Li positions while the blue arrows highlight the regions where no Co occupation in Li sites is monitored.

## Evaluation of melting stainless steel to obtain dispersed includes of yttrium oxide by induction melting with the adding metal

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Recent years have seen a marked resurgence of interest and innovation in nuclear power, with particular attention being paid to liquid metal-cooled fast reactor (LMFR) fuels and fuel cycle options [1]. This renewed interest transcends national boundaries and is part of a global initiative driven by projects such as the International Project on Innovative Reactors and Fuel Cycles (INPRO), the Generation IV International Forum (GIF) and the International Framework Program Nuclear Energy Cooperation (IFNEC). Leading countries including the US, France, UK, Russia, South Korea, Japan, India, China and Germany have played key roles in the development of LMFR fuels.

Structural elements susceptible to radiation-induced degradation fall into two main categories. First, these are long-lasting, largely irreplaceable components that enclose and support the core. Secondly, these are components designed to contain and support fuel exposed to the harshest nuclear environment. The latter components are designed so that they can be replaced either when target burn-in is reached or when failure is imminent. Therefore, a major challenge in the development of LMFR fuel cycles is the development of fuel assemblies that can withstand failure-free operation at or above 20 at. % burnout, which is approximately two times greater than when using conventional austenitic stainless steels [2].

Operational problems are exacerbated by high temperatures (300-700°C), variable voltages and intense radiation damage to the assembly components. Radiation exposure is combined with corrosion of liquid metals (for example, sodium, lead) and chemical interaction with fuel and fission products, which persists for 2-4 years.



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Addressing these issues is critical to the successful development and implementation of advanced LMFR fuel cycles, an important milestone in the development of nuclear power.

At the moment, ferritic and FM alloys strengthened by oxide dispersion (ODS) are the pinnacle of materials development. These alloys promise to overcome the shortcomings of previous materials while maintaining essential properties. However, industrial production of ODS alloys remains a challenge [3].

The main method for creating ODS steels is mechanical alloying followed by pressure treatment, such as rolling, extrusion, pressing and others. Despite the potential of this area of research, it remains poorly studied in the scientific community. An in-depth study of this topic could lead to important discoveries and significant progress in the field of structural materials for nuclear power. Existing work on this topic either does not adequately describe the process and results, or is of no practical value due to the inherent complexity of the procedure [4].

The study of inclusions formed during steel smelting using the ODS liquid metallurgy method is a poorly studied topic. In this work, the task was set to explore this topic, continuing the review article on steel smelting.

The study included the study of five steelmaking methods, including two methods of introducing yttrium oxide nanopowder into a liquid melt and three methods of producing yttrium oxide in steel by oxidizing yttrium metal. The most successful result was an experiment on the oxidation of yttrium metal with oxygen supplied to the furnace atmosphere.

Based on the successful method, an experimental plan was developed with the most effective content of yttrium oxide in the steel volume. This experiment was carried out without control of the furnace atmosphere, in an ambient atmosphere without additional oxygen injection, which, according to calculations, may give better results compared to previous works.

### References

- [1] K. T. Agbevanu, S. K. Debrah, E. M. Arthur, E. Shitsi Heliyon, 9 (2023) 16580.
- [2] J. Zhang, S. S. Yin, L. Chen Nuclear Engineering and Technology, 19(2021) 1436 – 1445.
- [3] Internationale Atomenergie-Organisation – Vienna : IAEA, (2012) 87.
- [4] V. Chumanov, I. Chumanov Chernaya Metallurgiya, 63(2020) 499-503.

## Energy and cost analysis of automotive batteries based on learning curve and configuration design

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The vast adoption of electric vehicles (EVs) depends on the reduction of cost and the improvement of energy density of automotive batteries [1]. The learning curve model is capable of quantitatively predicting the cost reduction through the installed battery capacity. The precision of predicted battery cost can be boosted and verified by the refined learning curve model that considers dual factors including economic scale and technological innovations. This report proposes an empirical analysis to accurately predict battery cost and energy density based on lithium iron phosphate (LFP) and ternary nickel-cobalt-manganese oxide (NCM) cathodes that are widely used in the Chinese EV market. We also provide a feasible path to illustrate how battery energy density is achieved by considering technological innovations for battery configuration design. Based on the above optimized cost and energy density of two battery technologies, the cost fluctuation of the entire EV is identified ultimately.



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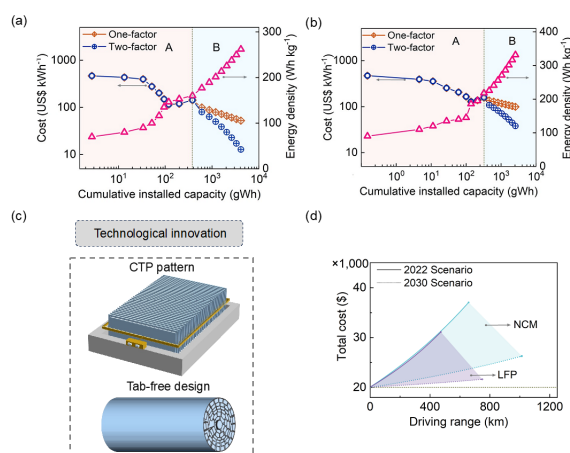


Figure 1. Cost and energy density predictions of (a) LFP and (b) NCM batteries enabled by single-/dual-factor learning curve models. (c) Benefiting battery energy efficiency by technological innovation for battery configuration design in terms of Cell-to-pack (CTP) pattern and Tab-free design. (d) Driving-range dependance of EV costs based on LFP/NCM battery routes with current and advanced development scenarios.

### References

- [1] M. Shahjalal, P. K. Roy, et al. *Energy*, 241 (2022) 122881.

## The origin of extraordinary selectivity in dehydrogenation of methylcyclohexane over NiSn catalysts

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The development of efficient and stable catalysts for the dehydrogenation of methylcyclohexane (MCH) is crucial for advancing hydrogen storage technologies. Liquid Organic Hydrogen Carriers (LOHCs), such as MCH, offer a viable solution for hydrogen storage and transportation due to their high hydrogen content and liquid state at ambient conditions. The dehydrogenation of MCH to toluene and hydrogen is a key step in this technology, requiring catalysts that provide high selectivity and stability under operational conditions [1]. That process typically catalyzed by Pt-based catalysts, however there are also promising examples of catalyst systems that do not contain noble metals. Currently Nickel-based catalysts are widely studied for their catalytic activity in hydrogenation and dehydrogenation reactions. However, their performance can be significantly enhanced by modifying them with other metals. Tin (Sn) has been identified as an effective promoter for nickel catalysts, improving their selectivity and stability. This study focuses on the synthesis, characterization, and testing of Sn-modified high-loaded nickel catalysts (HLNC, 75 wt% Ni) for MCH dehydrogenation. The primary goal is to optimize the composition and reduction conditions of the Sn/Ni catalysts to achieve high selectivity and conversion rates while maintaining long-term stability. The hypothesis is that Sn modification reduces the adsorption energy of the reaction product, toluene, thereby facilitating its rapid removal from the catalyst surface and preventing further decomposition [2-4].

The HLNC was prepared using a heterophase sol-gel technique, with SiO<sub>2</sub> as a stabilizing agent [2]. Sn was introduced via wetness impregnation, followed by reduction in hydrogen flow at different temperatures (400°C, 500°C or 600°C). Catalytic testing was conducted in a fixed-bed continuous flow reactor at 250-350°C under ambient pressure, with a WHSV of 18.5 h<sup>-1</sup>. Characterizations included TPD, XRD, and HRTEM to analyze the structural and compositional changes in the catalysts [4].

The Sn-modified nickel catalysts exhibited remarkable performance in MCH dehydrogenation. The optimal composition of Sn:Ni 1:4, reduced at 500°C, achieved a dehydrogenation selectivity of 99.0% at a 92% MCH conversion and a WHSV of 6.0 h<sup>-1</sup>. This composition also maintained a 99.9% selectivity at a 60.4% conversion and WHSV of 18.5 h<sup>-1</sup> over a 100-hour run, demonstrating excellent stability. XRD analysis revealed the formation of intermetallic compounds Ni<sub>3</sub>Sn and Ni<sub>3</sub>Sn<sub>2</sub> upon reduction, with a more uniform distribution



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of Sn observed at higher reduction temperatures. The lattice parameter of metallic Ni in the NiSn solid solutions deviated from the standard value, indicating the formation of cubic structured  $\text{Ni}_x\text{Sn}_{1-x}$  solid solutions. These structural changes are critical for the enhanced performance of the catalyst. HRTEM analysis showed that the Sn-HLNC catalyst consisted of submicron agglomerates with a  $\text{SiO}_2$  matrix embedding NiSn nanoparticles (5–10 nm). The uniform distribution of Sn in the catalyst matrix, especially after reduction at  $500^\circ\text{C}$ , contributed to the high stability and selectivity observed during the catalytic tests. TPD experiments of toluene revealed three distinct peaks corresponding to the evaporation of physisorbed toluene, desorption of physisorbed toluene, and desorption of chemisorbed toluene. The initial HLNC catalyst showed stronger chemisorption of toluene, with a chemisorbed toluene fraction of 6.4%, compared to 1.5% for the Sn-HLNC sample. This lower chemisorption energy on the Sn-modified catalyst facilitated the rapid removal of toluene, preventing its further decomposition into benzene and methane. Theoretical calculations supported these findings, showing the adsorption energy of toluene on the initial HLNC catalyst to be  $-1.45$  eV, while on the Sn-HLNC, it was significantly reduced to  $-0.08$  eV. This reduced adsorption energy is key to the enhanced selectivity and performance of the Sn-modified catalysts.

The Sn-modified HLNC with a Sn:Ni 1:4 composition and reduction at  $500^\circ\text{C}$  exhibits superior dehydrogenation performance, achieving high selectivity and stability. The formation of NiSn solid solutions reduces the adsorption energy of toluene, facilitating its quick removal from the catalyst surface. These findings present Sn-modified Ni catalysts as promising candidates for efficient MCH dehydrogenation in hydrogen storage applications.

### References

- [1] M. Niermann, A. Beckendorff, M. Kaltschmitt, K. Bonhoff, *Int. J Hydrogen Energy*, 44 (2019) 6631–6654.
- [2] Y. Gulyaeva, M. Alekseeva, O. Bulavchenko, A. Kremneva, A. Saraev, E. Gerasimov, S. Selishcheva, V. Kaichev, V. Yakovlev, *Nanomaterials*. 11 (2021) 1-20.
- [3] M. V. Alekseeva (Bykova), Y.K. Gulyaeva, O.A. Bulavchenko, A.A. Saraev, A.M. Kremneva, S.A. Stepanenko, A.P. Koskin, V. V. Kaichev, V.A. Yakovlev. *Dalt. Trans.* 51 (2022) 6068–6085.
- [4] A. P. Koskin, S. A. Stepanenko, M. V. Alekseeva (Bykova), O. A. Bulavchenko, E. Y. Gerasimov, A. I. Lysikov, P. M. Yeletsky, V. V. Kaichev, V. A. Yakovlev, *Chemical Engineering Journal*, 476 (2023) 146629:1-13.

## Synthesis and investigation of $\text{LiCoPO}_4$ -based materials for lithium-ion batteries

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$\text{LiCoPO}_4$  (LCP) as a high-voltage cathode material for lithium-ion batteries is selected due to its high theoretical capacity (167 mAh/g) and elevated operating voltage (4.8 V vs.  $\text{Li}/\text{Li}^+$ ). The olivine crystal structure of  $\text{LiCoPO}_4$  offers thermal stability due to P-O covalent bonding, rendering it a promising candidate for applications requiring high energy density and enhanced safety compared to traditional cobalt-based alternatives such as  $\text{LiCoO}_2$ .

Despite its advantages,  $\text{LiCoPO}_4$  faces significant challenges that impede its practical application. These include low electronic conductivity, poor  $\text{Li}^+$  diffusion, and instability of electrolytes at high voltage. Furthermore, the material experiences structural degradation during cycling, which results in limited cycle stability and rate performance.

Mechanical activation (MA) and boron (B) doping are investigated as potential avenues for improving the electronic and ionic conductivities of the material. The MA process involves the mixing and calcination of the material under controlled atmospheres [1], while B-doping aims to enhance the electrochemical



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performance. Ultrasonic spray pyrolysis is a process that consists of atomizing a precursor solution into fine droplets using a gas stream, which are then directed into a high-temperature furnace. This method allows for precise control of particle size, morphology, and composition, ultimately improving the electrochemical performance of materials such as LiCoPO<sub>4</sub>.

The experimental results demonstrate that the B-doped LiCoPO<sub>4</sub> exhibits enhanced performance compared to the pristine samples. Nevertheless, both materials are susceptible to electrolyte decomposition under high potentials, which results in poor cycle stability. To address this issue, fluorinated ethylene carbonate (FEC) is proposed as an alternative to ethylene carbonate (EC) in the electrolyte composition. The addition of FEC to the electrolyte composition has been shown to enhance the formation of protective surface films on the cathode, thereby improving the battery's cycling stability and capacity retention [2].

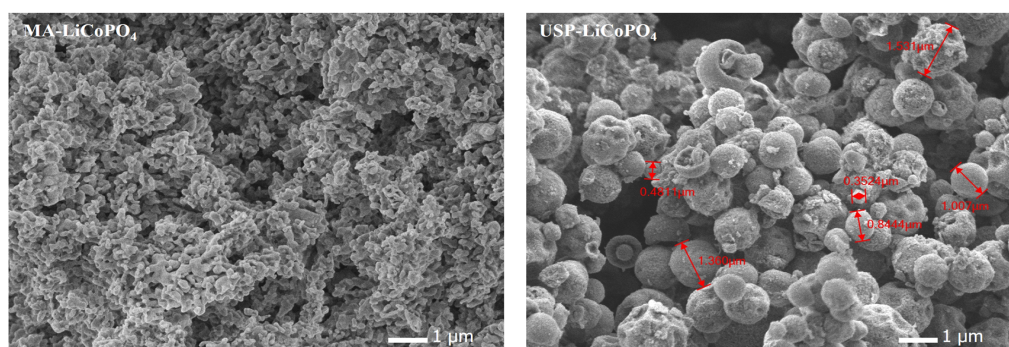


Figure 1. The SEM images of LiCoPO<sub>4</sub> synthesised by MA and USP methods

### References

- [1] Houyong Chen, Meng Chen, et al. "Synthesis and electrochemical performance of hierarchical nanocomposite of carbon coated LiCoPO<sub>4</sub> crosslinked by graphene." *Materials Chemistry and Physics*, 171 (2016): 6-10.
- [2] R. Sharabi, E. Markevich, K. Fridman, Gregory Gershinsky, et al. "Electrolyte solution for the improved cycling performance of LiCoPO<sub>4</sub>/C composite cathodes." *Electrochemistry Communications*, 28 (2013): 20-23.

## A parametric study on synthesis of Na<sub>x</sub>MnO<sub>2</sub> for advanced Na-ion batteries (SIBs) using custom-built ultrasonic spray pyrolysis (USP) framework

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Rapid Growth in the consumption of the lithium ion batteries has raised the demand of the lithium in international market which has generated alarming situation all over the globe due to scarcity of the resources of lithium which are already unevenly distributed resulting in the price hikes. This scenario has created the void for the innovations of the alternatives such as sodium (Na), zinc (Zn) and potassium (K) ion batteries. Among these competitors, sodium ion batteries (SIBs) have proved themselves as the future replacement of market leading LIBs [1]. For such breakthroughs, nanostructured structures have made substantial contributions to the field of material science, notably in the domain of energy storage, which is a serious problem in the world today due to the increasing rise in battery usage at all phases of life. A variety of techniques for synthesizing nanomaterials are available, such as the sol-gel method, solid state reaction, mechanochemical synthesis, and so on; however, in this work, ultrasonic spray pyrolysis (USP) was used, and a custom-built setup was fabricated with available resources, making it feasible for the low-cost generation of nanomaterials for inexpensive advanced sodium ion batteries (SIBs) for various applications. This study investigated the phenomenon of spray



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pyrolysis using a locally assembled setup with various possible variations to determine the effects of gas, flowrate, temperature distribution, and other factors on the morphology and crystal structure  $\text{Na}_x\text{MnO}_2$  particles intended to be used as electrode material in sodium ion batteries (SIBs).

This study might be useful for researchers working in the field of material synthesis in regions of the world where expensive equipment is lacking. This study generated significant findings in terms of crystal structure, which was P2 type and suitable for sodium ion batteries (SIB).

### References

[1] Konarov, Aishuak, Hee Jae Kim, Natalia Voronina, Zhumabay Bakenov, and Seung-Taek Myung. "P2- $\text{Na}_2/3\text{MnO}_2$  by Incorporation: as a cathode material of high capacity and long cycle life for sodium-ion batteries." ACS applied materials & interfaces 11, no. 32 (2019): 28928-28933.

## Polyacrylamide-based hydrogel electrolyte for modulating water activity in aqueous battery systems

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The limitations of lithium-ion battery systems, including lithium scarcity, demanding assembly conditions, and safety risks associated with flammable organic electrolytes, underscore the need for renewable, cost-effective, and safe alternatives. While zinc-ion or hybrid aqueous battery systems have garnered interest, challenges such as undesired side reactions, limited electrochemical stability, and electrolyte leakage persist, hindering large-scale adoption. Among electrolyte engineering approaches, hydrogel electrolytes have emerged as promising solutions, offering improved stability and relatively high ionic conductivity while mitigating leakage risks. Additionally, the modification opportunities of the hydrogel electrolytes present great potential for various applications.

Here, we synthesized a dual-function hydrogel electrolyte based on polyacrylamide and poly(ethylene dioxythiophene):polystyrene (Figure 1). This electrolyte effectively reduces water content and enhances stability by minimizing undesired side reactions. Moreover, the polymer network and its functional groups promote controlled ion transport. Swelling in a binary solution of ethylene glycol and water (EG 10%) further enhances the stability of the assembled battery system. The developed hydrogel exhibits relatively good ionic conductivity ( $1.6 \times 10^{-3} \text{ S cm}^{-1}$ ) and excellent electrochemical stability, surpassing 2.5 V on linear sweep voltammetry tests. An assembled aqueous lithium-ion hybrid battery with a zinc anode demonstrates high capacity ( $119.2 \text{ mAh g}^{-1}$ ), close to 100% coulombic efficiency, and good cycle stability, retaining 67.6% capacity after more than 400 cycles. This study highlights the potential of polyacrylamide-based hydrogel electrolytes with dual functionality as the electrolyte and separator, inspiring further development in hydrogel electrolytes for aqueous battery systems.





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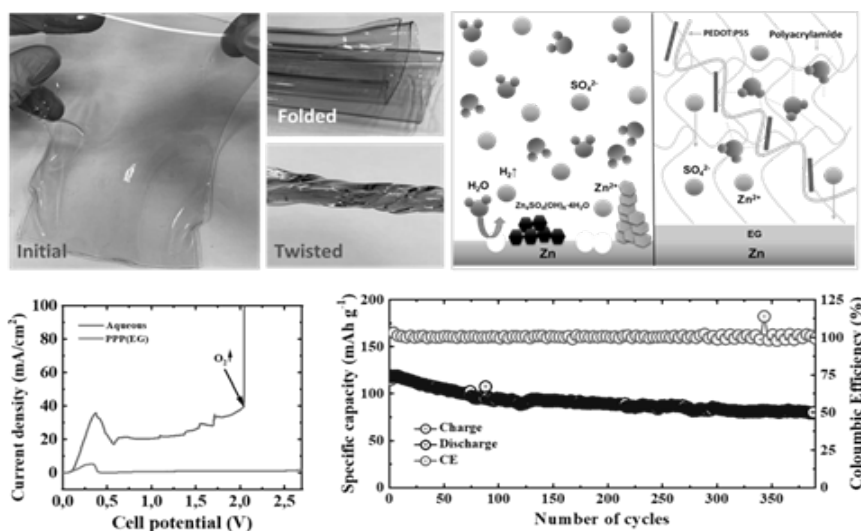


Figure 1. Polyacrylamide-Based Hydrogel Electrolyte images and results.

## A general strategy on biomass-derived hard carbons for boosting the energy densities of Na-ion batteries

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Na-ion battery is promising candidate of Li-ion battery for the next-generation scalable energy storage, due to its high abundance of an element, low costs of raw materials, and high sustainability.[1] Hard carbon anode is a promising anode for its high plateau capacity at low potential range, which boost the energy density of Na-ion full battery.[2] Hard carbons derived from different precursors show quite different capacities and plateau capacities. Design and manipulating approaches are necessary to enhance the plateau capacities based on precursor structures.

Herein, a densification strategy has been developed to boost the capacity of lignin, cellulose, and woodpowder-derived hard carbon anodes. Given the mechanical densification treatment, carbon radicals could be formed and recombined under a reduction atmosphere during pyrolysis, which assists to generate a disordered structure with a higher closed pore volume. The as-prepared lignin-derived hard carbon (O-HC<sub>4</sub>) anode displays an impressively high reversible capacity of 483 mAh g<sup>-1</sup> and a high plateau capacity of 282 mAh g<sup>-1</sup>, which are much higher than the reversible capacity of 360 mAh g<sup>-1</sup> and plateau capacity of 193 mAh g<sup>-1</sup> of the untreated lignin-derived hard carbon (O-HC<sub>0</sub>) anode. This Work Provides a general strategy to boost the plateau capacity of biomass-derived hard carbon anodes for high-energy-density Na-ion batteries.

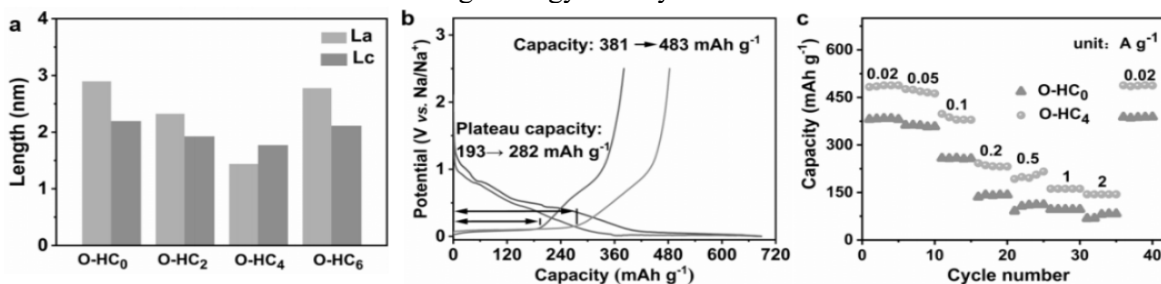


Figure 1. (a) The La and Lc (the length and the thickness of the graphitic nanodomains calculated from the XRD pattern of hard carbon materials), (b) the galvanostatic charge-discharge curves and (c) rate capability of hard carbon anodes.



### References

- [1] J. Yin, Y.S. Zhang, H. Liang, W. Zhang, Y. Zhu, Synthesis strategies of hard carbon anodes for sodium-ion batteries, *Mater. Reports Energy*. (2024) 100137. <https://doi.org/10.1016/j.jsamd.2023.100613>.
- [2] J. Yin, J. Jin, C. Chen, Y. Lei, Z. Tian, Y. Wang, Z. Zhao, A.-H. Emwas, Y. Zhu, Y. Han, U. Schwingenschlögl, W. Zhang, and H.N. Alshareef, Preferential Pyrolysis Construction of Carbon Anodes with 8400 h Lifespan for High-Energy-Density K-ion Batteries, *Angew. Chem. Int. Ed.* 62 (2023) e202301396. <https://doi.org/10.1002/anie.202301396>.

## Eco-Friendly Enhancement of Interfacial Strength in Aluminum-Polyurethane Adhesive Joints using Cellulose Nanofiber and Surface Treatment

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Adhesive joints play a crucial role in various industries due to their ability to bond dissimilar materials effectively. The strength of these joints is essential for ensuring the structural integrity and performance of the assembled components. The primary challenge in adhesive joints is the strength of interface between dissimilar materials. This research investigates the improvement of the interfacial strength in aluminum (Al 2024) and polyurethane adhesive joints by incorporating environmentally friendly cellulose nanofibers (CNF) within range 0.5–2 wt%, and employing chemical surface treatment (alkaline etching for 5, 15 and 45 min). The synergy of using both treatments on the interfacial strength is also investigated. Surface topography of treated Al2024 sheets was analyzed by profilometry while single lap shear joints were prepared for mechanical testing. Failure surfaces were studied *via* scanning electron microscopy.

The study reveals that the shear strength of adhesive joints can be significantly improved with addition of CNF; for example, 0.5 wt% CNF improves the interfacial strength by 86%. However, the positive effect of CNF diminishes after 1 wt% due to nanomaterials' agglomeration. Chemical surface treatment resulted in a 77% increment in the lap shear strength due to the obtained rough surface. Combining surface treatment and CNF led to further improvement of interfacial strength: when 0.5 wt% CNF and 45 min chemical surface treatment were applied simultaneously, the improvement reached a maximum of 137%. SEM images showed that the interface strengthening is due to mechanical interlock and nanofiber bridging. The study provides valuable insights into strengthening the interface between metallic surface and adhesives using eco-friendly nanomaterials and surface treatment. These findings can potentially be applied in high strength fibre-metal laminates for aerospace and automotive industry.



## Obtaining a volumetric nanostructured state of solid zirconium alloy rods by methods of severe plastic deformation

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Zirconium-based alloys are one of the main materials of nuclear engineering and are used for thermal neutron reactors such as a pressurized water reactor (PWR) or water-water energetic reactor (WVER) fuel elements (fuel rods) shells and plugs manufacturing [1]. The protecting of fuel rods shell surface and its mechanical properties improving is one of the most urgent problems of modern nuclear power engineering. The nanostructured ultrafine grained (UFG) structure provides improving the mechanical properties and enhanced radiation resistance due a lot of grain boundaries in material volume which is drain surface for defects [2].

Severe Plastic Deformation (SPD) methods provides the extremely total strain level (more than 30 mm/mm) in combination with the vortex metal flow character. The SPD have no tensile stresses in central zone. This fact and huge strain level makes real a significant structure changing by this method to the ultrafine-grained (UFG) state without cracking and grain size about 300-800 nm.

In the course of this study, a comprehensive finite element analysis of various schemes of intense plastic deformation was carried out. By modeling various deformation modes, it was possible to deepen the understanding of the mechanism of occurrence and development of the UFG structure, as well as to determine the optimal conditions and process parameters to achieve the best results.

As a result of a full-scale experiment, samples with submicron ultrafine-grained (UFG) structure were obtained. These samples have been extensively analyzed using various methods, including scanning electron microscopy with electron backscattering analysis and transmission electron microscopy (TEM). The SEM-EBSD method made it possible to study in detail the crystal structure and texture of the samples, revealing the distribution and orientation of the grains, as well as grain boundaries (Figure 1).

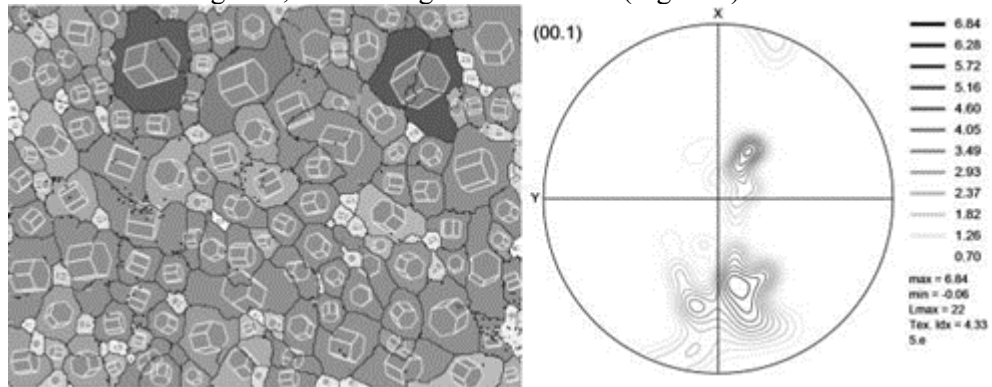


Figure 1. orientation map and pole figure from EBSD analysis

The combined application of these analysis methods confirmed the presence of a UFG structure in the studied samples and allowed us to obtain valuable data on the mechanisms of its formation, which is an important step in optimizing the processes of intensive plastic deformation to create materials with improved performance characteristics.



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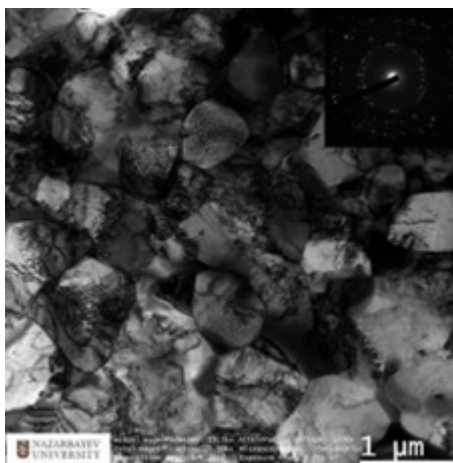


Figure 2. TEM image of UFG structure

### References

- [1] Zinkle, S.J.; Was, G.S. Materials challenges in nuclear energy. *Acta. Mater.* 2013, 61, 735–758.
- [2] Nita, N.; Schaeublin, R.; Victoria, M. Impact of irradiation on the microstructure of nanocrystalline materials. *J. Nucl. Mater.* 2004, 329–333, 953–957.
- [3] Galkin, S.P. Radial shear rolling as an optimal technology for lean production. *Steel Transl.* 2014, 44, 61–64.

## Effect of Bio-Waste Composition and Treatment Conditions on the Structure and Electrochemical Performance of Hard Carbon for Sodium-Ion Batteries

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Recently, significant investments have been devoted to supporting research and development for the production of relatively cheap energy storage systems through the commercialization of Sodium-Ion Batteries (SIBs) owing to their numerous advantages such as inexpensive cathode materials, wide operating temperature and safer transportation over Lithium-Ion Batteries. Hard Carbon has been identified as the most suitable anode material for SIBs owing to its large interlayer distance and low sodium-ion insertion voltage that improves sodium ion intercalation.

Conventionally, these Hard Carbon were synthesized from expensive carbon precursors which counters the production of cheap and sustainable energy storage systems, utilization of readily available bio-waste as carbon precursors for Hard Carbon synthesis reduces SIBs production cost while providing cheap and efficient waste disposal methods. However, the composition, treatment process and synthesis routes of the readily available carbon precursor (bio-waste) utilized for hard carbon synthesis largely influence the structure and electrochemical performance of the resulting SIBs.

This research investigates the effect of the biowaste composition and pre-treatment conditions (before and after thermal treatment) on the structure, porosity and overall electrochemical performances of these anode materials for SIBs. Material characterization techniques and Electrochemical tests like XRD, TEM, Raman Spectroscopy, Galvanostatic charge-discharge, C-rate and EIS were employed to study and compare the physical properties and electrochemical performances of the synthesized and commercial anode materials.

The synthesis of loose mesoporous anode material with over 20% yield, a reversible capacity of c.a 300 mAh g<sup>-1</sup> and ICE of 78% was achieved through pre-oxidation at 150 °C in air before carbonization at 1300 °C under an argon environment. This reveals the impact of pre-oxidation, material composition and enlarged inter-layer distance through hindered graphitization, the presence of metal oxides and improved sodium insertion on the electrochemical performance of the synthesized anode material.



### Acknowledgement

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## Development of Low-Temperature Supercapacitors with Bio-Waste Derived Activated Carbon and Safe Electrolytes

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Developing energy storage devices that prioritize safety and sustainability is essential to meet the rapidly increasing energy demands, including those for low-temperature applications. Addressing this challenge requires a comprehensive and integrated approach to designing electrolytes, with careful consideration of their toxicity, environmental impact, and cost. To target low-temperature applications while maintaining safety, non-toxicity, and affordability, we designed a ternary electrolyte system (TES) consisting of water, 1,2-propylene glycol as a co-solvent, and NaClO<sub>4</sub> salt. This TES is not only non-toxic and safe but also effective in maintaining high performance at low temperatures.

Aqueous electrolytes are known for their high ionic conductivity and low cost. However, their use at low temperatures is often limited by water's tendency to freeze, which adversely affects electrolyte performance. By incorporating 1,2-propylene glycol, we can lower the freezing point of the electrolyte solution, enabling its use at sub-zero temperatures [1,2]. This modification allows our TES to retain high ionic mobility and maintain efficient charge transfer, even at -40°C.

The NaClO<sub>4</sub> salt, chosen for its high oxidative stability and low toxicity, further enhances the safety profile of the electrolyte. NaClO<sub>4</sub>, unlike some other salts, does not pose significant health risks and is environmentally benign [3]. Combined with the use of water and 1,2-propylene glycol—a non-toxic, biodegradable solvent commonly used in food and pharmaceutical industries—our TES stands out as a particularly safe and sustainable choice for energy storage applications.

Additionally, we utilized high surface area electrodes (2423 m<sup>2</sup>/g) derived from bio-waste, specifically date seeds, as a carbon source. This approach not only leverages sustainable materials but also contributes to waste valorization, addressing both environmental and economic concerns. The use of bio-waste, such as date seeds, provides a renewable and cost-effective source of carbon material while reducing environmental pollution. The high surface area of these electrodes enhances the electrochemical performance of the supercapacitor, contributing to its efficiency and durability [4].

The combination of the TES and bio-waste-derived electrodes enabled a symmetric supercapacitor to operate efficiently at low temperatures, achieving a specific capacitance of 112 F/g at 0.2 A/g. The ternary electrolyte system demonstrated exceptional stability and conductivity at low temperatures, making it ideal for applications in extreme environments. Remarkably, this symmetric supercapacitor exhibited outstanding performance, maintaining 98.27% capacity retention over 10,000 cycles, even after being tested under different environmental conditions.

Furthermore, our study highlights the feasibility of integrating green chemistry principles in the development of advanced energy storage systems. The use of date seeds as a carbon source not only provides a sustainable and cost-effective material but also contributes to waste reduction and environmental sustainability. The inclusion of 1,2-propylene glycol, which is less toxic compared to many other organic solvents, enhances the safety profile of the electrolyte. This innovative approach to electrolyte design and sustainable electrode materials paves the way for the creation of high-performance, environmentally friendly energy storage devices suitable for a wide range of applications, particularly in low-temperature environments [5].



### References

- [1]. Gao X. et al. Recent progress of aqueous and organic/aqueous hybrid electrolytes for low-temperature rechargeable metal-ion batteries and supercapacitors // *Energy Storage Mater.* 2023. Vol. 54. P. 382–402.
- [2]. Teherpuria H. et al. Salt Effects on Ionic Conductivity Mechanisms in Ethylene Carbonate Electrolytes: Interplay of Viscosity and Ion-ion Relaxations. 2024.
- [3]. Chen Y., Zhang Y.-H., Zhao L.-J. ATR-FTIR spectroscopic studies on aqueous LiClO<sub>4</sub>, NaClO<sub>4</sub>, and Mg(ClO<sub>4</sub>)<sub>2</sub> solutions // *Physical Chemistry Chemical Physics.* 2004. Vol. 6, No 3. P. 537.
- [4]. Poonam et al. Review of supercapacitors: Materials and devices // *J Energy Storage.* 2019. Vol. 21. P. 801–825.
- [5]. Lan S. et al. Recent Advances in Low-Temperature Liquid Electrolyte for Supercapacitors // *Small.* 2024

## Quenched PVDF/PMMA Porous Matrix for Triboelectric Energy Harvesting and Sensing

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The increasing demand for flexible and wearable devices is driven by ongoing advancements in intelligent electronics technology, coupled with the growing importance of the Internet of Things (IoT) in biomedical applications. Modern electronics must exhibit specific characteristics, including a lightweight design, high conductivity, good dielectric permittivity, low dielectric loss, and exceptional breakdown strength. Polyvinylidene fluoride (PVDF), a polymer known for its high triboelectric charge density, is a common piezoelectric material used in nanogenerators like triboelectric nanogenerators (TENGs). However, obtaining PVDF with a high  $\beta$ -phase content using conventional methods, typically employed for membrane materials, poses a significant challenge due to its high resistance and the inherent difficulty in polarization.

Therefore, this research study employs a novel quenching method to prepare a PVDF/PMMA porous matrix with a predominant  $\beta$ -phase content of around 86%, offering a relatively simple and cost-effective approach. The fabricated TENG device exhibited an impressive output power of approximately 750 mW m<sup>-2</sup> and demonstrated excellent mechanical robustness, enduring more than 36,000 cycles. This mechanical robustness is three times higher than that of previous PVDF-based TENGs. Overall, this study demonstrates the potential application of a PVDF/PMMA porous matrix TENG device, fabricated through a simple and cost-effective method, highlighting its versatility and efficiency for various practical purposes.

### Acknowledgments

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## Effect of 2D Material and Surface Treatment on the Adhesive Strength of Aluminum-Polyurethane Joints

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Fiber metal laminates (FMLs) is a class of hybrid materials that combine the features of metal and fiber reinforced polymer resulting in remarkable strength and stiffness-to-weight ratios. Outstanding mechanical properties under quasi-static, dynamic and shock loads make them suitable for military and commercial aircraft applications. However, delamination arising from relatively weak polymer-metal interface region is a challenging issue remaining the scope of the ongoing research. In this study, a novel approach to improve aluminium (Al2024) and polyurethane interfacial adhesion by incorporating 2D-material ( $\alpha$ -Zirconium phosphate ( $\alpha$ -ZrP) with 0, 0.5, 1, 1.5 and 2 wt%), mechanical (sandpaper with #80, 100, 120 grit size) and electrochemical (H<sub>2</sub>SO<sub>4</sub> anodizing) treatments of the aluminum surface, and their synergetic effects was studied. Profilometry was used to measure the roughness of treated Al2024, while single lap joint was tested to evaluate the mechanical properties of aluminum-polyurethane adhesive joints.

Addition of 0.5 wt%  $\alpha$ -ZrP led to the highest shear strength recording 92% increment. Application of mechanical treatment increased the shear strength by 35%, while electrochemical treatment resulted in 217.8% increase. In addition, a combination of 0.5 wt%  $\alpha$ -ZrP and electrochemical surface treatment demonstrated superior performance, increasing lap shear strength by 498.3%. Improved stress transfer, achieved through the properties of  $\alpha$ -ZrP nanosheets and the development of a robust interface with a larger surface area through anodizing, were the main factors contributing to the enhancements in the adhesive joint strength. The results not only hold promise for industrial applications like high interlaminar strength in fiber metal laminates but also pave the way for enhancing the performance of adhesive joints in aerospace components and automotive structures.

## Composite of biomass-derived carbon and titanium nitride nanoparticles for lithium-sulfur batteries

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Nowadays, lithium-sulfur batteries (LSBs) have attracted considerable attention due to their high specific energy (2600 Wh·kg<sup>-1</sup>) and theoretical specific capacity (1675 mAh·g<sup>-1</sup>). In addition, elemental sulfur is inexpensive, widely available, environmentally friendly, and non-toxic. However, the application and development of LSBs face challenges such as the shuttle effect and volume expansion during long-term cycling. These issues lead to low electrochemical reversibility and rapid capacity loss during operation[1]. The main efforts to improve the electrochemical performance of LSBs have been directed towards the development of carbon-based sulfur composites, as it has been found that using biomass as a raw material allows the production of porous and highly reactive carbon materials with good physical and chemical stability[2]. Transition metal nitrides exhibit high electronic conductivity and strong chemisorption towards lithium polysulfides (LiPSs). In particular, titanium nitride (TiN) has attracted increasing attention for LSBs applications due to its high electronic conductivity and catalytic effect on the conversion of LiPSs[3].

In this study, we synthesized and characterized a composite that consist of carbon and TiN via carbothermal nitridization and subsequently utilized it as a porous matrix for the preparation of a sulfur cathode using the melt-diffusion technique. Additionally, composites based on graphene porous carbon (GPC) decorated



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with TiN nanoparticles were synthesized with varying GPC to TiCl<sub>4</sub> ratios and used as efficient separator modifiers.

The results indicate that the C-TiN composite has a dual function, physically interacting with LiPSs through carbon and chemically through TiN. Additionally, TiN can catalyze the redox reaction of sulfur. A cell featuring a GPC@S cathode and a GPC-TiN modified separator exhibited accelerated LiPSs redox reaction and suppressed the shuttle effect. Specifically, the GPC@S/GPC-TiN-10 cell showed an excellent initial discharge capacity of 1560.85 mAh·g<sup>-1</sup> at 0.2 C and demonstrated promising long-term cycling performance.

### Acknowledgements

This research was funded by the project AP1967770 “Development of all-solid-state lithium-sulfur full cells based on nanostructured carbon derived from plant waste” from the Ministry of Education and Science of the Republic of Kazakhstan.

### References

[1] Bruce, P.; Freunberger, S.; Hardwick, L.; Tarascon, J. Li-O<sub>2</sub> and Li-S batteries with high energy storage. *Nat. Mater.* 11 (2012) 19–29.

[2] Zhang, Y.; Zhao, Y.; Bakenov, Z.; Tuiyebayeva, M.; Konarov, A.; Chen, P. Synthesis of hierarchical porous sulfur/polypyrrole/multiwalled carbon nanotube composite cathode for lithium batteries. *Electrochim. Acta* 143 (2014) 49–55.

[3] F. Sultanov, N. Zhumasheva, A. Dangaliyeva, A. Zhaisanova, N. Baikalov, B. Tatykayev, M. Yeleuov, Z. Bakenov, A. Mentbayeva, Enhancing lithium-sulfur battery performance with biomass-derived graphene-like porous carbon and NiO nanoparticles composites, *J. Power Sources* 593 (2024) 233959.

## Production carbon nanomaterials based from brown coals for hydrogen storage

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Hydrogen energy is increasingly recognized for its potential to play a crucial role in the global transition to sustainable energy. Hydrogen's versatility extends from being able to store and deliver energy to being used directly as fuel for transport or for heating in residential and commercial buildings [1] [2]. In this work, sorbents were obtained from coals of the Maikuben lignite basin, the Shoptkyol deposit. The physicochemical properties of the resulting porous carbon materials were studied. In figure 1 SEM analysis showed that a large number of CNTs with a diameter from ~69.5 nm to ~200.2 nm were formed on the surface of the carbon sample.

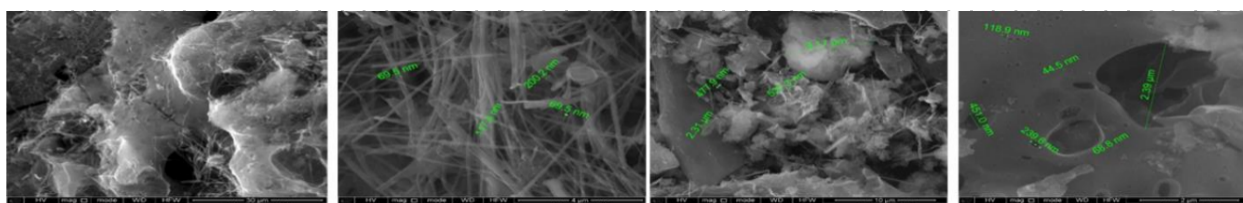


Figure 1. Electron microscopic images of activated adsorbents based on carbon

The study examined the dynamics of the hydrogen adsorption process on a porous carbon material at a temperature of 77 K. Based on the results of studying the adsorption characteristics, it can be concluded that the adsorbents have a high specific surface area for hydrogen of 1165.97 m<sup>2</sup>/g, respectively, hydrogen adsorption was 1.49%. The study provided important data on the dynamics of the hydrogen adsorption process on porous carbon material, its speed and efficiency. These results (figure 2 and table 1) can be useful in the development and optimization of hydrogen adsorption processes for various industrial and scientific applications.





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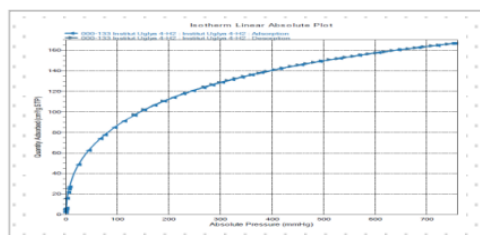


Figure 2. Adsorption curve of the activated adsorbent

Table 1. Results of the study of hydrogen sorption with PCM

Name	S(DFT) specific, m <sup>2</sup> /g	Mass H <sub>2</sub> , % 77 K	Heat of adsorption of H <sub>2</sub> , kJ/mol
Carbon adsorbent	1165.97	1.49	15.66

Thus, when assessing the efficiency of an adsorption process, it is important to consider not only the potential improvement in adsorption properties at low temperatures, but also the energy costs associated with maintaining these conditions. This balance between improving the adsorption process and the energy costs of creating and maintaining optimal temperatures is a key aspect of the development and optimization of adsorption-based technologies and plays an important role in assessing their economic feasibility.

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### References

- [1] S. Schaefer, A. Jeder, G. Sdanghi Int. J. Hydrogen Energy, 45 (2020) 30767-30782. [2] C. Liu, Y. Chen, H.M. Cheng Carbon, 48 (2010) 452-455.

## Practical Investigation of Si Alloy Anode for High-Energy Li-Ion Batteries

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Recent market trends have increasingly focused on the introduction of silicon-based (Si-based) materials, particularly silicon oxide (SiO<sub>x</sub>) and silicon-carbon (Si-C) composites, to address performance challenges in energy storage applications. Despite notable advancements, unresolved issues such as significant volume expansion and low initial Coulombic efficiency (ICE) persist [1]. To enhance the reversibility during the initial cycle and mitigate volume variation issues of Si-based materials, numerous research groups have explored solutions including pre-lithiation, alloying with heteroelements, and optimizing particle size and morphology [2].

Among the various approaches, the use of silicon alloys with nano-Si grains embedded in inactive matrixes shows substantial promise for commercialization. These inactive phases act as a buffer, accommodating volume changes and providing a stable electronic conduction path during cycling. The electrochemical stability of Si alloys, however, is highly dependent on microstructural homogeneity, composition quality, and synthesis methods [3]. Although some strategies have achieved electrochemical improvements under mild conditions, practical testing under high mass loadings and electrode densification remains insufficient, hindering feasibility confirmation.

Furthermore, the co-utilization of graphite and silicon has shown limited success in commercial applications, with the use of Si-based materials in industrial anodes remaining below 5 wt% due to performance degradation and significant volume expansion under high densification. This underscores the need for further development in Si-graphite (Si-Gr) co-utilization, focusing on materials that offer improved initial cycle reversibility and optimized thickness variations to meet energy density requirements [4].



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In this study, we have designed a graphite-blended silicon alloy composite electrode that surpasses the energy performance of commercial graphite materials. Our approach aims to enhance the practical application of Si-based materials in high-energy density anodes, addressing current limitations and paving the way for more robust and commercially viable energy storage solutions. Extensive testing and analysis under practical conditions have been conducted to validate the feasibility and performance improvements of our proposed composite electrode.

### Acknowledgement

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### References

- [1] T. Chen, J. Wu, Q. Zhang, X. Su, *Journal of Power Sources*, 363 (2017) 126-144.
- [2] S. Chae, M. Ko, K. Kim, K. Ahn, J. Cho, *Joule*, 1 (2020) 47-60.
- [3] M.N. Obrovac, *Current Opinion in Electrochemistry*, 9 (2018) 8-17.
- [4] N. Kim, Y. Kim, J. Sung, J. Cho, *Nature Energy*, 8 (2023) 921-933

## Electrochemical characterisation of RF sputtered Co-, Li-doped ZnO nanofilms as anode material for lithium-ion batteries

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Zinc oxide (ZnO) has emerged as a promising anode material for lithium-ion batteries (LIBs) due to its low cost, wide bandgap, non-toxicity, and high theoretical capacity of 987 mAh g<sup>-1</sup>. However, pure ZnO anodes suffer from significant drawbacks, including rapid capacity degradation upon cycling and poor rate capability. These issues arise from ZnO's low electronic conductivity, severe agglomeration, and substantial volume expansion (228%) during lithiation/delithiation processes [1]. Additionally, the formation of expansion-induced nanocracks undermines electrode performance and disrupts the formation of the stable solid electrolyte interphase [2]. To address these challenges, this study explores zinc oxide thin film dual-doped with lithium and cobalt (Zn<sub>0.872</sub>Li<sub>0.099</sub>Co<sub>0.029</sub>O, referred to as LCZO) anodes prepared via RF magnetron sputtering. The improvement of polycrystallinity can be achieved by the optimization of content, morphology, and crystallization circumstances [3-4]. During the deposition process key parameters such as RF power and pressure were varied. Additionally, the annealing temperature was adjusted across 400°C, 450°C, and 500°C. Pure ZnO, Li doped ZnO (Zn<sub>0.901</sub>Li<sub>0.099</sub>O, referred to as LZO) and Co-doped ZnO (Zn<sub>0.9695</sub>Co<sub>0.0305</sub>O, referred to as CZO) thin films were fabricated for comparative study. Electrochemical tests of LCZO, annealed at 450 °C, showed good reversible specific capacity of 400 mAhg<sup>-1</sup> at 0.1C rate over 100 cycles. In contrast, the obtained ZnO, LZO and CZO thin films and annealed at 500 °C showed highest specific capacities of 160 mAh g<sup>-1</sup>, 300 mAh g<sup>-1</sup> and 185 mAh g<sup>-1</sup>, respectively. Further investigation will explore the role of magnetron deposition conditions. This research highlights the impact of lithium and cobalt doping in ZnO anode material and the effect of thermal post-processing on its stability in lithium-ion batteries.

### Acknowledgments

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### References

- [1] Singh R., Ichikawa T., & Jain A. (2021). Zinc oxide as promising anode material for Li-ion battery. In *Elsevier eBooks* (pp. 575–603).



The 12<sup>th</sup> International Conference on Nanomaterials and Advanced Energy Storage Systems (INESS - 2024)

[2] Bui V. K. H., Pham T. N., Hur J., & Lee Y. (2021). Review of ZNO Binary and Ternary Composite anodes for Lithium-Ion batteries. *Nanomaterials*, 11(8), 2001.

[3] Sun W., Li Z., Li D., Gao K., Miao Z., Han Y., Guan S., Li Z., & Sun C. (2024). Pre-lithiation strategy to design high-performance zinc oxide anode for lithium-ion batteries.

[4] Li Y., Li W., Fang M., Yao X., Chen C., Shui M., Shu J., & Ren Y. (2017). The preparation, performance and lithiation mechanism of cobalt-doped zinc oxide as a high performance anode material for LIB. *Current Applied Physics*, 17(8), 1050–1057.

## Surface segregation of metal dopants at electrochemically active surface of layered oxide for Li-ion batteries: a computational study

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In recent years, there has been significant interest in the surface segregation of doping elements within layered oxide cathode materials for metal-ion batteries. It has been observed that altering the surface concentration of a specific element can impact stability of the electrochemically active surface, resulting in decreased or improved electrochemical performance. However, the underlying physical and chemical mechanisms behind this segregation phenomenon are not clear. To elucidate the role of commercially important doping elements, such as Mg, Al, Ti, V, Cr, Mn, Fe, and Ni, we conducted a density functional theory study on their segregation at the (104) low-energy surface of LiCoO<sub>2</sub> (Figure 1a). Through precise control of the local oxidation states and magnetic moments of surface atoms, we identified their most stable configurations. Our findings reveal that all elements, except Al and Cr, exhibit a propensity for segregation, primarily driven by differences in surface energies between the host and solute lattices (Figure 1b). This phenomenon is further explained by crystal-field stabilization energies. Finally, we provide a rationalization of available experimental results and offer several predictions regarding highly segregating and non-segregating dopants [1].

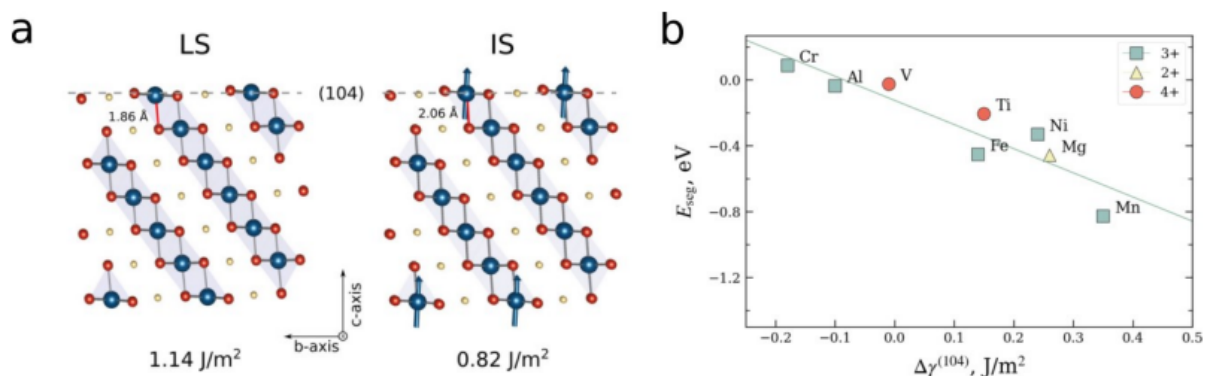


Figure 1. a) Atomic and magnetic structure of the (104) LiCoO<sub>2</sub> surface with LS and IS Co 3+ ions. Surface energies and M-O distances are also shown. b) Segregation energy of dopants as a function of differential surface energy  $\Delta\gamma^{(104)} = \gamma^{(104)}(\text{LiCoO}_2) - \gamma^{(104)}(\text{LiMO}_2)$ . For Ti and V, the segregation energy of the small polaron electron (-0.74 eV) is subtracted. The Pearson correlation coefficient is -0.872.

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### References

[1] A.O. Boev, S.S. Fedotov, A.M. Abakumov, D.A. Aksyonov *Phys. Rev. Materials* 8 (2024) 055403



## Li-Ion Transfer Mechanism of Gel Polymer Electrolyte with Sole Fluoroethylene Carbonate Solvent

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Gel polymer electrolytes (GPEs) are deemed as the most promising candidates to address the individual limitations of liquid and solid electrolytes. [1-2] However, the extensive development is still hindered due to the veiled Li-ion conduction mechanism. Herein, the related mechanism in GPEs is extensively studied by developing an in situ polymerized GPE comprising fluoroethylene carbonate (FEC) solvent and carbonate ester segments (F-GPE). Practically, although with high dielectric constant, FEC fails to effectively transport Li ions when acting as the sole solvent. By sharp contrast, F-GPE demonstrates superior electrochemical performances. The related Li-ion transfer mechanism is investigated using molecular dynamics simulations and <sup>7</sup>Li/<sup>6</sup>Li solid-state nNMR spectroscopy. The polymer segments are extended with the swelling of FEC, then an electron-delocalization interface layer is generated between abundant electron-rich groups of FEC and the polymer ingredients, which works as an electron-rich “Milky Way” and therefore the rapid transfer of Li ions is facilitated by lowering the diffusion barrier dramatically. A high conductivity of  $2.47 \times 10^{-4} \text{ S cm}^{-1}$  and a small polarization of about 20 mV for Li//Li symmetric cell after 8000 h are achieved (Fig. 1). Remarkably, FEC provides high flame-retardancy and makes F-GPE remains stable under ignition and puncture tests.

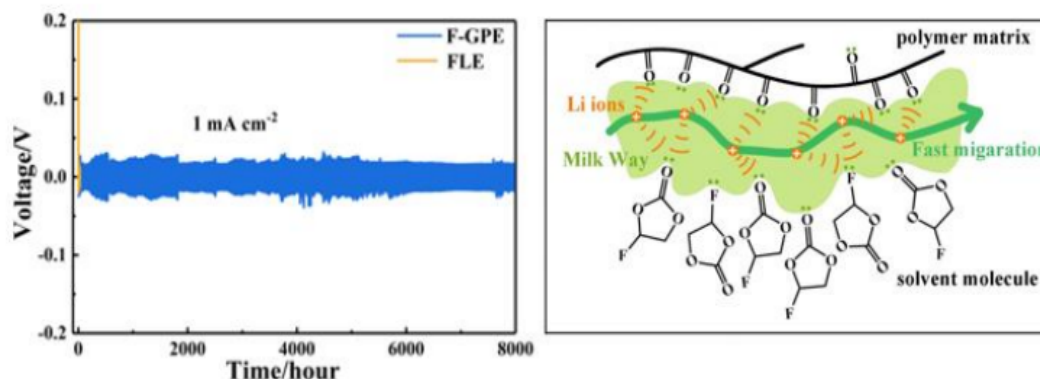


Fig. 1. Galvanostatic cycling profiles of Li/F-GPE/Li and Li/FLE/Li symmetrical cells with current densities of  $1 \text{ mA cm}^{-2}$  and Schematic diagram of Li-ion transfer mechanism for F-GPE

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### References

- [1] S. Wang, Q. F. Sun, L.Q. Zhang\*, et al. *Advanced Energy Materials* (2023) 2204036.
- [2] Q.F. Sun, S. Wang, L.Q. Zhang\*, et al. *Energy Storage Materials* 44 (2022) 537-546.



## Exploring the impact of $\gamma$ -rays on stability of a wide bandgap perovskite

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Complex lead halides with perovskite structure and general formula APbX<sub>3</sub> (A is a cation, either organic methylammonium (MA<sup>+</sup>) or formamidinium (FA<sup>+</sup>), or inorganic Cs<sup>+</sup>; and X is an anion of Br, Cl halogen or I) has been extensively studied last years in terms of radiation hardness. Many researchers found surprisingly high resistance of various perovskite materials towards highenergy electrons [1, 2], protons [3, 4], and hard ionization such as X-rays [5-7] and gamma-rays [8, 9]. Superior radiation hardness makes a family of perovskite semiconductors an attractive candidate for single and multijunction solar cells for space environment [10, 11] and as X-ray and gamma-ray detectors [12,13].

In this work, the recombination dynamics and defect concentration of a mixed cation mixed halide perovskite with 1.7 eV bandgap after exposure to  $\gamma$ -ray source (0-21 kGy) was studied. Such methods as photoluminescent spectroscopy, impedance spectroscopy and admittance spectroscopy were used to reveal the effect of hard ionization in absorber material. It was found that moderate doses (up to 10 kGy) passivate defects with activation energy  $\approx 0.5$  eV and at the same time form new vacancies that cause dramatic growth of the diffusion coefficient and migration of mobile ions. Doses above 10 kGy are detrimental for perovskite solar cells mainly due to growing role of interface recombination. The results encourage to use the wide bandgap perovskite Cs<sub>0.17</sub>FA<sub>0.83</sub>PbI<sub>1.8</sub>Br<sub>1.2</sub> as a material for tandem solar cells with potential application in space environment.

### References

- [1] Y. Miyazawa, M. Ikegami, T. Miyasaka, T. Ohshima, M. Imaizumi and K. Hirose, 2015 IEEE 42nd Photovolt. Spec. Conf. (2015) 1–4.
- [2] Y. Miyazawa, M. Ikegami, H. Chen, T. Ohshima, M. Imaizumi, K. Hirose and T. Miyasaka, ISCIENCE, 2 (2018) 148–155.
- [3] V. V. Brus, F. Lang, J. Bundesmann, S. Seidel, A. Denker, B. Rech, G. Landi, H. C. Neitzert, J. Rappich and N. H. Nickel, Adv. Electron. Mater., 3 (2017) 1600438
- [4] F. Lang, N. H. Nickel, J. Bundesmann, S. Seidel, A. Denker, S. Albrecht, V. V. Brus, J. Rappich, B. Rech, G. Landi and H. C. Neitzert, Adv. Mater., 28 (2016) 8726–8731.
- [5] K. Sakhatskyi and M. V. Kovalenko, Light Sci. Appl., 11 (2022) 41377.
- [6] A. Garcia-Fernandez, B. Kammlander and S. Riva, Phys. Chem. Chem. Phys., 26 (2024) 1000–1010.
- [7] V. Milotti, S. Cacovich, D. R. Ceratti, D. Ory, J. Barichello, F. Matteocci, A. Di Carlo, P. M. Sheverdyayeva, P. Schulz and P. Moras, Small Methods, 7 (2023) 1–9.
- [8] A. G. Boldyreva, A. F. Akbulatov, S. A. Tsarev, S. Y. Luchkin, I. S. Zhidkov, E. Z. Kurmaev, K. J. Stevenson, V. G. Petrov and P. A. Troshin, J. Phys. Chem. Lett., 10 (2019) 813–818.
- [9] A. G. Boldyreva, A. F. Akbulatov, M. Elnaggar, S. Y. Luchkin, A. V. Danilov, I. S. Zhidkov, O. R. Yamilova, Y. S. Fedotov, S. I. Bredikhin, E. Z. Kurmaev, K. J. Stevenson and P. A. Troshin, Sustain. Energy Fuels, 3 (2019) 2705–2716.
- [10] A. R. Kirmani, K. Brandon, J. Grandidier, D. M. Wilt, T. Kaitlyn, J. M. Luther, A. R. Kirmani, B. K. Durant, J. Grandidier, N. M. Haegel, M. D. Kelzenberg, Y. M. Lao, M. D. McGehee, L. Mcmillon-brown, D. P. Ostrowski, T. J. Peshek, B. Rout, I. R. Sellers, M. Steger, D. Walker, D. M. Wilt, K. T. Vansant and J. M. Luther, (2022) 1015–1031.
- [11] I. Cardinaletti, T. Vangerven, S. Nagels, R. Cornelissen, D. Schreurs, J. Hruby, J. Vodnik, D. Devisscher, J. Kesters, J. D’Haen, A. Franquet, V. Spampinato, T. Conard, W. Maes, W. Deferme and J. V. Manca, Sol. Energy Mater. Sol. Cells, 182 (2018) 121–127.
- [12] C. C. Stoumpos, C. D. Malliakas, J. A. Peters, Z. Liu, M. Sebastian, J. Im, T. C. Chasapis, A. C. Wibowo, D. Y. Chung, A. J. Freeman, B. W. Wessels and M. G. Kanatzidis, Cryst. Growth Des., 13 (2013) 2722–2727.



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[13] Y. He, L. Matei, H. J. Jung, K. M. McCall, M. Chen, C. C. Stoumpos, Z. Liu, J. A. Peters, D. Y. Chung, B. W. Wessels, M. R. Wasielewski, V. P. Dravid, A. Burger and M. G. Kanatzidis, *Nat. Commun.*, 9 (2018) 1–8.

## Enhanced electrochemical performance of phosphorus-doped hard carbon anodes derived from upcycled PET-bottles for lithium-ion batteries

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The modern world faces a critical challenge with plastic pollution, necessitating innovative solutions for sustainable management. One promising approach is the upcycling of plastic materials into more valuable products, thereby reducing the generation of microplastics associated with conventional recycling [1]. Among various plastics, polyethylene terephthalate (PET) from single-use beverage bottles has been identified as a potential raw material for the production of carbon anodes in lithium-ion batteries (LIBs) due to its high carbon content and abundance of ester bonds [2].

In this study, we upcycled waste PET into phosphorus-doped hard carbon (P-HC) through a single-step pyrolysis process with orthophosphoric acid ( $H_3PO_4$ ), aiming to enhance the electrochemical properties of the resultant carbon. The synthesized P-HC was characterized using Fourier-transform infrared spectroscopy (FTIR), thermogravimetric analysis (TGA-DSC), X-ray diffraction (XRD), scanning electron microscopy (SEM), and transmission electron microscopy (TEM) to elucidate its structural and thermal properties.

Electrochemical characterizations revealed that the P-HC anodes exhibit superior lithium storage capabilities, including high specific capacity and excellent rate capability ( $492 \text{ mAhg}^{-1}$  at  $0.1 \text{ Ag}^{-1}$  and  $131 \text{ mAhg}^{-1}$  at  $3.5 \text{ Ag}^{-1}$ , respectively), significantly outperforming non-doped PET-derived carbon. This enhancement is attributed to the improved electrical conductivity and structural stability imparted by phosphorus doping [3]. The P-HC anodes retained a high specific capacity after numerous cycles, demonstrating their potential for long-term application in LIBs.

This study presents a dual solution to plastic pollution and energy storage challenges by converting PET waste into high-performance anode materials for next-generation LIBs. This sustainable approach not only mitigates environmental impact but also contributes to the advancement of energy storage technologies.

### References

[1] Suzuki, G., Uchida, N., Tuyen, L. H., Tanaka, K., Matsukami, H., Kunisue, T., Takahashi, S., Viet, P. H., Kuramochi, H.; Osako, M. (2022). Mechanical recycling of plastic waste as a point source of microplastic pollution. *Environmental Pollution*, 303. <https://doi.org/10.1016/j.envpol.2022.119114>

[2] Chen, D., Luo, K., Yang, Z., Zhong, Y., Wu, Z., Song, Y., Chen, G., Wang, G., Zhong, B.; Guo, X. (2021). Direct conversion of ester bond-rich waste plastics into hard carbon for high-performance sodium storage. *Carbon*, 173, 253–261. <https://doi.org/10.1016/j.carbon.2020.11.004>

[3] Wang, H., Liu, S. T., Lei, C., Qiu, H. R., Jiang, W. Q., Sun, X. J., Zhang, Y. Q.; He, W. X. (2024). P-doped hard carbon material for anode of sodium ion battery was prepared by using polyphosphoric acid modified petroleum asphalt as precursor. *Electrochimica Acta*, 477. <https://doi.org/10.1016/j.electacta.2024.143812>



## Effect of hydrogen on flow stress in Al-Cu alloy: a multiscale approach

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In the present work, a multiscale study of the effect of hydrogen accumulated in  $\theta'$  phases on the mechanical properties of Al-Cu alloy is carried out. The mechanisms of the dislocation-precipitate interaction are studied depending on the hydrogen content in the inclusion at the level of atomistic simulation. It is shown that in a system without hydrogen, the interaction occurs by the mechanism of the Orowan loop formation around the inclusion. Energetically preferable places for hydrogen location near strengthening inclusions of the  $\theta'$ -phase in the Al-Cu alloy are determined. The system with the maximum hydrogen content exhibits at room temperature a tendency to absorb hydrogen atoms initially located at the interface. It is shown that the accumulation of hydrogen in the volume  $\theta'$  causes a decrease in the resistance of the inclusion to shear and causes a change in the mechanism of interaction from the formation of an Orowan loop to the cutting of the inclusion. This result was obtained in MD for two considered inclusion sizes: 5 and 10 nm. Features registered at the atomistic level are transferred to the level of continuum modeling. We construct a simplified model of the interaction of dislocations with precipitates, taking into account hydrogen softening. The mechanism of softening of inclusions associated with a change from looping to cutting is transferred to the DDD level. The DDD results demonstrate that H charging of Al-Cu alloy can substantially decrease its shear strength. Molecular dynamics (MD) calculations are performed using LAMMPS package. [1]. To describe interatomic interactions in the Al-Cu-H ternary system, the BOP potential proposed by [2] is used.

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### References

- [1] S. Plimpton, J. Comput. Phys. 117 (1995).
- [2] X. Zhou, D. Ward, M. Foster. New J. Chem. 42, 5215-5228 (2018).

## Fe-doped SnO<sub>2</sub> based gas sensor produced by SILAR for acetone gas sensing

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Volatile organic compounds (VOCs) are a significant concern due to their widespread presence as indoor air pollutants. These chemical vapors pose a detrimental impact on human health. Research has confirmed a strong correlation between the emission of VOCs and the incidence of certain types of cancers. [1]. Acetone, also known as propanone, dimethyl ketone, 2-propanone, propan-2-one, and  $\beta$ -ketopropane, is a versatile chemical with extensive applications in both laboratory and industrial contexts. [2]. Acetone, a volatile organic compound (VOC), can be detected in the exhaled breath of individuals with diabetes. The elevated levels of acetone in diabetic patients' breath make it a potential biomarker for non-invasive diagnosis of the condition [3]. Research has shown that measuring the concentration of acetone in a person's exhaled breath can serve as a viable alternative to traditional invasive blood tests for diagnosing and monitoring diabetes [4]. Thus, there is a great deal of interest in accurately determining the amounts of acetone.

Metal-oxide-semiconductor (MOS) materials have garnered significant attention as chemoresistive sensors for environmental monitoring applications. These sensors are capable of detecting and responding to a wide range of gases and volatile organic compounds (VOCs) by undergoing changes in their electrical resistance upon interaction with the target molecules. [5–6]. In recent years, considerable efforts have been focused on developing gas sensors using various oxide semiconductors like SnO<sub>2</sub>, WO<sub>3</sub>, In<sub>2</sub>O<sub>3</sub>, ZnO, NiO, MnO<sub>2</sub>, and V<sub>2</sub>O<sub>5</sub>.



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Among these oxide semiconductors, SnO<sub>2</sub> stands out as an n-type semiconductor with a broad band gap of 3.6 eV, attracting significant interest due to its exceptional performance and impressive chemical durability. Doping is a highly promising approach to improve the gas sensitivity and selectivity of oxide semiconductor gas sensors. This technique entails the introduction of particular impurities or foreign elements into the semiconductor material to modify its electrical and chemical characteristics. The desired gas sensors can be fabricated using the successive ionic layer adsorption and reaction (SILAR) method. Specifically, Fe-doped/ SnO<sub>2</sub> heterostructure gas sensors have been synthesized via the SILAR technique, utilizing SnCl<sub>2</sub> as the source of tin (Sn) and FeCl<sub>2</sub> as the source of iron (Fe). Doping can alter the grain size, crystal structure, oxygen distribution, and carrier concentration of gas sensing materials, enhancing the sensing capabilities of SnO<sub>2</sub> sensors. The gas selectivity assessments were conducted under uniform conditions of 100 ppm gases at 175°C, demonstrating the effectiveness of using Fe-doped SnO<sub>2</sub> sensors for detecting volatile organic compounds, particularly acetone. The study reveals that 0.5 mol.% Fe-doped SnO<sub>2</sub> exhibits exceptional response and selectivity to acetone among the tested gases, accompanied by a rapid recovery time of approximately 14 seconds. The research findings suggest that Fe-doped/SnO<sub>2</sub> sensors synthesized via the SILAR method demonstrate high selectivity to acetone vapors in air and fast recovery times. This implies that incorporating Fe ions into SnO<sub>2</sub> can be a highly effective strategy for developing high-performance gas sensors that are highly selective to acetone.

### Acknowledgements

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### References:

- [1] Al-Hardan, N. H.; Abdullah, M. J.; Abdul Aziz, A.; Ahmad, H.; Low, L. Y. ZnO Thin Films for VOC Sensing Applications. *Vacuum* 2010, 85 (1), 101–106. <https://doi.org/10.1016/j.vacuum.2010.04.009>.
- [2] Allen, P. W.; Bowen, H. J. M.; Sutton, L. E.; Bastiansen, O. The Molecular Structure of Acetone. *Trans. Faraday Soc.* 1952, 48, 991. <https://doi.org/10.1039/tf9524800991>.
- [3] Gardner, J. W.; Shin, H. W.; Hines, E. L. An Electronic Nose System to Diagnose Illness. *Sensors and Actuators B: Chemical* 2000, 70 (1–3), 19–24. [https://doi.org/10.1016/S0925-4005\(00\)00548-7](https://doi.org/10.1016/S0925-4005(00)00548-7).
- [4] Righettoni, M.; Tricoli, A.; Pratsinis, S. E. Si:WO<sub>3</sub> Sensors for Highly Selective Detection of Acetone for Easy Diagnosis of Diabetes by Breath Analysis. *Anal. Chem.* 2010, 82 (9), 3581–3587. <https://doi.org/10.1021/ac902695n>.
- [5] Lee, D.-S.; Lim, J.-W.; Lee, S.-M.; Huh, J.-S.; Lee, D.-D. Fabrication and Characterization of Micro-Gas Sensor for Nitrogen Oxides Gas Detection. *Sensors and Actuators B: Chemical* 2000, 64 (1–3), 31–36. [https://doi.org/10.1016/S0925-4005\(99\)00479-7](https://doi.org/10.1016/S0925-4005(99)00479-7).
- [6] Alizadeh, N.; Jamalabadi, H.; Tavoli, F. Breath Acetone Sensors as Non-Invasive Health Monitoring Systems: A Review. *IEEE Sensors Journal* 2020, 20 (1), 5–31. <https://doi.org/10.1109/JSEN.2019.2942693>.





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## Synthesis of N-heterocyclic compounds from renewable plant raw materials and their use as liquid organic hydrogen carriers

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Currently, the search and study of alternative energy sources is becoming increasingly relevant, and from this point of view, hydrogen is a renewable and environmentally friendly energy carrier. However, the key problem of the successful development of the hydrogen economy lies in the development of safe and efficient methods of transportation and storage of the hydrogen produced. This task is quite difficult, since the low liquefaction temperature, the high explosive content of hydrogen in gaseous form, as well as the low gravimetric energy density per unit volume lead to a high cost of hydrogen infrastructure [1].

Hydrogen can be written in covalently bound form in various chemical compounds, with subsequent release under certain conditions (metal hydrides; catalytic decomposition of methanol or formic acid). Currently, one of the most promising technologies is the use of liquid organic hydrogen carriers (liquid hydrogen carriers). The technology is based on the reversible chemical binding of H<sub>2</sub> in organic molecules (aromatic compounds and N-heterocycles). The use of LOHC such as toluene, mono- and dibenzyltoluenes allows for high energy consumption comparable to liquefied H<sub>2</sub>, as well as low cost due to the possibility of using the existing infrastructure for storage/transportation of liquid fuels. However, the endothermicity and energy consumption of the LOHC-substrate dehydrogenation stage complicate the technical implementation and reduce the energy efficiency of this process.

It is well known that H<sub>2</sub>-saturated N-heterocycles are characterized by low dehydrogenation temperatures (140-250° C) compared to cyclic hydrocarbons (350° C), and are also less volatile compounds, which allows the extraction of high purity H<sub>2</sub>. However, the disadvantage of N-heterocycles as LOHC is their lower availability, and from this point of view, one of the most promising N-heterocycles is tetradecahydrophenazine (14H-Ph), characterized by good thermal stability and high H<sub>2</sub> weight capacity (7.2 wt. %). In addition, 14H-Ph can be obtained from the decomposition products of lignin (which makes up 15-30% of lignocellulose biomass), which in the future makes 14H-Ph one of the most accessible heterocycles [2].

This report will present the results of the development of a method for the synthesis of 14H-Ph from lignin decomposition products. The process was carried out using hydrogenation reactions and, subsequently, amination of guaiacol in the presence of hydrogen, using catalysts based on nickel and/or palladium. The resulting 14H-Ph was investigated in the key process of the LOHC technology, the dehydrogenation reaction. A series of Pd-containing catalysts was used for this process. A series of highly loaded nickel catalysts (HLNC, 50-75 wt. % Ni-SiO<sub>2</sub>), previously studied in detail for the processes of toluene hydrogenation and methylcyclohexane dehydrogenation [3]. The results of the studies demonstrated a high, comparable with commercially available palladium analogues (1% Pd/C), the effectiveness of HLNC in the process of dehydrogenation of 14H-Ph. Cyclic tests of successive stages of hydrogen storage and extraction were also carried out for the most active catalyst from the Pd-containing series and various HLNC. It was shown that during five cycles of hydrogenation/dehydrogenation of 14H-Ph, only a slight loss of substrate was observed (less than 0.5 wt. %) while maintaining sufficient activity of the catalysts. Thus, it was found that when hydrogen is obtained from heterocyclic compounds, it is permissible to significantly reduce the process temperature, which ensures high purity of the extracted H<sub>2</sub> and reduces energy consumption for the dehydrogenation process.

### References

- [1] M. Niermann, A. Beckendorff, M. Kaltschmitt, K. Bonhoff, *Int. J Hydrogen Energy*, 44 (2019) 6631–6654.
- [2] D. Forberg, T. Schwob, M. Zaheer, M. Friedrich, N. Miyajima, R. Kempe, *Nature communications*, 7 (2016) 13201:1-6.
- [3] A. P. Koskin, S. A. Stepanenko, M. V. Alekseeva (Bykova), O. A. Bulavchenko, E. Y. Gerasimov, A. I. Lysikov, P. M. Yeletsky, V. V. Kaichev, V. A. Yakovlev, *Chemical Engineering Journal*, 476 (2023) 146629:1-13.



## Reforming of Steam Methane Analysis

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Steam methane reforming (SMR) is, by far, the largest source of hydrogen production. Globally, approximately 95% of all hydrogen is produced by the SMR process. This process involves reacting fossil fuels (usually natural gas), with steam at high temperature to produce hydrogen and carbon dioxide. If carbon dioxide capture is part of the process 'blue hydrogen' is produced. The hydrogen-rich gas at the outlet of the reformer is sent to a pressure swing absorber (PSA), which cleans the impurities from the gas. Hydrogen emerging from the PSA is typically 99.999% pure and this is known as the H<sub>2</sub> product gas.

In this research, steam methane reforming is analysed using thermodynamic principles followed by regression analysis. For the thermodynamics part, use is made of the Gibbs free energy minimizing technique, to find the effect of temperature, pressure and feed composition on methane conversion. The three variables, pressure, temperature and inlet gas composition, together with the methane conversion take the form of four column matrices. The thermodynamics analysis is followed by regression analysis to explore the relationship between an observed response to the various conditions. The combining of this statistical approach and the thermodynamic analysis concerning the steam reforming of methane equilibrium conditions gives results for the combined factors affecting the reactions.

The regressions used are, linear regression, parabolic regression and logarithmic regression, with the view to finding which type of regression is optimal and with the least error, to show how the conditions affect the response. This technique elucidates the behavior of reactors under different operational conditions, which makes it possible to quantitatively analyze the variation in methane conversion with changes in operational conditions.

### References

- [1] J. Moore et al. Compressors and expanders, in Machinery and Energy Systems for the Hydrogen Economy, Elsevier, 2022.
- [2] D. V. Demidov, I. V. Mishin, M. N. Mikhailov Int. J Hydrogen Energy, 36 (2011) 5941-5950.
- [3] C. Samprit, S. H. Ali, P. Bertram Regression Analysis by E, John Wiley & Sons, New York, 2006.

## Construction of better carbon anodes for K-ion batteries by defect engineering

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Due to their abundant potassium resources, potassium ion batteries are potential next-generation rechargeable alkali metal ion batteries [1]. Carbon-based materials are the most promising negative electrode materials for potassium ion batteries due to their low embedding/deintercalation potentials, high capacity and stability. The conventional graphite electrode has a low theoretical capacity (KC<sub>8</sub>, 278 mAh/g) and a large volume change (61%) during the K-intercalation process, so its application is limited.

Amorphous carbon materials have large layer spacing and abundant defect structure, which can break through the theoretical capacity limit of graphite (>300 mAh/g), and are potential carbon anode materials for potassium ion batteries. Pyrrolic nitrogen and pyridinic nitrogen exist at the edge defects of carbon materials and are considered to be effective K-storage active sites [1]. Therefore, by controllable preparation of amorphous carbon materials with abundant edge nitrogen doping sites, high capacity carbon anode materials can be developed.



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The generation of marginal nitrogen-doped sites is achieved through controlled pyrolytic carbonization of copolymers (polypyrrole-polyaniline) [2] and supramolecules [3] by selectively decomposing specific structures to expose nitrogen-doped sites. This strategy enables the preparation of high-edge nitrogen doped carbon materials at a higher carbonization temperature ( $>600\text{ }^{\circ}\text{C}$ ). By controlling the pyrolysis carbonization temperature, we achieved the regulation from edge nitrogen doping to graphitized nitrogen doping. When the carbonization temperature is  $700\text{ }^{\circ}\text{C}$ , the nitrogen doping at the edge of the prepared carbon material reaches 16.8at %, and the carbon material shows a reversible K storage capacity of up to 473mAh/g, and has good cyclic stability [3]. Further, we studied the energy storage mechanisms of Na and K in amorphous carbon materials with high edge nitrogen doping defects, and used electrochemical impedance technology to characterize different storage mechanisms of Na and K in amorphous carbon materials [4].

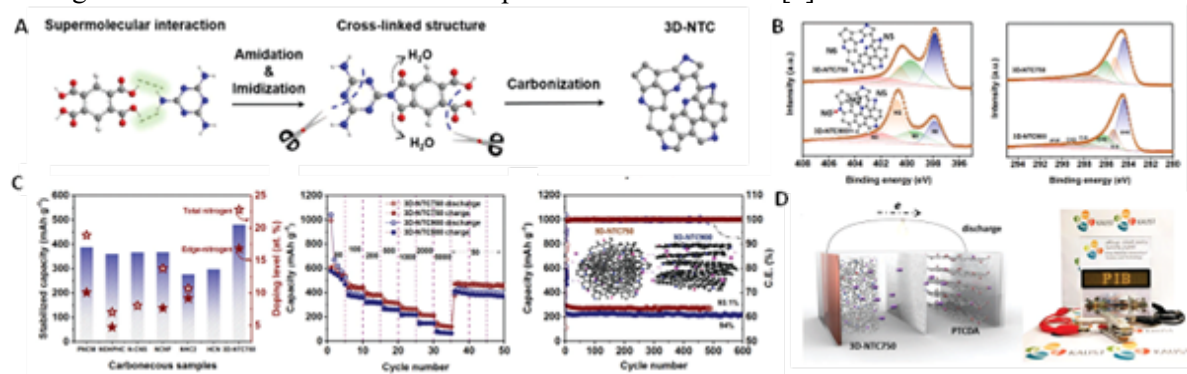


Figure 1. Methods for controlling the edge nitrogen doping in carbonaceous materials toward enhanced K-ion storage.

### References

- [1] Zhang, W.; Yin, J.; Wang, W.; Bayhan, Z.; Alshareef, H.N. Status of Rechargeable Potassium Batteries. *Nano Energy* 2021, 83, 105792.
- [2] Zhang, W.; Cao, Z.; Wang, W.; Alhajji, E.; Emwas, A.-H.; Costa, P.M.F.J.; Cavallo, L.; Alshareef, H.N. *Angew. Chem. Int. Ed.* 2020, 59, 4448–4455.
- [3] Zhang, W.; Yin, J.; Sun, M.; Wang, W.; Chen, C.; Altunkaya, M.; Emwas, A.H.; Han, Y.; Schwingschlögl, U.; Alshareef, H.N. *Adv. Mater.* 2020, 32, 2000732.
- [4] Zhang, W.; Sun, M.; Yin, J.; Wang, W.; Huang, G.; Qiu, X.; Schwingschlögl, U.; Alshareef, H.N. *Nano Energy* 2021, 87, 106184.

## Evaluation of Indoor Power Performance of Emerging Photovoltaic Technology for IoT Device Application

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The power conversion efficiency (PCE) of perovskite solar cell (PSC) has increased significantly over the last decades, obtaining a record efficiency of 25% comparable to already established PVs such as silicon based solar cells [1]. The rapid rise in power conversion efficiency (PCE) of perovskite solar cells has opened the door for enormous possibilities for powering indoor internet of Things (IoT) devices autonomously. An energy harvesting system powered by perovskite solar cell with a back-up li-ion based battery is presented as shown in Figure 1. During moments of high irradiation the battery storage system stores excess power generated by the PSC module and delivers the stored power to drive the load during scenarios of low irradiation. A DC-DC



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boost converter is engaged to match the voltage of the PSC and battery storage, a maximum power point tracking (MPPT) is achieved by perturb and observe (P&O) algorithm which perturbs the photovoltaic (PV) system by adjusting the operating voltage and observing its impact on the PV array output power.

Furthermore, the charging and discharging rate of the battery storage is controlled by the DC-DC buck-boost bi-directional converter with the incorporation of proportional integral controller (PI). A bidirectional DC-DC power flow converter is created by connecting buck and boost converters in anti-parallel to one another because conventional buck or boost converters are incapable of producing bidirectional power flow. The case scenarios for high, and low irradiance condition were modelled by varying irradiances value to  $1000 \text{ W/m}^2$ , and  $200 \text{ W/m}^2$  respectively at a constant temperature of  $25^\circ\text{C}$  with diverse battery operating state. The result obtained in this work demonstrates the promising potentials of powering low-power consumption IoT devices under indoor condition using perovskite solar cell.

**Keywords:** Photovoltaic (PV); Internet of Things (IoT); Perovskite solar cell (PSC); Maximum power point tracking (MPPT); Perturb and Observe (P&O); Proportional integral controller (PI)

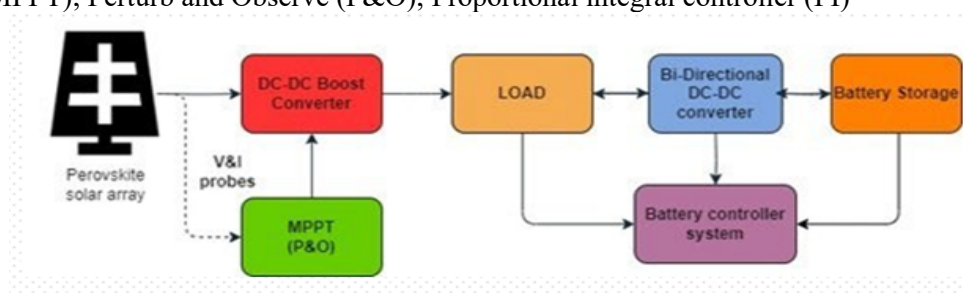


Figure 1. PSC harvesting system block diagram

### References

- [1] A. Hicks, "NREL Best Research Cell Efficiencies Chart."

## Study on effect of carbon nanomaterials as conductive additives in EDLCs

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Effects of various carbon nanomaterials using as conductive additives (5 wt%) in activated carbon-based electrodes for electrical double layer capacitors (EDLCs) were investigated. A variety of carbon nanomaterials including carbon black (CB), single-walled carbon nanotubes (SWCNT), graphene nanoplatelets (GNP), fullerenes (C<sub>60</sub>), and activated carbon nanofibers (ACNF) are considered in this work as they provide a diverse combination of intrinsic properties such as specific surface area, conductivity, micro-mesoporous structures, and geometry of nanomaterials. The results show that each carbon additive has its own strengths and limitations for different performance parameters considered. A reduction in capacitance at high current densities and material degradation during long-term cycling are observed for CB samples, which could be attributed to the high dispersibility of CB causing limited interparticle voids and thus increasing diffusion resistance. In contrast, the use of ACNFs significantly reduces the diffusion resistance and improves the cyclic stability compared with CB based samples due to the advantages of larger specific surface area and superior micro-mesoporous structures of ACNFs. In particular, EDLCs with ACNFs demonstrate an increase in specific capacitance and energy density by 99 % and 76 %, respectively compared to CB based EDLCs at a current density of 20 A/g [1].

### References

- [1] Zhanibek Ayaganov, et al. Journal of Energy Storage 78 (2024) 110035



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## Harnessing the Energy of Sun by Cost -Effective and Improved Stability Dye-sensitized Solar Cells

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Solar energy is the most promising and fast-growing field of renewable energy. The share of energy produced by photovoltaics is steadily increasing. Nevertheless, fossil fuels remain the main source of energy. The main reason for this is the cost of production. Energy produced from sunlight is more expensive than the power generated from fossil fuels. Third generation photovoltaics which includes dye-sensitized solar cells (DSSCs), perovskite solar cells, polymer solar cells and quantum dot sensitized solar cells are considered highly promising photovoltaic technology to replace traditional expensive silicon-based photovoltaics. Among 3G photovoltaic technologies dye-sensitized solar cell is unique due to their ease of preparation, affordable cost and flexibility. Further development of dye-sensitized solar cells requires new engineering solutions to improve its stability and to reduce its cost. In this work we present the development of novel materials for highly stable and cost-effective dye-sensitized solar cells. Platinum is traditionally used counter electrode material in DSSCs. Its high price may inhibit the widespread application of DSSCs. To address this issue, we present the novel Pt-free electrocatalysts such as ZnCo<sub>2</sub>S<sub>4</sub>/MWCNT [1], doped-PEDOT, FeCo<sub>2</sub>S<sub>4</sub> [2] and etc. for the use in DSSCs as counter electrode materials, see Fig. 1. Another problem related to the performance of DSSCs is poor stability caused by the use of liquid electrolyte. In this regard, we present the development of quasi-solid electrolyte made of metal-organic framework which can significantly enhance the stability of DSSCs.

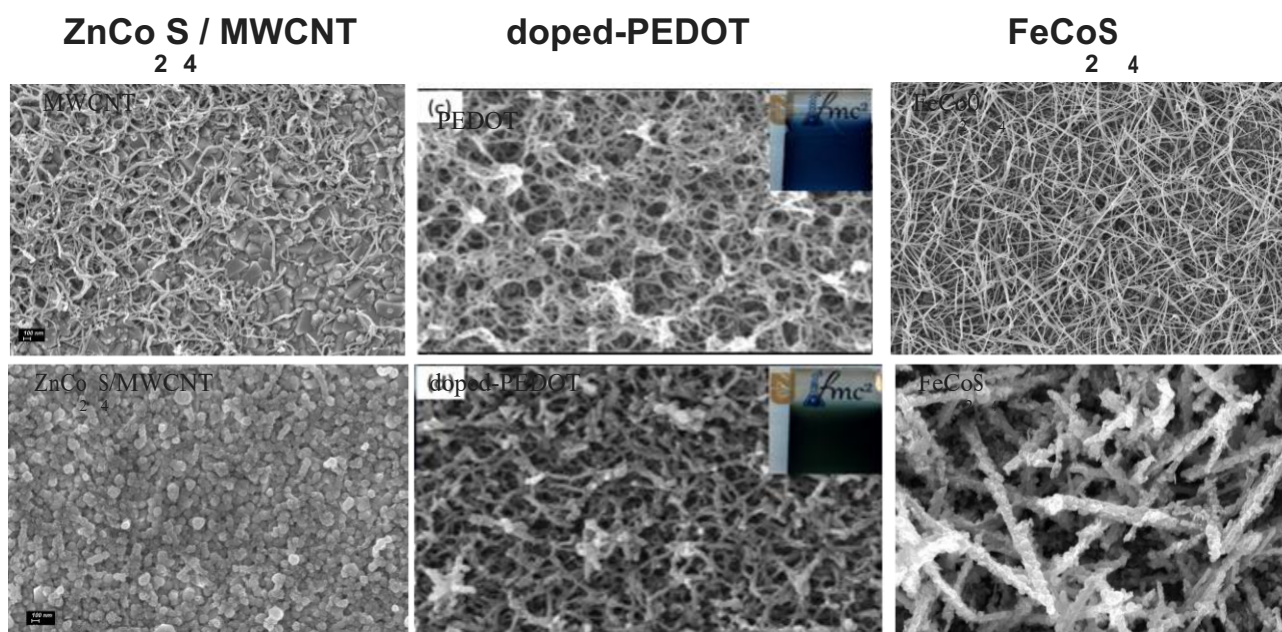


Figure 1. Cost-effective counter electrodes for dye-sensitized solar cells [1], [2].

### References

- [1] B. Bapayev, Y. Tashenov, S. Adilov, M. P. Balanay. *Surfaces and Interfaces*, V.37, 2023, 102699.  
[2] D. Suleimenova, Y. Tashenov, B. Bapayev, M. P. Balanay. *J. of Photochem. and Photobiol. A: Chemistry*, V.457, 2024, 115908.



## Enhancing the electrochemical performance of sodium-ion batteries with an external magnetic field

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A sodium-ion battery (SIB) is a promising cost-effective and more environmentally friendly alternative to lithium-ion batteries (LIB). Although SIB has lower capacity and energy density than LIB, sodium still offers a competitive advantage of being largely abundant and evenly distributed around the world [1]. The deficient performance of SIB is being tackled by a number of chemical and physical methods, among which is the application of an external field [2]. An external magnetic field has been used several times to improve the electrochemical performance of LIB by stabilising lithium metal anode by decreasing the intensity of dendritic growth. A similar phenomenon has been observed for zinc metal anode [3].

Sodium symmetrical cells containing two sodium metal discs were assembled in Argon-filled glovebox with sodium hexafluorate as an electrolyte. They were studied in this work to check the possibility of inhibiting dendrites formation and preventing related safety concerns. The long-term galvanostatic cycling (GC) of symmetrical cells under magnetic field (MF) of different strengths shown in Figure 1 indicate that under the MF influence, the cells demonstrate reduced potential polarization, which means less kinetic hindrances in the cell open operation [3]. The strength of MF did not have a linear correlation with this reduction in the polarization. The ac impedance spectra show reduced charge-transfer resistance and bulk resistance for the cell under MF, which is consistent with reduced polarization in GC. It is possible that this change in polarization is the consequence of the enhancement of mass transfer and diffusion of sodium ions with the help of MF [3], and is the subject of further investigations. Postmortem analysis of the sodium electrodes showed more uniform deposition of sodium ions under MF.

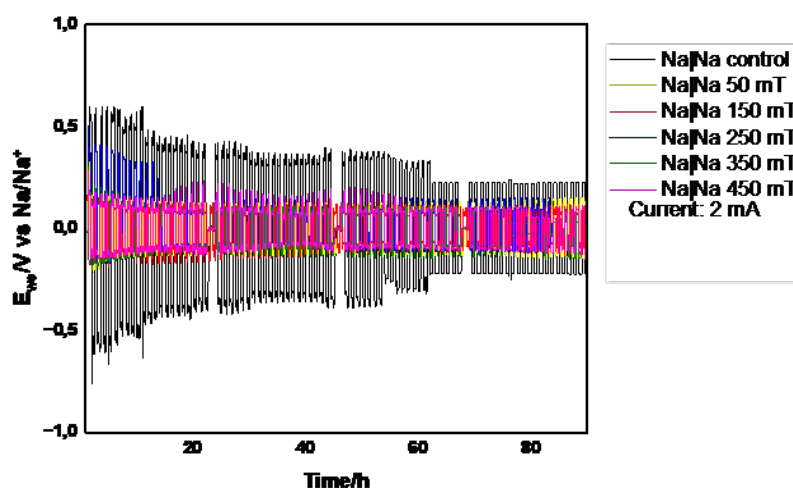


Figure 1. Galvanostatic charge-discharge of sodium symmetrical cells in the presence of MF of different strengths

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### References



## The 12<sup>th</sup> International Conference on Nanomaterials and Advanced Energy Storage Systems (INESS - 2024)

- [1] C. Bao *et al.*, ‘Solid Electrolyte Interphases on Sodium Metal Anodes’, *Adv Funct Materials*, vol. 30, no. 52, p. 2004891, Dec. 2020, doi: 10.1002/adfm.202004891.
- [2] C. Y. Zhang *et al.*, ‘Sodium-Sulfur Batteries with Unprecedented Capacity, Cycling Stability and Operation Temperature Range Enabled by a  $\text{CoFe}_2\text{O}_4$  Catalytic Additive Under an External Magnetic Field’, *Adv Funct Materials*, p. 2305908, Jul. 2023, doi: 10.1002/adfm.202305908.
- [3] Y. Chen, X. Dou, K. Wang, and Y. Han, ‘Magnetically enhancing diffusion for dendrite-free and long-term stable lithium metal anodes’, *Green Energy & Environment*, vol. 7, no. 5, pp. 965–974, Oct. 2022, doi: 10.1016/j.gee.2020.12.014.

### Effect of Zn modification on the low-temperature performance of graphite and hard carbon anodes in lithium-ion batteries

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Graphite is the first and the most widely used anode in commercial lithium-ion batteries (LIBs) because of charge/discharge profiles, resembling the lithium metal, and the safety of the material at room temperature [1]. However, it is admitted as one of the critical limiting factors for applying LIBs under harsh conditions, especially in low-temperature (LT) environments [2]. The main challenges in graphite anode at low temperatures include decreased electrical conductivity, restricted diffusion of  $\text{Li}^+$ , and formation of unstable or too thick solid electrolyte interphase (SEI) layer with low conductivity [3].

Modification of electrode materials by metals is one of the most effective ways in promoting the LT performance of LIBs, as it comprehensively improves the properties of the active material [4]. In particular, the addition of metal to the graphite anode can increase the conductivities and stabilize the SEI layer by catalyzing the formation of components with high ionic conductivities and restricting their overgrowth. The effect of different metals, including Au, Ag, Ni, Cu, Al, and Sn, on the LT performance of the graphite anode, has been studied [5]. On the other hand, to the best of our knowledge, the effect of Zn addition has not been reported yet.

In this work, Zn-modified graphite and hard carbon electrodes were prepared by partially substituting conducting agent Acetylene Black with Zn. Effect of 1 wt.% Zn addition on the LT performance of graphite and hard carbon anodes and SEI formation was studied in comparison to pristine Zn-free electrodes.

#### Acknowledgments

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#### References

- [1] F. Nobili, M. Mancini, S. Dsoke, R. Tossici, R. Marassi, J. Power Sources. 195 (2010) 7090–7097.
- [2] Y. Yan, L. Ben, Y. Zhan, X. Huang, *Electrochim. Acta.* 187 (2016) 186–192.
- [3] A. Belgibayeva, A. Rakhmetova, M. Rakhatkyzy, M. Kairova, I. Mukushev, N. Issatayev, G. Kalimuldina, A. Nurpeissova, Y.K. Sun, Z. Bakenov, *J. Power Sources.* 557 (2023) 232550.
- [4] M. Marinaro, F. Nobili, A. Birrozzi, S.K. Eswara Moorthy, U. Kaiser, R. Tossici, R. Marassi, *Electrochim. Acta.* 109 (2013) 207–213.
- [5] F. Nobili, S. Dsoke, T. Mecozzi, R. Marassi, *Electrochim. Acta.* 51 (2005) 536–544.



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## Synthesis of $\text{LiCoPO}_4@\text{C}$ composite nanofibers and their application as high-voltage cathode materials for lithium-ion batteries

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The rapid growth of lithium-ion battery (LIB) technology has led to an increase in demand for promising high-voltage cathode materials that are stable at high temperatures, nontoxic and are low cost [1]. Despite increasing use of LIBs due to their promising long cyclability and negligible memory effect, there is still room for further investigations to tackle challenges of lower power density, thermal runaway risks, and the ageing effect [2].

In order to address those challenges, lithium cobalt phosphate ( $\text{LiCoPO}_4$ , LCP) – a high-voltage cathode material with promising high energy density was chosen [3]. In comparison to widely commercialised  $\text{LiFePO}_4$  (LFP), having similar specific capacity as of LCP, the latter offers much higher operating voltage [3]. However, the absence of essential understanding about material crystal characteristics hinders the development of LCP in addition to electrolyte interfacial reaction caused by high voltage range [3]. Therefore, this research aims to enhance the overall characteristics of  $\text{LCP}@\text{C}$  materials using the nanosize structure improving ionic diffusivity and the synthesis of free-standing nanofibers utilising the environmentally friendly electrospinning process [4].

With the exception of adding a stoichiometric quantity of lithium nitrate and electrospinning at predetermined electrospinning parameters, the electrospinning solution was prepared as previously reported [5]. The fibres were dried at 150 °C and pre-oxidized at different temperatures, as mentioned in the sample names, before undergoing heat treatment at 700 °C in a nitrogen atmosphere. The molecular structure of nanofibers was obtained from Fourier Transform Infrared (FTIR) analysis using Nicolet iS10 FT-IR Spectrometer, while morphology of nanofibers were examined using scanning electron microscopy (SEM, Crossbeam500, Zeiss). The electrochemical performance was evaluated using CR2032 coin-type cells. Li chips were used as reference electrodes, along with polypropylene separators, ~50  $\mu\text{L}$  of an electrolyte solution that contained 1 M  $\text{LiPF}_6$  in a solvent mixture of ethylene carbonate and dimethyl carbonate (EC:DMC=1:1 vol.), and  $\text{LCP}@\text{C}$  composite nanofibers which served as free-standing cathodes with a mass loading of about 2  $\text{mg cm}^{-2}$ . The cells were evaluated in the potential range of 3.5–5.3 V vs.  $\text{Li/Li}^+$  at a current density of 0.1 C.

The FTIR plot is shown in Figure 1a, showing clear disparities between annealed samples varying only with pre-oxidation temperatures. The peaks at around 900-1100  $\text{cm}^{-1}$  are prescribed for the formation of phosphate groups while the peaks differences for the  $\text{LCP}@\text{C}$ -280 sample might indicate the presence of lithium phosphate. The SEM images in Figure 1b depict the formation of nanofibers with beads; the fibers' average diameter is between 280 and 330 nm. The detailed electrochemical performance of synthesised  $\text{LCP}@\text{C}$  nanofibers will be demonstrated at the conference.

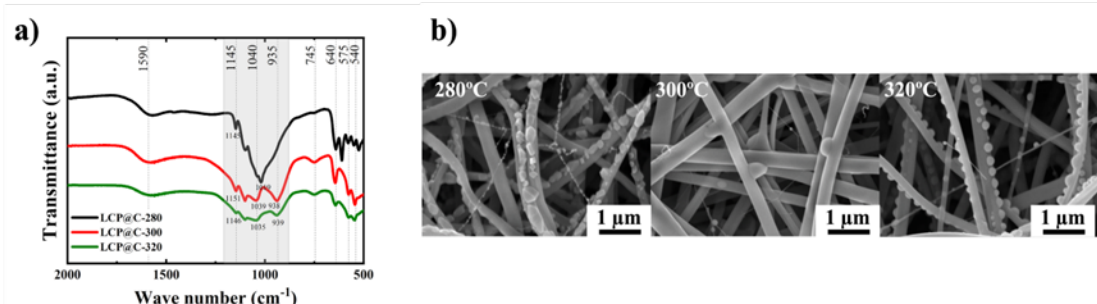


Figure 1. FTIR spectra (a) and SEM images (b) of  $\text{LCP}@\text{C}$  cathode materials pre-oxidized in the temperature range of 280-320 °C.





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### References

- [1]Ren et al., *Electrochim. Acta* 461 (2023) 142630
- [2]Liu et al., *J. of Cleaner Production* 423 (2023) 138678
- [3]Woo et al., *Mater. Adv.*, 4 (2023) 4823
- [4]Belgibayeva et al., *Electrochim. Acta* 419 (2022) 140400
- [5]Belgibayeva et al., *ChemElectroChem.* 9 (2022) e202200458

## Three-Dimensional Carbon Coated and High Mass-Loaded NiO/Ni Anode with High Specific Capacity for Lithium Ion Battery

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Nickel oxide (NiO) is notable for its impressive theoretical specific capacity, making it a highly attractive candidate for electrode materials in electrochemical energy storage applications. However, its practical application is hindered by subpar electrochemical performance and complex electrode fabrication processes. To address these challenges, we propose a porous three-dimensional NiO/Ni anode with a high mass loading of 6-7 mg/cm<sup>2</sup>, fabricated through thermal oxidation followed by carbon coating.

The resulting porous NiO/Ni anode was thoroughly characterized using scanning electron microscopy (SEM), X-ray diffraction (XRD), and energy-dispersive X-ray spectroscopy (EDS). When employed as an anode material for lithium-ion batteries (LIBs), this anode demonstrated an impressive reversible capacity of 715 mAh/g at 0.1C after 100 cycles. Additionally, it exhibited excellent electrochemical performance at high current, maintaining a specific capacity of 350 mAh/g at 1C after 100 cycles.

## Green Synthesis of SnO<sub>2</sub> Microspheres and Their Excellent Performance as an Active Anode Material in Low-Temperature Lithium-ion Batteries

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The green method is rapidly becoming the preferred approach to nanomaterial production to overcome problems with chemical synthesis, such as the use of hazardous chemicals and the creation of undesired by-products. Here we offer an environmentally friendly synthesis of a composite (SnO<sub>2</sub> nanopowder coated with



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carbon) and its application in sub-zero lithium-ion battery (LIB) anode. The synthesis technique is based on the conversion of the tin chloride dihydrate precursor into tin oxide nanopowder in plant extract media and its coating with biomass-derived carbon. The banana peel served as our source of both plant extract and carbon source.

When the composite was used as an anode in LIB, a stable specific capacity of 1150 mAh/g after 100 cycles was demonstrated. In addition, it showed outstanding capacity retention when charging and discharging at -20 °C, showing 750 mAh/g after 100 cycles. Composite SnO<sub>2</sub>/C microspheres are a viable anode material for the next generation of high-performance LIBs due to their improved specific capacity, reliable cyclic stability, and superb electrode performance.

### Effect of electrospinning solution concentration on the electrochemical properties of carbon composite nanofibers of zinc compounds as anode materials for lithium-ion batteries

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Zinc (Zn) is recognized for its abundance and eco-friendliness, presenting a range of compounds such as zinc oxide, sulfide, selenide, phosphides, and phosphates [1]. Although research on zinc phosphate as an anode material is limited, its distinctive properties have been acknowledged in various applications [2,3]. This study explores carbon composite nanofibers of zinc phosphate-based compounds synthesized using the facile electrospinning method directly from polyvinylpyrrolidone (PVP)-containing precursors.

Zinc compounds were synthesized through electrospinning combined with a two-step heat treatment process. Electrospinning solutions were prepared with varying concentrations of zinc nitrate, PVP, and phosphoric acid to identify the optimal spinnable concentration yielding the best physical and electrochemical properties. The electrospinning was conducted at a voltage of 18 kV, 1.0 mL h<sup>-1</sup> flow rate, and 10 cm tip-to-collector distance, using flat collector. The resulting fibers were dried at 120 °C for 12 h, and pre-oxidized at 280 °C for 1 h, and then annealed for 1 h at 750 °C in N<sub>2</sub> + H<sub>2</sub> (4%).

The formation of the desired materials was verified using X-Ray diffraction (XRD, Miniflex, Rigaku) and scanning electron microscopy (SEM, Crossbeam500, Zeiss). XRD patterns of ZnPO@C samples with different concentrations indicated the formation of Zn<sub>2</sub>P<sub>2</sub>O<sub>7</sub> with some *a*-Zn<sub>3</sub>(PO<sub>4</sub>)<sub>2</sub> impurities shown in. SEM images confirmed the fibrous morphology of the ZnPO@C nanofibers shown in.

CR2032 coin-type cells with lithium were assembled in a glove box under argon gas, using approximately ~50 µL of 1 M LiPF<sub>6</sub> dissolved in a mixture of ethylene carbonate, diethyl carbonate, and ethyl methyl carbonate (EC:DEC:EMC=1:1:1 vol.) as the electrolyte, with a polypropylene separator. The electrochemical properties of coin-type cells were evaluated using ZnPO@C nanofibers. The cells were tested at a current density of 100 mA g<sup>-1</sup> within a potential range of 0.01–3.0 V vs. Li/Li<sup>+</sup>. The results demonstrated that the sample prepared from a solution with optimal concentration of precursors exhibited the best electrochemical performance with an initial charge capacity of 772 mAh g<sup>-1</sup> (based on the mass of the composite including 45 wt% carbon).

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#### References

- [1] Y. Zhang, J. Wang, M. Alfred, P. Lv, F. Huang, Y. Cai, H. Qiao, Q. Wei, *Energy Storage Materials* 51 (2022) 2405-8297
- [2] Y. Guo, Y. Liu, Y. Li, S. Hou, T. Liu, L. Zhao, *Applied Surface Science* 508 (2020) 145288.
- [3] Y. Li, Z.T. Wang, G. Liu, J. Wang, J. Wang, *Advanced Powder Technology* 32 (2021) 4651–4657.f



## Synthesis and electrochemical characterization of hollow silica-embedded dehydrogenated polyacrylonitrile fibers as anode for lithium-ion batteries

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Lithium-ion batteries (LIBs) have become the cornerstone of portable electronic devices and electric vehicles due to their high energy density and long cycle life. However, the current demand for higher energy density and faster charging rates necessitates the development of advanced electrode materials. Among various electrode materials, silica (SiO<sub>2</sub>) as an anode material offers high theoretical capacity of 1965 mAh g<sup>-1</sup>, low cost, and minimal environmental impact [1,2]. On the other hand, in practice, bulk SiO<sub>2</sub> possesses poor electrochemical characteristics, originating from its high volume expansion during lithiation and delithiation, as well as low electrical conductivity. One solution to this problem is the compositing nanostructured SiO<sub>2</sub> with dehydrogenated polyacrylonitrile (DPAN), which is one of the most common electroforming matrices and carbon sources due to its high carbon yield and excellent mechanical properties [3].

In this work, we obtained hollow silica-embedded DPAN fibers (denoted as SiO<sub>2</sub>@DPAN) using electrospinning method and further heat treatment at 300 °C in the reduced atmosphere. Additionally, pristine hollow SiO<sub>2</sub> and DPAN with KB fibers without SiO<sub>2</sub> were obtained for comparative purposes.

The physical and electrochemical characteristics of the obtained samples were performed using various analytical techniques such as Scanning electron microscope (SEM), Transmission Electron Microscope (TEM), X-ray diffractometer (XRD), Brunauer–Emmett–Teller (BET).

Electrochemical characterizations reveal that the SiO<sub>2</sub>@DPAN fibers exhibit superior lithium storage properties, including high specific capacity, excellent cycling stability, retaining 940 mAh g<sup>-1</sup> after 100 cycles at a current density of 0.1 A g<sup>-1</sup>. The incorporation of hollow SiO<sub>2</sub> nanoparticles into DPAN fibers not only creates a porous architecture for enhanced lithium-ion diffusion but also mitigates volume expansion during lithiation, thereby improving the structural stability of the electrode. This study demonstrates the potential of SiO<sub>2</sub>@DPAN fibers as promising anode materials for next-generation LIBs, paving the way for the development of high-performance energy storage devices.

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### References

- [1] D. Sui, M. Yao, L. Si, K. Yan, J. Shi, J. Wang, C.C. Xu, Y. Zhang, Carbon N Y 205 (2023) 510–518.
- [2] L. Li, Y. Deng, K. Hu, B. Xu, N. Wang, Z. Bai, X. Xu, J. Yang, Progress in Natural Science: Materials International 33 (2023) 16–36.
- [3] S. Kalybekkyzy, A. Mentbayeva, M.V. Kahraman, Y. Zhang, Z. Bakenov, J Electrochem Soc 166 (2019) A5396–A5402.



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## **V<sub>2</sub>C MXene as an alternative anode material for low-temperature lithium-ion batteries**

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Lithium-ion batteries (LIBs) are a crucial energy storage technology, utilized in a wide range of devices from mobile phones and laptops to electric vehicles and stationary storage systems. However, their electrochemical performance significantly deteriorates in low-temperature (LT) environments, presenting a major obstacle to their widespread practical use. The conventional structure of LIBs reveals several issues that impact their performance at low temperatures. Notably, the rapid diffusion of lithium ions within the anode is commonly identified as a bottleneck for improving LT LIB performance.

In this context, we propose V<sub>2</sub>C Mxene as a promising alternative anode material for LT LIBs. V<sub>2</sub>C Mxene possesses properties such as high energy density, excellent electrical conductivity, structural stability and ductility, and a large surface area, making it a potentially more efficient and safer anode material capable of operating at low temperatures without reducing battery life. When utilized as an anode in LIBs, V<sub>2</sub>C Mxene demonstrated impressive characteristics, achieving a specific capacity of 420 mAh/g at a current of 0.1 A/g after 100 cycles at room temperature. Additionally, it maintained a significant capacity of 65 mAh/g at a current of 0.1 A/g after 100 cycles at -20 °C. The morphological and structural properties of the synthesized Mxene were thoroughly investigated using scanning electron microscopy (SEM), X-ray diffraction (XRD), Raman spectroscopy, and X-ray photoelectron spectroscopy (XPS).

## **PTHF-based solid polymer electrolyte through UV cross-linking**

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The development of lithium-ion batteries (LIBs) has become increasingly important in recent years due to growing demand for sustainable energy solutions, smaller smart electronics, wearable devices, and the expanding portable electronics market. Efforts have focused on improving the electrochemical performance and safety of LIBs. Safety concerns such as leakage, flammability, and toxicity, often associated with liquid electrolytes, underscore the necessity for secure solid-state batteries utilizing solvent-free electrolytes [1]. In this study, we present a thermally stable SPE fabricated by UV-induced cross-linking of acrylated PTHF (a-PTHF), poly(ethyleneglycol) diacrylate (PEGDA), trimethylolpropane ethoxylate triacrylate (ETPTA), and lithium bis(trifluoromethanesulfonyl)imide salt (LiTFSI), exploring various ratios of EO:Li. To fabricate solid polymer electrolyte films, polytetrahydrofuran's terminal groups were modified by incorporating acrylate-groups, known for their photosensitivity in cross-linking processes. The completeness of the acrylation was confirmed by observing peaks corresponding to acrylic (C=C) and C=O bends at 1636 and 1724 cm<sup>-1</sup>, respectively, in the FTIR spectrum of the product.

Subsequently, cross-linked flexible polymer films were prepared by UV irradiation of a polymer blend comprising a-PTHF, PEGDA, and ETPTA at various EO ratios. The disappearance of peaks at 1636 and 750



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cm<sup>-1</sup>, attributed to C=C and =C-H bends, indicated successful cross-linking process. These solid polymer electrolytes, based on acrylated polytetrahydrofuran, produced flexible and transparent films. SEM analysis confirmed that the lithium salt was fully dissolved in the polymer, resulting in smooth SEM images.

The outstanding mechanical strength and flexibility of these solid polymer electrolytes enabled the production of thin films, measuring 60 microns in thickness. Ionic conductivity studies revealed that the obtained solid polymer electrolytes using a-PTHF exhibited moderate ionic conductivity. Notably, among the polymer films, those with EO ratios of 6 and 8 demonstrated ionic conductivities of  $1.1 \cdot 10^{-5} \text{ S} \cdot \text{cm}^{-1}$  and  $1.65 \cdot 10^{-5} \text{ S} \cdot \text{cm}^{-1}$  at 80 °C, respectively.

Electrochemical studies conducted on Li/LFP coin cells using these solid polymer electrolytes showed favorable electrochemical performance. The samples exhibited exceptional mechanical strength and flexibility, highlighting their promising potential for use in Li-ion batteries.

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### References

[1] Y. Zhao, L. Wang, Y. Zhou, Zh. Liang, N. Tavajohi, B. Li, T. Li *Adv. Science*, 8 (2021) 2003675.

## Synthesis and electrochemical characterization of sulfur hosted in hybrid carbon composition as a cathode for lithium-sulfur batteries

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Lithium-Sulfur energy storage technology is considered “next-generation” battery technology, due to environmental sustainability, cost-effectiveness, and potential for high specific energy [1]. However, a low practical difficulties comes with LSB integration including the polysulfide shuttle effects, the low conductivity of sulfur, and low coulombic efficiency, which prevent a high and stable performance of batteries [2-3]. To overcome such obstacles, we examined commercial carbon black (Super P), buckwheat-derived hard carbon and single-walled carbon nanotubes (Tuball) in the hybrid substrate, which cooperate well with each other in an appropriate mass ratio as a sulfur host.

In this work, different sulfur/hybrid carbon composites were obtained via dissolving in CS<sub>2</sub>:ISO and further heat treatment at 155 °C for 12 h. The microstructure and morphology of the sulfur/carbon composites were performed using Scanning electron microscope (SEM), Transmission Electron Microscope (TEM), X-ray diffractometer (XRD).

Electrochemical characterizations revealed, when the mass ratio of hard carbon:Super P:Tuball is 3.3:2.3:1, it achieves the highest initial capacities of 1144.50 and 1161.35 mAh g<sup>-1</sup> when utilized as a cathode-active material. The discharge capacity drops to 822.8 mAh g<sup>-1</sup> (composite) after 25 cycles, indicating a capacity fading of about 1.1% per cycle. Besides, the cathode offers a high Coulombic efficiency of about 100%. The significant improvements in the electrochemical performance are associated with the desirable combination of Hard carbon:SuperP:Tuball in the hybrid carbon substrate. Thus, this work provides an innovative, non-complicated and low-cost strategy to synthesize high-performance sulfur/carbon composites as cathode materials for LSBs.



### Acknowledgments

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### References

- [1] Ould Ely, T., Kamzabek, D., Chakraborty, D., & Doherty, M. F. (2018). Lithium-Sulfur Batteries: State of the Art and Future Directions. In ACS Applied Energy Materials (Vol. 1, Issue 5, pp. 1783–1814). American Chemical Society. <https://doi.org/10.1021/acsaem.7b00153>
- [2] Seh, Z. W., Sun, Y., Zhang, Q., & Cui, Y. (2016). Designing high-energy lithium-sulfur batteries. *Chemical Society Reviews*, 45(20), 5605–5634. <https://doi.org/10.1039/c5cs00410a>
- [3] Imtiaz, S., Zhang, J., Zafar, Z. A., Ji, S., Huang, T., Anderson, J. A., Zhang, Z., & Huang, Y. (2016). Biomass-derived nanostructured porous carbons for lithium-sulfur batteries. *Science China Materials*, 59(5), 389–407. <https://doi.org/10.1007/s40843-016-5047-8>

## UV-crosslinked PTHF-based ultrathin composite polymer electrolytes with LATP nanoparticles

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Improvements in the safety and performance of lithium-ion batteries have given rise to the idea of using a solid electrolyte to create all-solid-state batteries. Developing solid electrolytes with high ionic conductivity, high electrochemical and thermal stability, and excellent electrode compatibility is a critical challenge for high-performance all-solid-state Li-ion batteries (1).

Solid electrolytes are considered a promising candidate to replace liquid electrolytes due to their superior mechanical properties (helpful in suppressing or eliminating uneven lithium electrodeposition and slowing subsequent dendrite formation) and a wide range of electrochemical stability. In addition to solid inorganic ceramic electrolytes, solid polymer electrolytes are becoming increasingly attractive, in which polymers are mixed with lithium salts. Unfortunately, the low ionic conductivity of such electrolytes at room temperature limits their use in commercial lithium-ion batteries. To overcome this problem, several strategies have been widely investigated, including the use of copolymers, the introduction of plasticizers, and the addition of ceramic fillers (5).

One promising candidate for a loosely coordinating solid polymer electrolyte (SPE) is poly(tetrahydrofuran) (PTHF). Adding structured ceramic fillers to modified PTHF can significantly increase the ionic conductivity of the solid polymer electrolyte. Our work studies the preparation and characterization of a composite solid polymer electrolyte based on  $\text{Li}_{1+x}\text{Al}_x\text{Ti}_{2-x}(\text{PO}_4)_3$  (LATP) and methacrylated polytetrahydrofuran (m-PTHF) as a matrix.

Polytetrahydrofuran (PTHF) is structurally similar to PEO, which is commonly used polymer in electrolyte development, but has fewer oxygen heteroatoms in the main chain (2). The PTHF polymer exhibits poor thermal stability and a low melting temperature, resulting in significant degradation at temperatures as low as 60 °C (3). In this work, to address the mentioned issues, to improve the mechanical stability of the PTHF polymer, a methacrylation reaction was carried out using 2-isocynoethylmethacrylate and adding dibutyltin diacetate catalyst, where the solvent used was dichloromethane (3). To fabricate composite electrolytes, LATP ceramic filler was synthesized by evaporation-induced self-assembly (EISA) (4). If x is 0.4 in the LATP structure, it has the highest ionic conductivity of all NASICON structured electrolytes according to previous studies [4.5]. Modified PTHF was mixed in different ratios with LiTFSI salt and LATP ceramic nanofiller and



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then exposed to UV radiation (365 nm). The components were poured between two glass slides and exposed to UV radiation for 15 minutes. All work was done in a glove box filled with argon.

The chemical structure of synthesized m-PTHF was confirmed by FTIR analysis. Obtained composite polymer electrolytes electrochemical performance was tested by systematic electrochemical impedance spectroscopy (EIS), cyclic voltammetry and cyclability tests. The highest ionic conductivity of the resulting composite electrolyte is reached  $1.57 \times 10^{-5}$  S/cm at 80 °C, making it a promising value for application in LIBs.

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### References

- [1] Zhengkun Xie, Zhijun Wu, Xiaowei An, Xiyan Yue, Pairuzha Xiaokaiti, Akihiro Yoshida, Abuliti Abudula, Guoqing Guan, Journal of Membrane Science, February 2020.
- [2] M. Alamgir, R. D. Moulton, K. M. Abraham, Electrochim. Acta 1991, 36, 773.
- [3] David G. Mackanic, Wesley Michaels, Minah Lee, Dawei Feng, Jeffrey Lopez, Jian Qin, Advanced Energy Materials, July 2018.
- [4] Xingang Liu, Ju Fu and Chuhong Zhang, Nanoscale Research Letters (2016), 11, 551
- [5] Qian Zhang, Kun Liu, Kang Liu, Junpeng Li, Chunjie Ma, Liang Zhou, Yaping Du, Journal of Colloid and Interface Science, November 2020, 389-398.
- [6] Yang Li, Wei Zhang, Qianqian Dou, Ka Wai Wong, Ka Ming Ng, The Royal Society of Chemistry, 2019, 7, 3391–3398

## Optimizing sulfur thin-film cathodes for Li|S microbatteries

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Lithium-Sulfur (Li|S) batteries offer substantial potential for high-energy-density and cost-effective energy storage, positioning them as promising candidates for next-generation portable and sustainable energy solutions. However, their application in microdevices has been limited due to challenges in integrating sulfur thin-film cathodes. Sulfur's high theoretical capacity of 1675 mAh/g and energy density of 2600 Wh/kg is counterbalanced by issues such as poor electrical conductivity, polysulfide dissolution, and significant volume changes during cycling, which lead to rapid capacity degradation and short cycle life.

Our research addresses these challenges by exploring advanced fabrication techniques and composite materials to optimize sulfur thin-film cathodes for Li|S microbatteries. We focus on enhancing cathode performance through the incorporation of carbon materials, using mechanochemical synthesis and spin-coating methods. These strategies aim to improve conductivity, encapsulate soluble polysulfides, and increase overall battery stability.

We also investigate the role of gel-polymer electrolytes based on polyethylene oxide (PEO) cross-linked with oxide electrolytes such as Li<sub>7</sub>La<sub>3</sub>Zr<sub>2</sub>O<sub>12</sub> (LLZO), which enhance ionic conductivity and mechanical robustness. Our results demonstrate significant improvements in electrochemical performance, including initial discharge capacities of up to 1829 mAh/g and high coulombic efficiencies (CE) of 97-99% over extended cycling.

Material characterization using SEM, TEM, XRD, and FTIR confirms the uniform distribution and stability of the composite materials. Figure 1 illustrates the detailed schematic representation of the cathode preparation process, highlighting the sequential steps involved in synthesizing the S/CNT/SP composite precursor and the subsequent spin-coating of the sulfur cathode slurries onto ultra-high vacuum (UHV) Al foil.



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The optimized spin-coating parameters ensure a dense slurry of minimal thickness, which is crucial for enhancing battery performance and stability.



Figure 1. Schematic representation of cathode preparation

Electrochemical testing of the Li|S cells with additional PEO/PVDF/LLZO/LiTFSI coating layers reveals substantial improvements in capacity retention and cycle life, reaching a specific capacity of 1230 mAh/g after 100 cycles.

Our study led to the successful assembly of a Li|S microbattery prototype, demonstrating promising performance metrics. The prototype achieved an initial areal capacity of approximately 110  $\mu\text{Ah}/\text{cm}^2$  and maintained a stable coulombic efficiency (CE) of 97%. This innovative approach to Li|S microbatteries paves the way for reliable, high-performance energy storage solutions for microdevices.

### Acknowledgements

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## Synthesis of carbon composite nanofibers of germanium-based compounds and their electrochemical performance as anode materials for lithium-ion batteries

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Lithium-ion batteries (LIBs) have advantages including high energy density, large output power, minimal self-discharge, and long cycle life. LIBs are frequently employed in electric vehicles and mobile devices as a type of energy technology. However, low theoretical capacity of commercially-used graphite anode is limiting the further advancement of LIBs [1].

Germanium-based compounds, including germanium oxide and nitride, are promising anode materials due to their high theoretical capacity (1126 mA h g<sup>-1</sup> for GeO<sub>2</sub>), achieved by creating Li<sub>4.4</sub>Ge alloy [2]. However, Ge-based compounds have weak electrical conductivity and substantial volume expansion and contraction during the charging and discharging operations, which reduces electrode cyclic performance. Other inactive or less active compositions are employed in these situations as a supporting and conducting matrix to dampen the volume shift [3].





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In this work, carbon composite nanofibers of Ge-based compounds were synthesized by electrospinning with heat treatments and applied as anode materials for LIBs.

Electrospinning solutions were prepared by mixing different concentrations of GeO<sub>2</sub> with distilled water, and ammonium nitrate, and PVP dissolved in ethanol, to determine the optimal concentration of spinning substances providing the best physical and electrochemical properties. The electrospinning process was carried out under certain conditions, such as a relative humidity of 30%, the electrospinning voltage of 18 kV, and the liquid flow rate of 0.8 ml h<sup>-1</sup>. Subsequently, a nanofiber sheet was dried for ten hours, pre-oxidized at 280 °C, and then annealed for 2 hours at 600 °C in N<sub>2</sub> + H<sub>2</sub>.

X-ray diffraction (XRD, Miniflex, Rigaku) and scanning electron microscopy (SEM, Crossbeam500, Zeiss) revealed the development of the desired material. Other characterization results will be presented at the conference.

### Acknowledgements

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### References

- [1] Mei, L., Mao, M., Chou, S., Liu, H., Dou, S., Ng, D. H. L., & Ma, J. *Journal of Materials Chemistry A*, 3(43)(2015), 21699–21705.
- [2] Guan, Z., Guan, Z., Li, Z., Liu, J., & Yu, K. *Nanoscale Research Letters*, 14 (2019) 2-3.
- [3] Roselin, L. S., Juang, R. S., Hsieh, C. T., Sagadevan, S., Umar, A., Selvin, R., & Hegazy, H. H. *Materials (Basel, Switzerland)*, 12(8) (2019), 1229.

## Investigation of the effect of binders on lithium-ion batteries operating at low temperatures

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Lithium-ion batteries (LIBs) are widely used in energy storage systems due to their high reversible capacity, outstanding rate performance and cycling stability. However, LIBs without sufficient thermal protection may not provide optimal power density and durability at low temperatures, limiting their use in harsh environments. To mitigate this problem, researchers have mainly focused on studying the influence of electrolytes and active electrode materials on the electrochemical performance of LIBs at low temperatures. However, less attention has been paid to the influence of binding materials on the performance of LIBs under extreme conditions. Therefore, in this study, various polymers such as polyvinylidene fluoride (PVDF), polyethylene oxide (PEO), and carboxymethylcellulose (CMC) were comparatively investigated as binders for hard carbon LIB anode operating at sub-zero temperatures.

The study investigates the physical and electrochemical characteristics of anodes utilizing various binders such as PVdF, PEO, and CMC to evaluate their efficiency in low-temperature environments. Anodes incorporating PEO and PVdF binders exhibit enhanced electrochemical properties attributed to their lower glass transition temperatures, higher ionic conductivity, and superior electrolyte absorption in comparison to those employing CMC binder. These specific attributes of PEO and PVdF anodes lead to decreased impedance and faster lithium-ion diffusion, resulting in improved discharge behavior and cycle performance under low-temperature conditions when compared to anodes with CMC binders.



## The methodological investigation of sulfur immobilization to commercial carbon

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Cathodes based on sulfur represent a promising class of electrodes for lithium-sulfur batteries, thanks to their high theoretical energy density and low raw material cost [1]. However, sulfur's intrinsic insulating nature poses a significant obstacle [2], limiting its ability to function as an effective electrode material. The incorporation of sulfur into a conductive additive is a way to overcome this challenge. The most common methods of sulfur loading include chemical precipitation, ball milling, and melt diffusion. We investigate the advantages and limitations of each technique.

Various experimental and analytical analysis including scanning electron microscopy (SEM), X-ray diffraction (XRD), thermogravimetric analysis (TGA), cyclic voltammetry (CV), and galvanostatic charge-discharge tests are employed to identify the physical, chemical, and electrochemical properties of the obtained cathode composites.

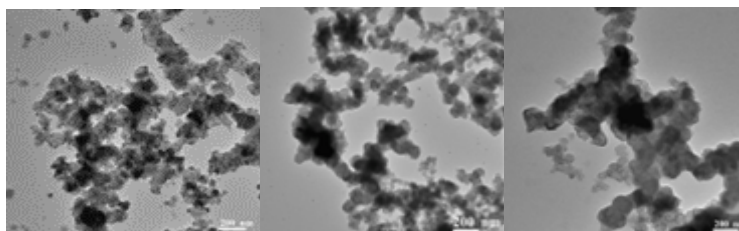


Figure 1. TEM images of AB@S composite made by chemical precipitation (a), ball milling (b), and melt diffusion (c)

Sulfur was successfully immobilized by each method, as demonstrated by TGA, SEM, and TEM analysis. Characteristic dark spots in the TEM images indicate effective sulfur incorporation into AB. To study the electrochemical characteristics of the prepared cathodes, a CP2032 coin-type configuration was used. A homogeneous suspension with a mass ratio of AB@S composite, Acetylene Black, and PVDF (8:1:1) was mixed with NMP. This slurry was applied to aluminum foil with a defined layer thickness using a Doctor Blade. To examine how the method of sulfur immobilizing affects the battery's electrochemical properties and stability during repeated charging and discharging, a charge-discharge test using a Neware Battery Tester was performed.

As can be seen on Fig.2, the cathode made by chemical precipitation exhibited an initial discharge capacity of 568.34 mAh/g and maintained a capacity above 504.50 mAh/g after the 15th cycle. The cathode made from ball milling showed the most stable results. The initial discharge capacity was 584.06 mAh/g and reduced to 551.78 mAh/g after the 15th cycle. Melt diffusion demonstrated the highest initial specific capacity, reaching 944.33 mAh/g and maintained a capacity above 731.97 mAh/g after the 15th cycle, demonstrating its potential as a promising method for Li-S batteries.

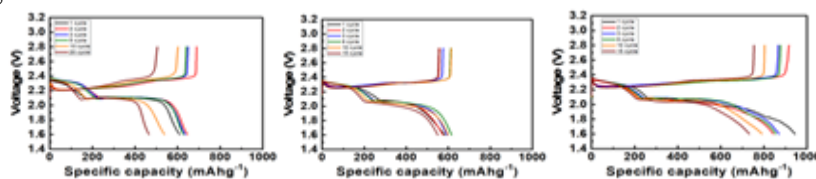


Figure 2. Galvanostatic charge-discharge tests of AB@S composite made by chemical precipitation (a), ball milling (b), and melt diffusion (c)

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### References

- [1] Huang, Lei, Jiaojiao Li, Bo Liu, Yahao Li, Shenghui Shen, Shengjue Deng, Chengwei Lu, et al. *Advanced Functional Materials* 30, no. 22 (2020).
- [2] Wang, Chong, Jia-Jia Chen, Yi-Ning Shi, Ming-Sen Zheng, and Quan-Feng Dong. *Electrochimica Acta* 55, no. 23 (2010): 7010–15.

## Enhancing the Electrical Conductivity and Performance of LiFePO<sub>4</sub>: Synthesis Methods and Doping Techniques

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Recent research has focused extensively on improving the electrical conductivity of LiFePO<sub>4</sub> through various innovative techniques. Significant advances have been made in doping with metal cations, synthesizing nanocrystalline grains, and applying carbon coatings [1]. These methods have led to remarkable improvements in the material's mass transfer rate and overall electrical performance [2].

One of the most effective techniques has been depositing conductive carbon coatings on active material particles. This process has significantly improved the mass transfer rate, which is critical for high-energy-density batteries. In addition, doping with supervalent cations has proven effective in narrowing the energy gap and increasing the electrical conductivity of LiFePO<sub>4</sub> [3]. These approaches have revolutionized the synthesis and modification of the material, demonstrating the viability of two primary synthesis methods: solid phase synthesis by planetary ball milling (PBM) and ultrasonic spray pyrolysis (USP).

The synthesis of LiFePO<sub>4</sub>/C active cathode materials has shown promising results. The morphology and structure of the synthesized materials have been analyzed by scanning electron microscopy (SEM) and transmission electron microscopy (TEM). At the same time, the crystallinity was studied using X-ray diffraction (XRD). Charge-discharge profiles have also been studied to assess performance.

Despite these advances, challenges remain in the form of performance limitations, in particular, the low electronic conductivity of the material and suboptimal performance at high C-rates. A reduction in the size of LiFePO<sub>4</sub> to the nanoscale has been identified as a strategic method. This approach shortens the diffusion length of Li ions and accelerates electron-conducting pathways during charging and discharging cycles, ultimately improving the material's overall performance.

Comparative studies have highlighted the potential of multidoping methods to produce LiFePO<sub>4</sub> materials with specific capacitance approaching theoretical values. Solid-phase synthesis in a planetary ball mill has emerged as a viable method for doping processes. This synthesis and modification technique holds significant potential for overcoming existing limitations and unlocking the full potential of LiFePO<sub>4</sub> for integration into high-energy-density batteries.

In summary, enhancing LiFePO<sub>4</sub>'s electrical conductivity and performance through advanced synthesis methods and doping techniques represents a critical area of research. The continued development and optimization of these methods are essential for fully exploiting the potential of LiFePO<sub>4</sub> in next-generation battery technologies

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### References

- [1] Qiu, S., Zhang, X., Li, Y. et al. Facile synthesis and electrochemical performances of secondary carbon-coated LiFePO<sub>4</sub>-C composite for Li-ion capacitors based on neutral aqueous electrolytes. *J Mater Sci: Mater Electron* 27, 7255–7264 (2016). <https://doi.org/10.1007/s10854-016-4692-1>



[2] Xuetian Li, Lina Yu, Yonghui Cui, Axiang Li, Hongmei Shao, Zhongcai Shao, Wei Zhang, Zhongbao Shao, Enhanced properties of LiFePO<sub>4</sub>/C cathode materials co-doped with V and F ions via high-temperature ball milling route, *International Journal of Hydrogen Energy*, Volume 44, Issue 50, 2019, Pages 27204-27213, 0360-3199, <https://doi.org/10.1016/j.ijhydene.2019.08.187>.

[3] Xu, Z.; Gao, L.; Liu, Y.; Li, L. Review—Recent Developments in the Doped LiFePO<sub>4</sub> Cathode Materials for Power Lithium Ion Batteries. *J. Electrochem. Soc.* 2016,163, A2600–A2610, <http://dx.doi.org/10.1149/2.0411613jes>

## Electrophoretic deposition of composite multilayer gel-polymer electrolyte for 3D lithium-ion batteries

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Electrochemical energy storage via batteries is pivotal in the global shift away from carbon-based fuel dependence. Although current electrochemical technologies are adequate for energy storage applications, including powering portable electronic devices, there is widespread agreement that new advancements in electrochemical power sources are crucial to meet future energy demands. Lithium-ion (Li-ion) batteries have demonstrated considerable promise in this area and possess significant potential for enhancing electrochemical performance [1].

A primary challenge of Li-ion batteries is the low areal capacity of their electrodes. Conventional two-dimensional (2D) electrodes exhibit limited areal capacity due to their surface area and structural configuration. Additionally, Li-ion batteries typically use a liquid electrolyte to facilitate ionic conductivity between the electrodes. While liquid electrolytes provide excellent ionic conductivity, they also present significant drawbacks, such as flammability.

To address these issues, three-dimensional (3D) Li-ion batteries with gel polymer electrolytes have gained substantial attention from researchers over the past decade. Studies have shown that 3D architecture batteries possess higher areal capacity compared to traditional 2D batteries, as they can incorporate more active material within the same footprint. Several types of 3D structured lithium-ion batteries (LIBs) have been developed, including interdigitated, foam-type (porous), core-shell, and nanowire architectures, each offering unique characteristics and benefits [1].

Notably, foam-type 3D batteries utilize a porous foam structure as the electrode material, which significantly increases the surface area available for lithium-ion (Li<sup>+</sup>) exchange. This configuration enhances the battery's energy density and charging rate due to the shortened pathways for Li<sup>+</sup> ions. However, due to their intricate 3D structure, these batteries cannot accommodate a conventional separator between the electrodes. Gel polymer electrolytes offer a solution to this problem, providing high ionic conductivity and non-evaporation properties, while simultaneously functioning as both separator and electrolyte.

To uniformly coat the diverse 3D structures of these batteries, the electrophoretic deposition (EPD) method can be employed. EPD is a highly effective technique for fabricating polymer and composite film coatings, distinguished by its rapid deposition rate and ability to produce relatively thin layers.

This method excels in uniformly coating complex and porous structures in a controlled manner using an electric field. Furthermore, the properties of the deposited layer can be precisely tailored by adjusting the suspension composition and deposition parameters. The mechanism of EPD involves the electrophoretic movement of charged polymer molecules and the subsequent formation of a film at the electrode surface under the influence of an electric field, typically within a two-electrode cell system [2].

In addition to its application in battery technology, EPD is widely used in various fields such as biomedical devices, corrosion protection, and advanced ceramics, due to its versatility and efficiency in creating uniform coatings on intricate surfaces. The ongoing research and development in EPD and 3D Li-ion batteries underscore their potential to significantly enhance the performance and longevity of next-generation energy storage systems, thereby contributing to the broader goal of sustainable energy solutions.



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This research aims to elucidate the impact of poly(ethylene oxide) (PEO) deposition on the electrochemical performance of Zn/ZnO foam electrodes. By investigating the electrode's interaction with a gel polymer electrolyte, we anticipate uncovering insights that could enhance the efficiency and stability of energy storage devices. Future experiments will focus on characterizing the material properties and assessing the electrochemical behavior under various conditions.

### References

- [1] Arthur T. S. et al. Three-dimensional electrodes and battery architectures //MRS bulletin. – 2011. – T. 36. – №. 7. – C. 523-531.
- [2] Hajizadeh A. et al. Electrophoretic deposition as a fabrication method for Li-ion battery electrodes and separators—a review //Journal of Power Sources. – 2022. – T. 535. – C. 231448.

## Synthesis and Study of Composite Aerogels Based on Graphene Oxide and MXene for Lithium-Sulfur Batteries

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Lithium-sulfur (Li-S) batteries have gained significant interest for their potential high energy density, affordability, and eco-friendly nature. However, the practical use of these batteries is hindered by sulfur's poor conductivity, volume change of up to 80%, and the shuttle effect of polysulfides. Various solutions have been proposed to address these challenges, such as combining sulfur with carbon materials, modifying the separator, etc [1].

GO serves as a preferred host for LiS because of its remarkable electronic conductivity, ample specific surface area, and favorable mechanical flexibility. These characteristics render GO highly suitable for accommodating Sulfur particles, thereby promoting enhanced electron transfer and elevating the composite material's overall efficacy [2].

Recently, MXenes, a novel category of two-dimensional materials, have been receiving growing interest for their potential applications in energy storage. Titanium-based MXenes, in particular, have attracted significant attention due to their distinctive two-dimensional structure characterized by high polarity and remarkable conductivity. Combining MXene with biomass carbon derived from renewable sources, which offers notable porosity, excellent electrical conductivity, and chemical stability, is considered an optimal choice for modifying separators in energy storage systems.

Considering the benefits outlined earlier, the study employed Graphene oxide as the host material, and utilized a composite of Biomass carbon and Mxene (GPC/Mxene) to coat the separator aiming to mitigate the shuttle effect and improve conductivity.

GO@S and GPC/MXene composites were synthesized and subsequently characterized using SEM, TEM, and XPS techniques. The SEM images demonstrate the successful removal of the "A" layers from the MAX phases, as evidenced by the observed structural changes in Figure 1.

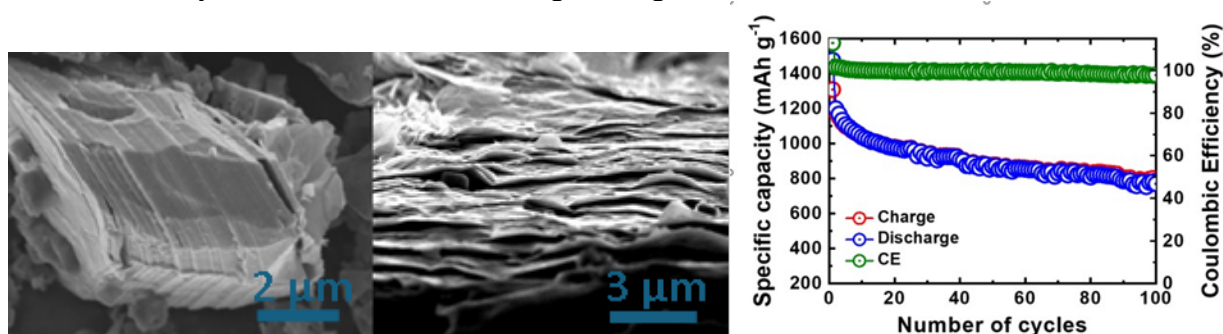


Figure 1. SEM images and cycling performance of the coin cell



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Electrochemical measurements were conducted using CR2032 coin-type cells. A uniform slurry containing the synthesized composites GO/S mentioned earlier (80 wt%), conductive acetylene black (10 wt%), and polyvinylidene fluoride binder (10 wt%) dispersed in N-methyl-2-pyrrolidone was coated onto carbon-coated aluminum foil to prepare the cathode. Furthermore, the GPC/Mxene composite was coated on a commercial Celgard 2400 separator. The resulting cathode, GO/S with bare separator and GO/S with GPC/Mxene coated separator exhibited an initial discharge capacity of 1008 mAh/g and 1476 mAh/g maintaining a capacity of 590 mAh/g and 769 mAh/g after the 100 th cycles respectively. These results underscore the material's potential as a promising candidate for application in Li-S batteries.

### Acknowledgments

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### References

- [1] A Manthiram, et. al., ACS Publications Acc. Chem. Res. 2013, 46, 5, 1125–1134.
- [2] Y Zhang, et. al., Materials today energy, 2018 – Elsevier

## Investigation of sputtered nanocomposite $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>-NiO-Ni<sub>2</sub>N anode with PEO- PVDF-co-HFP gel-polymer electrolyte for lithium-ion micro-batteries

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Research efforts to create novel materials with high charge capacity and excellent cycle ability appropriate for high-energy capacity lithium-ion batteries (LIBs) have been heightened due to the growing need for higher capacity batteries in electronics products. The low cycle stability, severe polarization, low initial coulombic efficiency, and other issues of transition metal oxides prevent their practical use as the lithium ion battery (LIB) anode, despite their high specific capacities. Due to their high theoretical energy densities transition metal oxides such as NiO electrode materials have been investigated as candidates for negative electrodes in the past few years.

In this work, we focus on development of new nanocomposite thin film electrodes via RF magnetron sputtering for lithium-ion microbatteries. In order to improve charge transfer kinetics and enhance cycling stability the chamber of the RF magnetron sputtering system was injected with argon, oxygen and nitrogen gases for the growth of the nanocomposite thin film electrodes based on  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>- NiO-Ni<sub>2</sub>N. We report a new nanocomposite anode fabricated by thermal treatment after magnetron sputtering. Poly(ethylene oxide)-poly(vinylidene fluoride-co-hexafluoropropylene) (PEO-PVDF-co-HFP) membranes with addition of graphene oxide nanoparticles (0.5, 1.0, 1.5 wt%) were used as separators in order to improve cycling stability. PEO was selected for its high ionic conductivity and PVDF-co-HFP was selected as a polymer with stable interfacial contact with an electrode. Nanoscale graphene oxide nanoparticles were utilized to suppress the formation of crystalline nuclei of polymers, thus increasing the amorphous regions and improving the movement ability of the polymer segments. The polymer film was activated by adding 4-5 drops of electrolyte solution 1 M LiPF<sub>6</sub> in EC and DMC [1:1 (v/v) ratio] to form gel-polymer electrolyte. The obtained results will be discussed at the conference.

### Acknowledgement

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## Impact of humidity on the synthesis of nickel phosphide carbon composite nanofibers and their polysulfide-mediating properties in lithium-sulfur batteries

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Lithium-sulfur batteries (LSB) have attracted widespread attention as a promising candidate for the next generation energy storage systems because of high theoretical capacity (1675 mAh g<sup>-1</sup>) and energy density (2600 Wh kg<sup>-1</sup>) of sulfur. However, the dissolution and shuttle of lithium polysulfides pose significant challenges in LSB [1]. Metal phosphide-based materials have shown potential in addressing these issues by efficiently trapping polysulfides and catalyzing their conversion [2]. The surface oxidation layer of metal phosphides is critical to their ability to mediate polysulfides, yet its composition and impact are not well understood [3].

In this study, we synthesize and characterize nickel phosphide carbon composite nanofibers with controlled surface oxidation layers using electrospinning and heat treatment, adjusting the electrospinning humidity (RH 20%, 25%, and 30%). We assessed the performance of these materials as multifunctional interlayers and sulfur host in LSB.

The physical and electrochemical properties of the prepared samples were evaluated using various analytical techniques.

Results show that humidity affects the main physical and electrical properties of composites, including chemical composition and crystallinity, content and graphitization degree of carbon, surface oxidation degree, specific surface area, and electrical conductivity. Subsequently, all samples have strong lithium polysulfide adsorption ability, with differences in polysulfide solution decolorization based on humidity with the highest adsorption ability corresponding to fibers prepared at RH 25%. However, polysulfide mediation properties differ, with RH 30% fibers showing stronger catalytic effects. Such variations in the physical properties further affect their electrochemical properties both as interlayer and sulfur host in LSB.

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### References

- [1] R. Kumar, J. Liu, J.Y. Hwang, Y.K. Sun, J. Mater. Chem. A. 6 (2018) 11582–11605.
- [2] A. Belgibayeva, M. Rakhatkyzy, A. Adi, I. Taniguchi, ChemElectroChem 9 (17), e202200458.
- [3] Y. Zhong, L. Yin, P. He, W. Liu, Z. Wu, H. Wang, J. Am. Chem. Soc. 140 (2018) 1455–1459.

## Precursor effects on layered Li-Mn-O based cathode material for lithium-ion batteries

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The need for sophisticated lithium-ion battery (LIB) systems is growing urgently because of the energy storage sector's and electric vehicles' quick development. Li-rich Mn-based (LRM) oxide electrodes have garnered interest due to their ability to produce a significantly high reversible discharge capacity greater than 250 mAh g<sup>-1</sup> in comparison to conventional electrode materials like LiFePO<sub>4</sub> and LiCoO<sub>2</sub> [1]. Transition metal ion redox reactions and oxygen anion redox reactions offer great energy density. Considering a crucial



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component,  $\text{Li}_2\text{MnO}_3$  is the primary source of capacity, inexpensive, abundant in resources, and ecologically benign. The primary techniques for activating  $\text{Li}_2\text{MnO}_3$  entail the introduction of structural defects, including oxygen vacancies and lithium faults [2]. The low initial Coulombic efficiency (ICE), low-rate capacity, and severe voltage fading of LRM cathode materials prevent them from being used in more practical applications. These issues must be resolved before their practical use. The electrochemical reaction mechanism and electrochemical performance of LRM cathode materials are heavily affected by their structure [1]. By adjusting the coordination environment of the alkali metal within developing structures and oxygen stacking patterns, a Li/Na-ion exchange technique can be thought of as an efficient solution to overcome irreversible lattice oxygen loss. Ion exchange depends on developing a required structure of layered Na precursors since this process only causes the transition metal (TM) layer to shift without breaking down the TM–O bond, enabling it to inherit the structural characteristics of  $\text{Na}_x\text{TMO}_2$  [3]. Using the ion exchange approach, R-3m type of  $\text{Li}_2\text{Mn}_3\text{O}_7$  cathodes (Figure 1) are synthesized and benefitted from limited lattice oxygen loss, reversible structure evolution, and stable Li migration, yielding better structural stability and electrochemical performance.

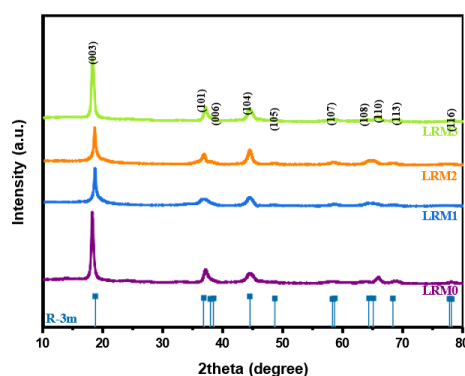


Figure 1. XRD patterns of  $\text{Li}_2\text{Mn}_3\text{O}_7$ .

### References

- [1] W. Zuo, M. Luo, X. Liu, J. Wu, H. Liu, J. Li, M. Winter, R. Eu, W. Yang, Y. Yang *Energy Environ. Sci.*, 13 (2020) 4450-4497.
- [2] C. Huang, Z. Q. Fang, Z. J. Wang, J. W. Zhao, S. X. Zhao, L. J. Ci *Nanoscale*, 13 (2021) 4921-4930.
- [3] J. M. Paulsen, R. A. Donaberger, J. R. Dahn *Chem. Mater.* 12 (2000) 2257-2267.

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## Synthesis of polypropylene carbonate-based composite electrolyte with LLZTO nanoparticles

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Solid state electrolytes (SSEs) represent a transformative advancement in energy storage technologies, particularly solid-state batteries, which offer substantial improvements over conventional liquid electrolyte systems. SSEs provide significant safety benefits by eliminating issues such as leakage, flammability, and thermal runaway, making them ideal for high-demand applications including electric vehicles and portable electronics. These electrolytes enable higher energy densities and longer operational lifespans by facilitating efficient ion transport within a solid matrix. Compared to liquid electrolytes, SSEs also offer enhanced mechanical strength and thermal stability, allowing for a broader operational temperature range.





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The development of SSEs focuses on overcoming challenges related to ionic conductivity, interfacial stability, and mechanical robustness. Advances in materials science have led to the exploration of various SSE types, including ceramics, polymers, and composite materials. To address the low ionic conductivity of solid state electrolytes at room temperature, strategies such as incorporating copolymers, introducing plasticizers, and adding ceramic fillers have been explored.

Designing solid state electrolytes ceramic components with a polypropylene carbonate (PPC) polymer matrix can increase ionic conductivity at room temperature (RT) and provide good ion transport capability at the electrode/electrolyte interface. Mengyang's research group has devised an innovative method to mitigate the agglomeration of LLZTO particles within SPEs. They selected poly-dopamine as a coating agent for LLZTO particles due to its excellent stability [2].

Polypropylene carbonate (PPC) is a biodegradable, amorphous polymer known for its high flexibility, good film-forming ability, and compatibility with lithium salts [3]. In this research work, we combined PPC-based polymer materials and ceramic components lithium lanthanum zirconium oxide ( $\text{Li}_{6.4}\text{La}_3\text{Zr}_{1.4}\text{Ta}_{0.3}\text{O}_{12}$ ). Garnet-type ceramic material  $\text{Li}_{6.4}\text{La}_3\text{Zr}_{1.4}\text{Ta}_{0.3}\text{O}_{12}$ ,  $x=0.6$  (LLZTO), was prepared by the traditional solid-phase method, through a two-step calcination process [4]. The resulting tablets reached a density of 92%, which had a positive effect on ionic conductivity. Powder X-ray diffraction (XRD) patterns of ground LLZTO powders are consistent with standard literature data of cubic garnet phase  $\text{Li}_{6.4}\text{La}_3\text{Zr}_{1.4}\text{Ta}_{0.3}\text{O}_{12}$ , confirming the successful synthesis of cubic phase LLZTO. The cross-section of LLZTO was discovered using scanning electron microscopy (SEM), in which particles have a dense structure built from crystals measuring 1-4 micrometers in size. To enhance the mechanical strength of PPC-based polymer film, the carboxyl groups of the polymer were modified with maleic anhydride [5]. Further, crosslinked PPC solid polymers were fabricated by incorporating methacryloxypropyltrimethoxysilane into the structure, along with LLZTO ceramic nanopowder and LiTFSI salt.

The electrochemical performance of obtained SPE was investigated and promising results were achieved by optimizing the composition of precursor materials.

### Acknowledgments

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### References

- [1] P. Yao , H. Yu , Z. Ding , Y. Liu , J. Lu , M. Lavorgna , J. Wu and X. Liu , *Front. Chem.*, 2019, 7 , 522
- [2] M. Jia, N. Zhao, Z. Bi, Z. Fu, F. Xu, C. Shi and X. Guo, *ACS Appl. Mater. Interfaces*, 2020, 12(41), 46162–4616
- [3] Li X., Meng L., Zhang Y., Qin Z., Meng L., Li C., Liu M, *Polymers*. 2022; 14:2159
- [4] R. Inada, K. Kusakabe, T. Tanaka, S. kudo, Y. Sakurai, *Solid State Ionics*, 262 (2014), pp. 568-572
- [5] M.Yao, F.Mai, H.Deng, N.Ning, K.Wang, Q.Fu. *J. Appl. Polym. Sci.*, 120, 3565 (2011)

## High-performance lithium storage using P-doped anode material derived from post-consumer PET plastic bottles

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Proper utilization and upcycling of plastic waste are imperative to minimizing the damage caused to the natural environment, promoting resource efficiency, and developing a circular economy [1]. Phosphorus doping



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of carbon material introduces a high number of active phosphorus-containing groups and creates larger interlayer distances, significantly contributing to the superior electrochemical performance of the obtained anode material [2].

Crushed post-consumer PET bottles were dissolved in a solvent mixture of dichloromethane and trifluoroacetic acid with varying amounts of phosphoric acid. The resulting mixture was dried into films and then annealed in the N<sub>2</sub> atmosphere to produce hard carbon materials. This material was assembled into lithium-ion half-cells for further electrochemical testing.

The XRD results reveal two significant peaks at  $2\theta \approx 21^\circ$  and  $2\theta \approx 43^\circ$ . The peak around  $2\theta \approx 21^\circ$  corresponds to the (002) plane, indicative of the interlayer spacing in turbostratic (disordered) carbon structures. The peak around  $2\theta \approx 43^\circ$  is assigned to the (101) plane, which reflects the in-plane ordering of carbon atoms. Variations in the intensity and width of this peak among different samples indicate structural changes in the in-plane order, influenced by the doping level of the material.

The P-doped hard carbon anode material exhibits high initial specific capacity and stable performance across multiple cycles: Subsequent cycling tests demonstrate stable specific capacity (~620 mAh/g) and overlapping CV and charge-discharge profiles, indicating consistent lithiation and delithiation processes.

### References

- [1] Wang, Y., Bailey, J., Zhu, Y., Zhang, Y., Boetcher, S. K. S., Li, Y., & Wu, C. (2022). Application of carbon nanotube prepared from waste plastic to phase change materials: The potential for battery thermal management. *Waste Management*, 154, 96–104. <https://doi.org/10.1016/j.wasman.2022.10.003>
- [2] Li, N., Yang, Q., Wei, Y., Rao, R., Wang, Y., Sha, M., ... & Qian, Y. (2020). Phosphorus-doped hard carbon with controlled active groups and microstructure for high-performance sodium-ion batteries. *Journal of Materials Chemistry A*, 8(39). <https://doi.org/10.1039/D0TA06910H>



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## Zinc Oxide decorated hollow carbon nanofibers for gas sensing applications

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Gas sensors play an important role in the developing world as they help to protect the environment and prevent leakages of gases. While zinc oxide (ZnO) has proven itself to be a promising gas sensing material, it still has disadvantages, one of which is a high operating temperature, which is reported to be around 200 oC or 350 oC [1]. To negate this disadvantage, combining ZnO with hollow carbon nanofibers, which are known for their flexibility, high surface area and operation at room temperature for gas response.

In this study, flexible core-shell structured highly porous carbon nanofibers decorated with ZnO nanoparticles were fabricated. The coaxial electrospinning technique is used for production core-shell structured nanofibers, with PAN and ZnO serving as the shell components and PMMA used as a sacrificial material. Following two consecutive heat treatments, including stabilization at 280 oC in an air environment and carbonization at 700 oC in an argon atmosphere, resulted in the production of hollow carbon nanofibers with ZnO embedded on their surface.

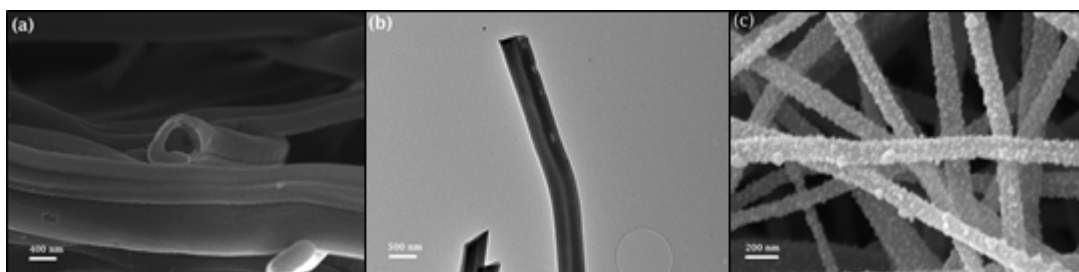


Figure 1. (a) SEM image of HCNF, (b) TEM image of HCNF, (c) SEM image of ZnO embedded CNF

Based on Fig. 1a. and Fig. 1b., hollow carbon nanofibers were successfully prepared via coaxial electrospinning from PAN and PMMA polymers where hollow inside carbon nanofiber is continuous. Fig. 3c. demonstrates ZnO decorated carbon nanofiber from precursor polymer of PAN. ZnO is evenly distributed on the surface of CNF which might indicate greater surface area in comparison with ordinary ZnO nanoparticles which is beneficial in gas sensing application. Integration of ZnO nanoparticles with porous flexible carbon fibers significantly increased the surface area of the material and improved gas-sensing performance towards CO<sub>2</sub> gas.

### Acknowledgments

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### References

[1] Franco, M. A., Conti, P. P., Andre, R. S., & Correa, D. S. (2022). A review on chemiresistive ZnO gas sensors. *Sensors and Actuators Reports*, 4, 100100. <https://doi.org/10.1016/j.snr.2022.100100>



## An Investigation Of The Use Of Hydroxy Carbonates For Electrochemical Glucose Sensor

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Given the importance of diabetes treatment and control of pre-diabetic states, the task of developing new materials for glucose sensors is urgent. Currently, a large number of different types of glucose sensors have been developed. However, due to the importance of this area, the intensity of research on the development of glucose sensors remains high, as evidenced by the large number of recent review papers [1-3]. Non-enzymatic glucose sensors are promising for reusable electrochemical test systems because of their high sensitivity, fast response and ease of operation. A wide class of materials such as noble metal nanoparticles, composites based on carbon nanomaterials, and metal oxides are used to create non-enzymatic glucose sensors. The search for new materials for the creation of highly sensitive glucose sensors is an urgent task. In the present work a new sensor material promising for the creation of glucose biosensors is investigated. Zinc, cobalt and copper hydroxy-carbonates were synthesized by hydrothermal method at 120°C and characterized by scanning electron microscopy, X-ray diffraction analysis, Raman spectroscopy and electrochemical methods.

The aim of this work was to search for new materials for glucose detection. It is shown that the material based on hydroxy-carbonates of zinc, cobalt and copper, which was synthesized by hydrothermal method, demonstrates high stability of the structure in a wide range of synthesis conditions, and also shows high sensitivity for glucose detection, so it is a new promising material for the creation of biosensors.

Glucose sensitivity was tested by CV cyclic voltammetry. Figure 1(a) show the CV curves for synthesized sample. It can be seen that significant changes in CV curves are observed when glucose is added. The current measured at a potential of 0.6 V with respect to Ag/AgCl increases in the range up to ~0.5 mM in a relationship close to linear, as shown in Figure 1 (b). The same figures show the concentration dependence of sensitivity. As can be seen, the sensitivity reaches ~13 mA mA mM<sup>-1</sup> cm<sup>-2</sup>, this value is very high compared to the data available in the literature.

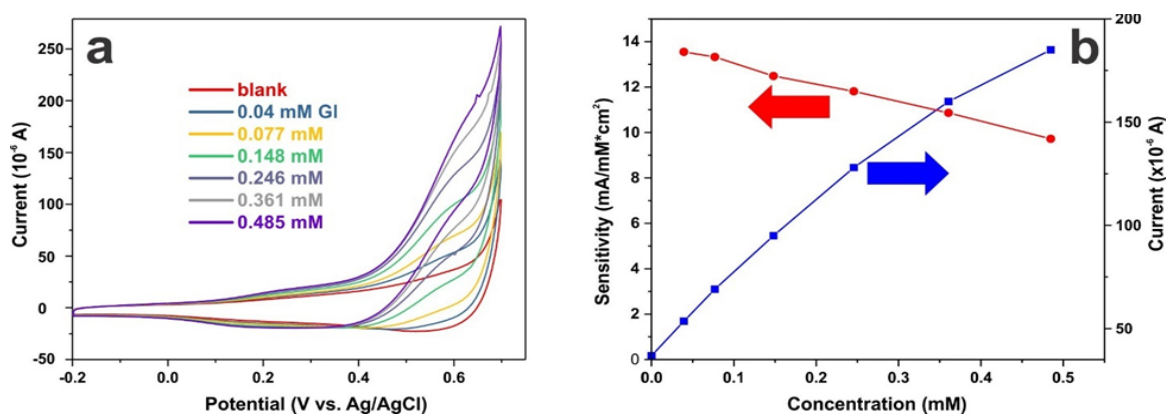


Figure 1. CV characteristics for synthesized sample in the glucose concentration range from 0 to 0.485 mM (a); Current dependence at 0.6 V potential versus Ag/AgCl and sensitivity versus glucose concentration (b).

Thus, the present work reports a new material for the fabrication of glucose sensor - hydroxy-carbonates of zinc and cobalt. The stable phase composition of this material is formed under a sufficiently wide range of synthesis conditions, and in the same range the high sensitivity of the sensor is maintained. The material demonstrated a sensitivity of ~13 mA mM<sup>-1</sup> cm<sup>-2</sup>, linear region up to 0.5 mM, in this region showed a detection limit of 0.007 mM glucose. The simplicity of the material synthesis and its high sensitivity make the obtained material promising for practical application in the development of non-enzymatic glucose detection sensors.



### References

- [1] Tamoghna Saha, Rafael Del Caño, Kuldeep Mahato, Ernesto De la Paz, Chuanrui Chen, Shichao Ding, Lu Yin, and Joseph Wang. Wearable Electrochemical Glucose Sensors in Diabetes Management: A Comprehensive Reviews 12 (2023) 7854–7889.
- [2] Yan Wang, You Wu and Yifeng Lei. Microneedle-based glucose monitoring: a review from sampling methods to wearable biosensors. *Biomater. Sci.*, 11 (2023) 5727-5757.
- [3] Kermue Vasco Jarnda, Danqi Wang, Qurrat-Ul-Ain, Richmond Anaman, Varney Edwin Johnson, Garmai Prosperity Roberts, Pauline Sammumah Johnson, Bob Wisdom Jallowide Jr, Tianhan Kai, Ping Ding. Recent advances in electrochemical non-enzymatic glucose sensor for the detection of glucose in tears and saliva: A Review. *Sensors and Actuators A: Physical* 363 (2023) 11.

## Development of a Flexible Strain Sensor Using a 2D Conductive Carbon Layer Integrated with Carbon Cloth

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Flexible strain sensors have garnered significant interest due to their potential applications across various fields, leveraging the exceptional electrical and mechanical properties of carbon nanotubes (CNTs). Despite advancements, achieving scalable fabrication of highly sensitive and stretchable strain sensors remains challenging, prompting the development of a novel sensor using overlapped CNT bundles integrated with a silicone elastomer.

In this study, we synthesized highly flexible strain sensors by combining various concentrations of multiwalled carbon nanotubes (MWCNTs) with a 2D conductive layer and Ecoflex. We analyzed critical performance parameters, including linearity, sensitivity, stretchability, hysteresis, durability, and sensing stability, to evaluate the effectiveness of the sensors.

The main results demonstrated that the highest sensitivity was achieved with 0.75 wt% MWCNT, exhibiting a gauge factor (GF) of 8.34 within the 0-100% strain range. Additionally, the synthesized nanocomposite showed a fast response time, low hysteresis, and high durability, maintaining performance over more than 10,000 cycles.

The developed strain sensors offer significant relevance and application potential for soft robotics, providing "stick-on" sensors that are soft, stretchable, and conformable, thus preserving the adaptivity and safety of these systems. These sensors can detect both large and subtle human movements, such as elbow rotation, wrist bending, knee bending, swallowing, and phonation, demonstrating their potential for human-machine interactions and personal health monitoring. This advancement addresses existing challenges in CNT strain sensors, paving the way for new functionalities in wearable robotics and sensing technologies.

**Keywords:** strain sensors, carbon nanotubes, 2D conductive layer

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## The effect of Ti doping on the structural and morphological properties of ZnO nanorods obtained through seeded hydrothermal method

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The advancement of technology necessitates the means of control over the emissions of different gases into the atmosphere. Fast and precise gas detection of emitted toxic gases is instrumental in keeping our health and the surrounding environment safe. Several means of monitoring have been developed over the years, such as optical, acoustic, and resistive gas sensors, to which metal oxide semiconductor (MOS)-based gas sensors belong [1]. Among MOS-based gas sensors, ZnO is a popular n-type material possessing tunable morphological and electrical properties that are highly suitable for the detection of toxic gases [2]. There are several methods of improving the sensitivity of ZnO to gases, such as structural modification by beam treatment, control over nano-architecture of the sensing material, decorating by noble metals and doping by different group elements to change band structure. Doping of ZnO by transition metal (TM) often results in the change of morphology and electrical properties that eventually result in higher response to toxic gases [3]. Soltabayev et al have shown that improved sensing response of nitric oxide was achieved through doping with titanium element obtained with magnetron sputtering method [4]. In this work, ZnO nanorods containing dopant titanium atoms were synthesized using the hydrothermal method. Initially, cleaned glass substrates were coated with seed layer using spin-coating method with varying thickness values. The process parameters consist of 40 microliter dosages applied to every cycle of coating that spun at 5000 rpm for 15 seconds. Further, the deposited layer was treated at 300 °C for 5 min after each cycle. It was found that the thickness of the seed layer for 2 cycles, 5 cycles, and 10 cycles was around 125 nm, 300 nm, and 500 nm, respectively. The nanorods were grown using a hydrothermal method with the solution containing 0.476 g zinc nitrate hexahydrate, 40 ml DI water, appropriate amount of titanium isopropoxide and regulated to pH value of 10 using ammonium hydroxide solution. The substrates were immersed in the solution while being vertically mounted on the wall of the Teflon liner and placed inside the stainless-steel autoclave. The growth conditions are 100 °C and 2 hours, after which the substrates were dried at 60 °C for 6 hours. It was further found that the placement of the substrate and its orientation influences the growth of nanorods, for example, the growth of nanorods through the transformation of the solution into gaseous state and reacting with the seed layer did not yield nanorod-like structure. The substrates in that case were placed above the solution inside the Teflon-liner. Meanwhile, horizontal position at the bottom of the liner resulted in the formation of nanorods along with flower-like structures that were significantly bigger in size. Mounting the substrate on the wall and positioning it vertically inside the solution yielded only nanorods that did not have flower-like structures. The effect of Ti doping on ZnO was characterized by XRD, SEM and XPS. Through the analysis of the obtained data, the changes in morphological and electrical properties will be discussed. Further research efforts will be focused on obtaining an improved response towards toxic gases.

### Acknowledgements

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### References

- [1] A. Ajjaq, Ö. Barin, A. Çağırtekin, B. Soltabayev, S. Acar, ZnO seed-mediated hydrothermal growth of advanced 1-D ZnO and 2-D CuO nanostructured oxide ceramics for gas sensing applications, *Ceram. Int.* 49 (2023). <https://doi.org/10.1016/j.ceramint.2023.10.071>.
- [2] M. Jiao, *Microfabricated Gas Sensors Based on Hydrothermally Grown 1-D ZnO Nanostructures*, 2017.
- [3] B. Soltabayev, Y. Raiymbekov, A. Nuftolla, A. Turlybekuly, G. Yergaliuly, A. Mentbayeva, Sensitivity Enhancement of CO<sub>2</sub> Sensors at Room Temperature Based on the CZO Nanorod Architecture, *ACS Sensors*. 9 (2024) 1227–1238. <https://doi.org/10.1021/acssensors.3c02059>.



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[4]B. Soltabayev, A. Ajjaq, G. Yergaliuly, Y. Kadyrov, A. Turlybekuly, S. Acar, A. Mentbayeva, Ultrasensitive nitric oxide gas sensors based on Ti-doped ZnO nanofilms prepared by RF magnetron sputtering system, *J. Alloys Compd.* 953 (2023) 170125. <https://doi.org/10.1016/j.jallcom.2023.170125>.

## Production and Characterization of Chemically-Activated Carbon, Together with an Investigation of Its Potential in Electroanalytical Applications

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Activated carbons (AC) have favourable characteristics, including high electrical conductivity, high thermal stability, corrosion resistance, high surface area, and well-developed porosity for several applications [1]. Moreover, the utilisation of biowastes as excellent precursors of AC due to their abundant availability, cost-effectiveness, and sustainability [2]. Local biomass sources, such as agricultural residues, forestry waste, and other organic materials, are renewable and can be replenished annually, reducing dependence on non-renewable resources for the production of AC [3-4]. Furthermore, utilising local biomass for AC production helps manage waste, reduce environmental pollution, and promote sustainable waste management practices. Converting such local biomass wastes into ACs and studying its electroanalytical application is essential to developing green chemistry and environmentally sustainable technologies [5-7].

Therefore, this work aims to synthesise AC from wheat wastes by a three-stage process. For this purpose, the biomass underwent a series of processes, including initial carbonisation, chemical activation with iron (III) chloride, and a secondary carbonisation stage. Then, material characterisation was performed through several analytical techniques (including elemental analysis, FT-IR spectroscopy, XRD, SEM-EDX, and TEM). Finally, the carbonaceous material was utilised as an electrode-active material for Fe<sup>2+,3+</sup> determination in aqueous solutions. According to the elemental analysis results, AC comprises mainly 73.04% C, 0.472% H, and 3.62% N. A decrease in the H/C and O/C ratios, as well as volatile substances, combined with an increase in the concentration of aromatic carbon in the structure, was observed. FT-IR and XRD results suggested the presence of highly crystalline graphite structure in AC, while TEM analysis revealed a chain structure of iron particles (Fig. 1a). SEM microscopy showed a heterogeneous porous AC with cubic morphology of Fe-based particles (Fig. 1b,c).

The activated carbon has been further tested as an electrode-active material in creating a carbon-paste electrode operating under direct potentiometry and potentiometric titration to determine Fe<sup>2+</sup> and Fe<sup>3+</sup> ions in aqueous solutions. The paper will provide detailed conditions for conducting a potentiometric analysis. These studies expand the horizons of using AC in electrochemistry, particularly in its electroanalytical applications.

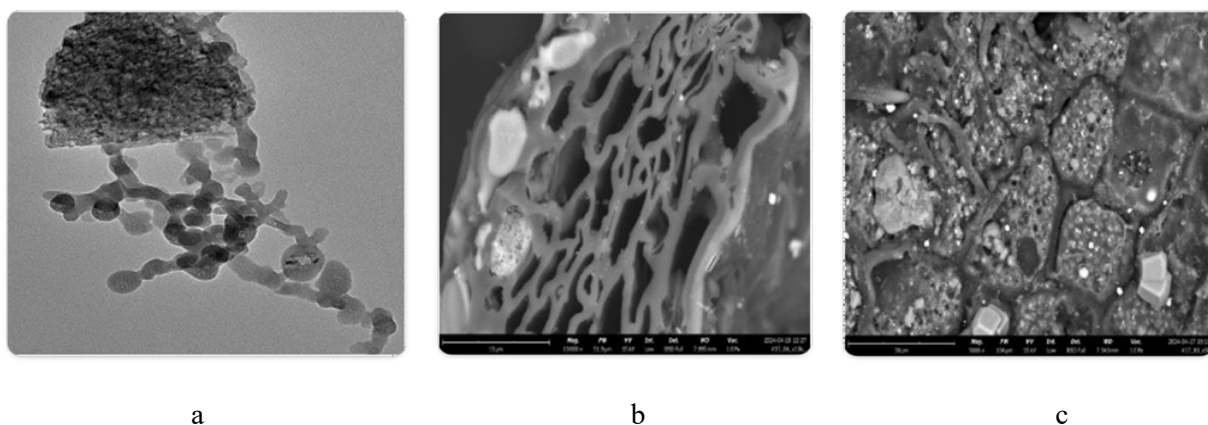


Figure 1. TEM (a) and SEM (b,c) images of AC



### References

- [1] T. Subramaniam, M. Ansari, S. Krishnan, M. Khalid *Chemosphere*, 354 (2024) 354.
- [2] P. Chaudhary, S. Bansal, B. Sharma, S. Saini, A. Joshi *Journal of Energy Storage*, 78 (2024) 109996.
- [3] G. Özsin, M. Kılıç, E. Apaydın-Varol, A. Pütün *Applied Water Science*, 9 (2019) 56.
- [4] M. Fazal-ur-Rehman *Current Trends in Chemical Engineering and Technology*, 1 (2018) 1-10.
- [5] C. Zhong, Y. Chen, Y. Zheng, Q. Tian, Y. Chen, M. Xie, Z. Tian *Analytical Sciences*, (2024).
- [6] A. Kangmenaa, R. Forkuo, E. Agorku *Sensing Technology*, 2 (2024) 1-40.
- [7] Z. Lucio-Rivera, R. Gudgel, A. Smith, W. Gorski *Journal of Electroanalytical Chemistry*, 956 (2024) 118094.

## Production of materials like graphene oxide from activated carbon obtained from agricultural waste

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Nowadays, it is urgent to develop a super-sensitive humidity sensor using a relatively cheap material and affordable manufacturing technology, which allows to determine a wide range of environmental humidity. As such a material can be called carbon materials such as graphite, graphene, graphene oxide and graphene-like materials derived from activated carbon. The peculiarity of graphene-like materials lies in their availability and economic viability. With the advent of graphene and graphene-like materials because of their physical and mechanical as well as the most important electronic properties, a lot of research has been done on the development of sensitive sensors to detect humidity and various gases [1-3].

In this research work, graphene-like materials were synthesized from activated carbon obtained from agricultural waste using Hammers method and brought to Ph~7. The physicochemical properties of this material were studied by IR spectroscopy, SEM, sorption properties, XRD, BET, XPS and moisture resistance. According to the results of physicochemical investigations, the following data were obtained: according to IR spectroscopic studies, C=C aromatic functional groups were detected in activated carbon in 1518 cm<sup>-1</sup> absorbed region, C-O carboxyl groups in 1054 cm<sup>-1</sup>, OH dimeric hydroxo groups were detected in 2902 and 2986 cm<sup>-1</sup> absorbed region. In the study of graphene-like material, C-O carboxyl functional groups were formed at 1097 cm<sup>-1</sup>, C-C aromatic groups at 1470 cm<sup>-1</sup>, C=O carbonyl groups at 1782 cm<sup>-1</sup>, OH hydroxo groups at 3325 cm<sup>-1</sup> absorbed region [1-5]. XRD analysis revealed a peak shift from  $2\theta=22.5^\circ$  to  $2\theta=11^\circ$ . These values show an increase in the interplanar spacing of the graphene-like material in contrast to the original material. The XPS analysis results revealed major peaks with binding energies of 284.1 eV, 288.8 eV. They are associated with aromatic and aliphatic carbon atoms sp<sup>2</sup> and sp<sup>3</sup> (C=C), epoxy groups (C-O-C) and carboxyl groups (C(O)-O-H), respectively, and peaks in the region of 292-295 eV, which are characteristic of the binding energies of  $\pi-\pi^*$  transitions in aromatic closed chains in not large amounts.

### References

- [1] F. Schedin, A. K. Geim, S. V. Morozov, E. W. Hill, P. Blake, N. I. Katsnelson and K. S. Novoselov (2007) Detection of Individual Gas Molecules Adsorbed on Graphene. *Nature Materials*, 6, 652-655.
- [2] Tilek Kuanyshbekov,\* Nazim Guseinov, Zhandos Tolepov, Bayan Kurbanova, Malika Tulegenova, Kydyrmolla Akatan, Nurgamit Kantay, and Elzhas Zhasasynov., Thermally Reduced Graphene Oxide Membranes From Local Kazakhstan Graphite “Ognevsky”, *ChemistrySelect*, 2023, 8, e202301746, 1 – 13, <https://doi.org/10.1002/slct.202301746>.
- [3] T. Kuanyshbekov, Z. Sagdollin, E. Zhasasynov, K. Akatan, B. Kurbanova, N. Guseinov, Z. Tolepov, N. Kantay, M. Beisebekov, Composite membrane based on graphene oxide and carboxymethylcellulose from local Kazakh raw materials for possible applications in electronic devices, *Journal of Composites Science*, 2023, 7, 342, doi: 10.3390/jcs7080342.
- [4] Tilek Kuanyshbekov\*, Nazim Guseinov, Bayan Kurbanova, Renata Nemkaeva, Kydyrmolla Akatan, Zhandos Tolepov, Malika Tulegenova, Madi Aitzhanov, Elzhas Zhasasynov, Sabu Thomas. Local





Natural Graphite as a Promising Raw Material for the Production of Thermally Reduced Graphene-Like Films. *Engineered Science*. 2024, 23, 1000, DOI:10.30919/esmm1000

[5] T.K. Kuanyshbekov, K. Akatan, S.K. Kabdrakhmanova, R. Nemkaeva, M. Aitzhanov, A. Imasheva, E. Kairatuly (2021) Synthesis of Graphene Oxide from Graphite by the Hummers' Method. *J Oxidation Communications* 44(2):356–365

## Highly Sensitive Composite Nanomaterials for Optical Fiber Sensors for the Detection of KIM1 Protein

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Biosensors are established as promising analytical tools for detecting various analytes important in biomedicine and environmental monitoring. Using fiber optic technology as a sensing element in biosensors offers low cost, high sensitivity, chemical inertness, and immunity to electromagnetic interference. [1]. The great diversity of current biosensor designs is based on the utilization of a wide format of analytical and technological strategies, detecting various regulatory and functional molecular markers associated with infectious pathogens. Current methods for detecting this protein use labeled assay reagents and are time consuming [2]. This work aimed to apply new materials to optical fiber sensors for KIM1 protein detection. A method of fabrication of optical biosensors is proposed for their modification with zinc, cobalt, and copper hydroxy-carbonates nanoparticles. Composite nanoparticles are increasing their sensitivity, stability, and repeatability. Zinc, cobalt, and copper hydroxy-carbonates were synthesized by hydrothermal method at 120°C for 6 hours and obtained in the form of powders. The biosensor uses a fiber-optical sensor with a uniform zinc, cobalt, and copper hydroxy-carbonates thin layer deposited by the dip-coating method as a modification sensor for detecting the KIM1 protein. The advantages of this biosensor include the ease of manufacture on a standard fiber, and the simplicity of applying zinc, cobalt, and copper hydroxy-carbonates in thin layers by the dip-coating method without the use of expensive equipment. The fabricated optical fiber biosensors were employed for the detection of KIM1 protein diluted in PBS (Phosphate-buffered saline). The transducer part of the optical fiber biosensor was applied with a zinc, cobalt, and copper hydroxy-carbonates layer and the KIM1 antibody was immersed in the analyte solution with KIM1 protein, while the other end of the optical fiber was connected to the Micron Optics device. The optical fiber's surface was immobilized with 2  $\mu\text{g}/\text{mL}$  KIM1 antibody for overnight and the unreacted biomolecules were blocked with the 1% BSA solution. The concentration range of KIM1 analyte was from 100 aM up to 100 nM. At the same time, the functionalized optical fiber sensors were immersed in a vial containing 500  $\mu\text{L}$  of a KIM1 protein solution. Measurements for each concentration were carried out for 10 min. The total number of measurements was 8, in the PBS solution, including all concentrations of KIM1 proteins.

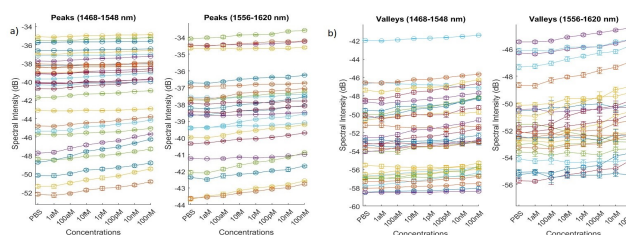


Figure 1. All local peaks in sensor response. Left subplot shows peaks range of wavelength 1468-1548 nm (a), right subplot shows peaks B range of wavelength 1556-1620 nm (b)



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In the wavelength range of 1548-1556 nm, the FBG response is observed, which is shown in Figure 1 (a). Each point indicates an average intensity value and standard deviations between 8 measurements. It can be seen that the intensity response improves as concentration increases which clearly shows the detection happening. In the case of valleys Figure 1 (b), the same can be seen. But there are a few fluctuations and the standard deviation is a little higher compared to the peaks. Consequently, a new type of optical biosensor was investigated and developed, which allows to detection of biomolecules of a substance with accuracy and determines the level of the required protein. Modification and optimization of optical biosensors allow for improvement of the characteristics of optical biosensors.

### References

- [1] Aliya Bekmurzayeva, Marzhan Nurlankyzy, Albina Abdossova, Zhuldyz Myrkhyyeva, and Daniele Tosi, "All-fiber label-free optical fiber biosensors: from modern technologies to current applications [Invited]," *Biomed. Opt. Express* 15 (2024) 1453-1473.
- [2] Paltusheva, Z.U.; Ashikbayeva, Z.; Tosi, D.; Gritsenko, L.V. Highly Sensitive Zinc Oxide Fiber-Optic Biosensor for the Detection of CD44 Protein. *Biosensors* 12 (2022) 1015.

## Nitrogen-doped carbon nanowalls electrode for hydrogen peroxide sensing

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The large surface area, highly active graphene edges, and catalyst-free fabrication have contributed to the extensive application of CNWs as electrode material for electrochemical sensors [1]. In recent years, the electrochemical properties of CNWs for detection of various analytes such as lactate, paracetamol, glucose, hydrogen peroxide, ascorbic acid, and uric acid have been studied in detail [2–4]. To improve the electrochemical properties of CNWs, electrochemical sensors were fabricated by incorporating Pt nanoparticles, manganese oxide, etc. However, the effectiveness of the sensors relies on the use of composite structure, expensive noble metal Pt and specific enzymes, which complicates the sensor fabrication technology. One of the simple methods to improve the electrochemical properties of the material is nitrogen doping. N-doped graphene has been found to exhibit higher electrocatalytic activity than the most other electrocatalysts [5].

In this study, RI-PECVD method is used to synthesize N-doped CNWs on TiSiO<sub>2</sub>/Si substrate at different nitrogen flow rates. The effect of different nitrogen flow rates on CNWs characteristics was analyzed by X-ray photoelectron spectroscopy (XPS), scanning electron microscopy (SEM), Raman spectroscopy. Then the sensor performance of the nitrogen-doped CNWs toward H<sub>2</sub>O<sub>2</sub> detection was investigated using cyclic voltammetry (CV) and amperometric techniques. An analysis of Raman spectra shows that the ratio of the G and D peak intensities (IG/ID) in CNWs synthesized at 20 sccm flow rate is greater than at 10 sccm, 0.75 and 0.66, respectively, indicating that CNWs synthesized at high nitrogen gas flow rate are less defective. Based on Raman analysis data, it can be concluded that with an increase in the nitrogen flow rate from 10 sccm to 20 sccm, the structure of CNW films becomes more graphitic, because of the substitution of nitrogen to the defect sites or by the etching of the amorphous carbon phase. It can be found that the graphitic N content of the N-CNWs increases with the increase of N<sub>2</sub> flow rate. On the other hand, pyridinic N and pyrrolic N components decrease with the increase of N<sub>2</sub> flow rate. The higher concentration of incorporated graphitic N can be due to the formation of multiple vacancy defects by higher etching of CNWs by N<sub>2</sub> atoms during the synthesis process. The electrochemical properties of CNWs with different nitrogen content were evaluated in a three-electrode system where a 0.1 M PBS solution was used as the electrolyte. CV of N-doped CNWs was measured from -0.8 V to 1 V at a scan rate of 20 mV/s in the absence of H<sub>2</sub>O<sub>2</sub> and in the presence of 5 mM H<sub>2</sub>O<sub>2</sub>. It can also be noticed that an increase in nitrogen flow rate from 10 to 20 sccm during doping leads to an increase in the reduction current. To further confirm the electrocatalytic activity of N-doped CNWs samples toward H<sub>2</sub>O<sub>2</sub>, amperometric



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measurement was performed. Based on the CV results,  $-0.45$  V was selected as an applied potential for the amperometric detection of  $\text{H}_2\text{O}_2$  as reduction peak increased sharply at this potential. The amperometric response of different samples was measured at  $-0.45$  V by adding  $\text{H}_2\text{O}_2$  with different concentrations from  $1 \mu\text{M}$  to  $20 \text{ mM}$  every 50s into PBS (100 ml). The volume of  $\text{H}_2\text{O}_2$  to be dropped was varied from  $10 \mu\text{l}$  to  $200 \text{ ml}$ . As it can be seen, the highest amperometric response was observed for the CNWs doped with  $20 \text{ sccm N}_2$ . It is found that all CNWs samples react quickly and reach a steady state about 5 s, indicating a good electrocatalytic performance and a fast electron exchange response. The CNWs sample doped at high nitrogen flow rate ( $\text{N}_2$ :  $20 \text{ sccm}$ ) exhibits a wide linear response range for reduction of  $\text{H}_2\text{O}_2$  concentration from  $1 \mu\text{M}$  to  $250 \mu\text{M}$ , low LOD value, and high sensitivity of  $679.6 \mu\text{AmM}^{-1} \text{ cm}^{-2}$ . This study demonstrates a new pathway for the application of nitrogen-doped carbon nanowalls in electrochemical sensing.

### References

- [1] M. Hiramatsu, M. Hori Springer Vienna, (2010) 1–161.
- [2] F. Bohlooli, A. Yamatogi, S. Mori Sens Biosens. Res., 31 (2021) 100392.
- [3] M. Tomatsu, M. Hiramatsu, J.S. Foord, H. Kondo, K. Ishikawa, M. Sekine, K. Takeda, M. Hori Jpn. J. Appl. Phys., 56 (2017) 06HF03.
- [4] Z. Zhai, B. Leng, N. Yang, B. Yang, L. Liu, N. Huang, X. Jiang Small., 15 (2019) 1901527.
- [5] Y. Shao, S. Zhang et al. J. Mater. Chem. 20 (2010) 7491-7496.

## ZnO/PVP@NiO nanofibers for gas sensing applications via combined electrospinning/SILAR technique

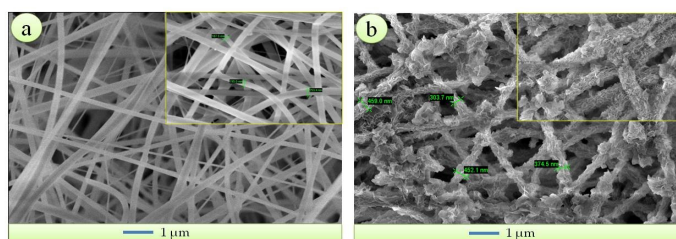
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Growing concerns about safety in laboratory and industrial settings have spurred significant interest in fast and reliable gas detection methods. Recently, metal oxide semiconducting (MOS) materials, such as  $\text{TiO}_2$ ,  $\text{SnO}_2$ ,  $\text{WO}_3$ , and  $\text{ZnO}$ , have been extensively studied for the fabrication of new semiconductor gas sensors due to their small particle size and large surface area [1]. The gas-sensing mechanism involves the chemisorption of oxygen on the surface of these oxides and charge transfer during the reaction of oxygen with target gas molecules [2], leading to a change in the sensor's surface resistance.  $\text{ZnO}$  is a crucial oxide semiconductor for sensing toxic and combustible gases, offering advantages like low cost, quick response time, ease of manufacturing, and compact size compared to traditional analytical instruments [3]. However,  $\text{ZnO}$  sensors typically operate at high temperatures ( $400\text{--}500 \text{ }^\circ\text{C}$ ) and have limited selectivity [4].



**Figure 1.** Scanning electron microscope (SEM) images of (a)  $\text{ZnO/PVP}$  and (b)  $\text{ZnO/PVP@NiO}$  nanocomposites

To date, research has primarily focused on enhancing the sensitivity of  $\text{ZnO}$  to various gases, with an emphasis on improving preparation methods and reducing operating temperatures. This work introduces a method for preparing  $\text{ZnO/PVP@NiO}$  core/shell nanofibers using a combined electrospinning/SILAR technique. Figure 1 shows images of (a)  $\text{ZnO/PVP}$  and (b)  $\text{ZnO/PVP@NiO}$  obtained using a SEM. This



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approach results in a significantly larger surface area compared to plain ZnO/PVP fibers. The increased surface area enhances the sensitivity, selectivity, and response/recovery time of the nanofibers, while also allowing for a lower operating temperature.

### Acknowledgements

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### References

- [1] A.K. Batra, A.K. Chilvery, P. Guggilla, M. Aggarwal, J.R. Currie. *Journal of Nanoscience and Nanotechnology*. 14 (2) (2014) 2065-85.
- [2] P. Shankar, J.B. Rayappan. *Sci. Lett. J.* 4 (2015) 126.
- [3] M.V. Nikolic, V. Milovanovic, Z.Z. Vasiljevic, Z. Stamenkovic. *Sensors*. 22 (2020) 6694.
- [4] H. Xu, X. Liu, D. Cui, M. Li, M. Jiang. *Sensors and Actuators B: Chemical*. 114 (2006) 301-7.

## Functionalization of the tribonegative layer to enhance the performance of the triboelectric nanogenerator

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Recently, it is believed that environmental energy associated with various activities such as human body movements, air and water flow, as well as sound waves, provides an alternative source of energy for portable and mobile devices [1]. This new technology, called a nanogenerator (NG), is a technology that converts mechanical and/or thermal energy produced as a result of small physical changes into electricity [2]. Among NGs, triboelectric nanogenerators (TENGs) are the most promising candidate for further application due to their advantages such as high output power, high efficiency, lightweight, production from economical materials, and ease of manufacturing [3].

Silicone as a tribonegative material has recently attracted attention in the production of TENG due to its low cost, flexibility, high chemical stability, and its ability to easily be turned into a composite structure by mixing micro/nanoparticles. Thus, the performance of TENG can be enhanced through structural improvements. Modification of the silicone matrix with fillers not only changes the surface electrification and dielectric permittivity of the material, but also makes them more effective in electrostatic induction to improve the characteristics of TENG.

In this work, we present a study of the output characteristics of a TENG based on the commercial silicone matrix Ecoflex and polyvinyl alcohol (PVA). The commercial silicone matrix was modified by adding synthesized hexachlorofullerene (C<sub>60</sub>Cl<sub>6</sub>). Furthermore, our electrical property analysis revealed that the PVA/Ecoflex composition with 0.25% fullerene group by weight was the optimal concentration, yielding output voltages 40% higher than the unmodified TENGs.

The TENG prototype we developed, which consisted of PVA/Ecoflex with a fullerene group, demonstrated robust and consistent performance. It showed no noticeable degradation even after undergoing 20,000 continuous cyclic tests. These empirical results underscore the potential of our approach. By selectively modifying specific functional groups in the polymer matrix, we cannot only enhance the output of TENG but also influence the permittivity and dielectric loss. This finding opens up new possibilities for improving the efficiency and practicality of TENGs, making them a more viable energy harvesting solution.

### References

- [1] M. M. Shulaker, G. Hills, R. S. Park, R. T. Howe, K. Saraswat, H. S. P. Wong, S. Mitra, *Nature*, 547(2017),: 74-78.
- [2] F. R. Fan, Z. Q. Tian, Z. L. Wang, *Nano Energy*, 1 (2012), 328-334.
- [3] K. Dong, X. Peng, Z. L. Wang, *Advanced Materials*, (32) 2020, 1902



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## Selective determination of cadmium (II) in extraction samples by fusion of low-melting organic substances

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Cadmium is widely used in the production of alloys, batteries, pigments, and metal coatings [1]. Cadmium compounds are highly toxic, so reliable monitoring of its content is necessary. The challenges of developing efficient selective methods for concentrating and extracting cadmium(II) from raw materials, soils, natural and waste waters, as well as highly sensitive rapid analysis methods with preliminary metal concentration, remain relevant. One of the promising and modern methods for determining cadmium(II) is atomic absorption spectroscopy, which is a reliable, rapid, and sensitive method for determining more than seventy elements.

Until now, there have been few research works using non-toxic, fire-safe, and inexpensive cadmium extractants, as well as studying the influence of major accompanying metals on its quantitative extraction. Systems with low-melting organic reagents provide a number of advantages: higher distribution and concentration coefficients of elements, the ability to carry out the process in the low pH range and a wide range of element concentrations, clear phase separation, practical insolubility in water, and non-toxicity of low-melting organic substances. Almost all low-melting organic substances are non-volatile, and therefore do not pollute the air in the workplace; many of them have a wide temperature range of existence of the liquid phase, are non-flammable, thermally and hydrolytically stable.

In this work, the extraction patterns of cadmium by low-melting organic substances with subsequent atomic absorption determination of cadmium(II) in aqueous solutions were established. The individual influence of major accompanying metals such as copper(II), zinc(II), and iron(III), as well as the influence of a mixture of accompanying metals on the conditions of quantitative extraction of cadmium into the melt of low-melting organic substances, were studied. This allows for the closest approximation of the composition of artificial models to the composition of natural objects in the environment of Kazakhstan. The obtained data can be used for monitoring cadmium in environmental objects and food products, as well as for the development of new combined methods for determining cadmium in the presence of major accompanying metals.

### References

[1] Occupational safety and health administration (OSHA). U.S. Department of Labor. (2024).

## Catalytic Dehydration of Biomass-Derived Feedstocks to Obtain 5-Hydroxymethylfurfural and Furfural

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Leave a blank line between each paragraph (do not **indent** the paragraph). The text should be **justified left and right**. Biomass- produced furanics, furfural and 5-hydroxymethylfurfural (5-HMF), are considered as vital platform chemicals used in the production of active pharmaceutical ingredients (APIs), nanomaterials, and fuels. The primary challenge associated with their production pertains to the high cost involved in scaling up to industrial levels. Consequently, it is essential to explore more cost-effective options that yield efficient end products. In this study, the use of Lewis and Brønsted acids such as HCl and AlCl<sub>3</sub> enhances the isomerization of glucose through catalytic dehydration into 5-HMF. It was observed that employing moderate reaction conditions increased the yield of 5-HMF to 44.94 % and 50.60 % respectively, with changes in HCl concentration and AlCl<sub>3</sub> mass loading. The suitable conditions to achieve the highest yield of 5-HMF were 100 μL of HCl, 0.75 g of AlCl<sub>3</sub>, reaction temperature 150 °C, and reaction time 4 h. In the second experiment,



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corn cob was converted into furfural in the presence of 20 % H<sub>2</sub>SO<sub>4</sub>, in combination with NaCl as a promoter. The optimal conditions under which a yield of 44.77 % was achieved were as follows: 50 mL of 20 % H<sub>2</sub>SO<sub>4</sub>, reaction temperature 140 °C, 0.5 g of NaCl, 5 g of corn cob, and reaction time 160 min. Furthermore, a proposed reaction mechanism was outlined to elucidate the pathway for the production of the aforementioned platform chemicals.

### **Extraction-atomic-absorption determination of iron(III) by molten tributyl phosphate in paraffin**

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The Republic of Kazakhstan ranks 8th (6%) in the world in terms of iron ore reserves (about 8.7 billion tons of proven reserves, 12.5% of the Republic's industrial volume) [1]. 70% of the produced goods are exported to 97 countries worldwide. Within the Republic's territory, the Sokolovsky-Sarbaysky and Lisakovskiy ore-dressing plants (ODP), Aktobe and Aksu ferroalloy plants, and JSC "Ispat Karmet" engaged in rolling and production of ferrous metallurgy products are operating. The Aksu ferroalloy plant is one of the world's largest producers of ferroalloys [2].

At present, there is no reason to extract iron from solutions after leaching, as it is more advantageous to obtain it from rich ores using conventional flotation and pyrometallurgy methods. However, iron removal and extraction are necessary for environmental protection reasons and the need to conserve natural resources. Iron removal from solutions is practiced only at a few plants; however, the main task of such processes is merely to remove it from the system to facilitate the extraction of the main metal in subsequent technological operations. Usually, for iron removal after leaching, this solution is oxidized and neutralized with lime. As a result, iron precipitates in the form of hydroxide, jarosite, or goethite. This process is highly inefficient. When iron is precipitated, a stoichiometric amount of gypsum is also formed. A significant problem arises in the daily removal of large quantities of gypsum and iron cake. Large tailings ponds are required for this. In addition, the bulky precipitate carries away a large amount of valuable metal, which is not extracted even by washing and is lost. Gradually, these metals are leached from the gypsum-iron cake by ordinary weathering. As a result, there are tailing dumps containing metals such as iron, nickel, cobalt, and zinc at concentrations of several hundred milligrams per liter. If there is no provision for returning these waters to the plant, they gradually pollute water bodies. There are grounds to expect that in the future, iron will be extracted from solutions not only due to environmental protection but also due to saving its natural resources.

Nowadays, iron extraction from chloride solutions is widely used. Along with diethyl ether and diisopropyl ether, which were previously most widely used, currently, tributyl phosphate, methyl isobutyl ketone, and other solvents are often used. This work is dedicated to the principles and establishment of optimal conditions for quantitative extraction of iron halide complexes by a tributyl phosphate molten in paraffin. The concentration of iron(III) in aqueous solutions was controlled by atomic absorption spectroscopy, which is a modern, reliable, rapid, and sensitive method for determining more than seventy elements. The influence of various factors was studied: temperature, duration of phase contact, volume ratio of phases, pH of the aqueous solution, metal concentration, concentration of hydrochloric acid on the degree of iron(III) extraction. The obtained data can be used for monitoring iron in various environmental objects and food products, as well as for the development of new combined methods for determining iron(III).

#### **References**

- [1] United States Geological Survey (USGS). Mineral commodity summaries. (2022) 99.
- [2] Gross domestic product for 2023 (data on a quarterly basis) // © 2023 Agency of the Republic of Kazakhstan on Statistics



## PCL-based hydrophobic nanofiber membrane preparation and optimization

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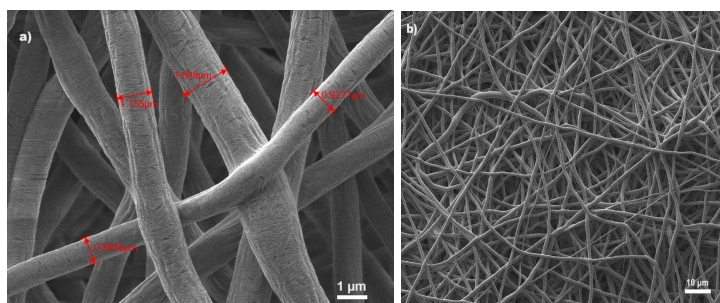
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Hydrophobic materials are increasingly in demand due to their unique set of functional properties, such as waterproof, corrosion-resistant, stability in biofouling and inorganic pollutants. Their ability to repel water and other liquids makes them valuable for applications in health and safety, environmental protection, energy efficiency and consumer products. In particular, air and water filtration techniques have been in high demand during the Covid-19 pandemic, and water-oil separation techniques remain relevant to reduce the environmental hazards of oil leaks.

Due to high stability and high chemical resistance of the nanofibers, the hydrophobic nanofibers are commonly utilized among the hydrophobic materials. With the use of electrospinning technique, the fibers with high porosity, small diameter, high strength to weight ratio, and high surface to volume ratio can be manufactured. [1] Moreover, the morphology of the fibers can be controlled by optimizing the electrospinning parameters. Versatility of nanofibers provides wide range of opportunities for creating the hydrophobic materials.

Hydrophobic nanofibers can be efficiently produced from polymers known for their water-repellent properties, such as polystyrene (PS), polyacrylonitrile (PAN), polymethyl methacrylate (PMMA), polydimethylsiloxane (PDMS) [2], [3], [4], [5]. However, the Polycaprolactone (PCL) was chosen for its unique combination biodegradability, biocompatibility and excellent mechanical properties. The semi-crystalline nature of PCL provides a balance of flexibility and strength, allowing the creation of strong nanofiber structures that maintain integrity under a variety of conditions.

In our research, we successfully fabricated polycaprolactone (PCL) nanofibers using the electrospinning technique. Chloroform (CF) is commonly used as a solvent for PCL; however the viscosity of solutions is barely controllable with the chloroform, which results in micrometric dimensions. In order to decrease the sizes to the nanoscale dimensions, the PCL was dissolved in binary solution of CF/ Dimethylformamide (DMF) with the ratio of 4:1. The optimized parameters of prepared hydrophobic PCL nanofibers with the diameter range of 885.8 nm – 1608.0 nm as following: flow rate of solution – 1.0ml/hour, tip-to-collector distance – 15cm, applied voltage – 20kV. According to the scanning electron microscope (SEM) images on Figure 1. the morphological analysis of the nanofibers – the surface of the fibers is homogeneous and fibers have uniform fibrous structure. The mechanical stability, hydrophobicity and filtration performance of the obtained membranes were investigated.



**Figure 1.** SEM images of nanofibers obtained from CF/DMF solution by electrospinning technique. a) morphology of separate nanofibers, b) morphology of nanofiber film.

### References

- [1] Alarif, Ibrahim M., et al. *Materials* 8.10 (2015): 7017-7031.
- [2] Lin, Jinyou, et al. *Nanoscale* 4.1 (2012): 176-182.
- [3] Kausar, A. *Advances in Materials Science* 19.1 (2019): 5-20.
- [4] Chang, T. C., et al. *Journal of Polymer Science Part A: Polymer Chemistry* 38.11 (2000): 1972-1980.
- [5] Li, Kunquan, et al. *Applied surface science* 279 (2013): 458-463.



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## Deep eutectic solvent-supported poly(vinyl) alcohol electrospun anion-exchange membrane for alkaline fuel cell application

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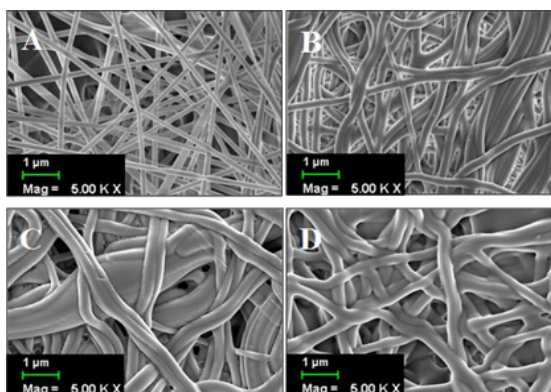
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Alkaline anion exchange membrane fuel cells (AEMFC) have gained interest due to their potential as electrochemical energy conversion devices and a competitive alternative to the more extensively studied commercialized proton exchange membrane fuel cells (PEMFCs). Nevertheless, their development impedes the limited ion conductivity and chemical and mechanical stability in an alkaline medium of anion exchange membranes (AEMs). The ionic conductivity of AEM is lower than that of a proton exchange membrane (PEM) because the mobility of hydroxide ions is inherently lower than that of protons [1]. Deep eutectic solvents (DESs) as green solvents can overcome this issue. In this work, a new fabrication approach for DES-supported AEMs for AEMFC application was developed. The obtained composite AEMs comprise a poly(vinyl) alcohol (PVA) polymer-based nanofiber mat prepared by the electrospinning method, crosslinked with glutaraldehyde (GA) solution, and impregnated with DES, which consists of choline chloride (ChCl) and ethylene glycol (EG). Poly(vinyl alcohol) (PVA) is one of the potential polymers for the development of AEM due to its water solubility, biodegradability, high fiber forming ability, non-toxicity, and high chemical and thermal stability [2]. DES might facilitate the conductivity of hydroxide ions, while the PVA-based nanofibers in the form of membranes are the platform for ion conduction. Overall, modification with DES could enhance the properties of the membrane without affecting the structure of the polymer by an environmentally friendly and straightforward approach. Thus, this work aims to achieve high ionic conductivity and chemical and mechanical stability by using DES as an additive within a PVA nanofibrous network. As a result, the cross-linking of pristine PVA fibers with GA solution (see Figure 1B), DES uptake, and the presence of voids as channels for ion conduction (see Figure 1C and 1D) were successfully confirmed with scanning electron microscopy (SEM, Crossbeam500, Zeiss). DES-supported composite AEM named DES3@PVA4 (crosslinked with a 4 wt.% GA solution) revealed a conductivity of 0.66 and

1.05 mS/cm at room temperature and 60 °C, respectively, with the help of electrochemical impedance spectroscopy (EIS, Metrohm Autolab). Along with high ionic conductivity, the DES3@PVA4 composite membrane maintained the original nanofiber structure's potential for avoiding areal swelling. The absence of swelling also impacted the moderate water uptake (364 %) and enhanced tensile characteristics with a tensile stress of 0.19 MPa and elongation at break of 1.08 %, particularly elongation that was adequate to maintain the membrane's integrity. Tensile test measurements were conducted using electronic universal testing equipment (WDW-3 Jinan HST Group Co.). So, the DES-supported PVA-based composite membrane demonstrated high hydroxide conductivity, flexibility, and mechanical stability in a fully hydrated state, showing potential to be utilized as an AEM for AEMFC applications.







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Figure 1. SEM images of the top views of (A) pristine PVA, (B) PVA4, (C) DES3@PVA4, and (D) DES3@PVA4 after immersion in potassium hydroxide solution.

### References

- [1] G. Das, J.-H. Choi, P. K. T. Nguyen, D.-J. Kim, and Y. S. Yoon, *Polymers (Basel)*. 14 (6) (2022) 1197.
- [2] C.-C. Yang, S.-J. Lin, and G.-M. Wu, *Mater. Chem. Phys.* 92 (2005) 251–255.

## Solid state synthesis of noble-metal-free micro/nanostructured g-C<sub>3</sub>N<sub>4</sub>/NiS/Bi<sub>2</sub>S<sub>3</sub> photocatalysts for hydrogen evolution

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The process of water splitting to produce hydrogen through photocatalysis has attracted significant interest due to its cost-effectiveness, low energy consumption, and environmental friendliness [1]. Numerous efforts have been undertaken to develop photocatalysts that are both active and highly efficient for this purpose. However, the incorporation of noble metals as co-catalysts increases the cost of hydrogen production, thereby restricting its practical applications [2]. In this study, we present all solid state approach for synthesizing noble-metal-free micro/nanostructured photocatalysts composed of g-C<sub>3</sub>N<sub>4</sub>, NiS, and Bi<sub>2</sub>S<sub>3</sub> for hydrogen evolution. The synthesis process comprises two steps: milling using a planetary ball mill followed by thermal treatment. This approach resulted in systems with component content by weight percent of g-C<sub>3</sub>N<sub>4</sub>/NiS/Bi<sub>2</sub>S<sub>3</sub> at (98-1-1) and (96-2-2). For comparison double systems g-C<sub>3</sub>N<sub>4</sub>/NiS (98-2) and g-C<sub>3</sub>N<sub>4</sub>/Bi<sub>2</sub>S<sub>3</sub> (98-2) were also synthesized. Our experimental findings from XRD analysis revealed the presence of the main characteristic peaks of g-C<sub>3</sub>N<sub>4</sub>, NiS, and Bi<sub>2</sub>S<sub>3</sub> (Figure 1). SEM and TEM analysis showed that the samples comprised layers of g-C<sub>3</sub>N<sub>4</sub> decorated with NiS nanoparticles (with diameters less than 20 nm) and rod-shaped Bi<sub>2</sub>S<sub>3</sub> (with lengths below 200 nm). Additionally, our photocatalysts demonstrated the capability to generate hydrogen from water-alcohol solutions, underscoring the importance of further investigation into this promising system.

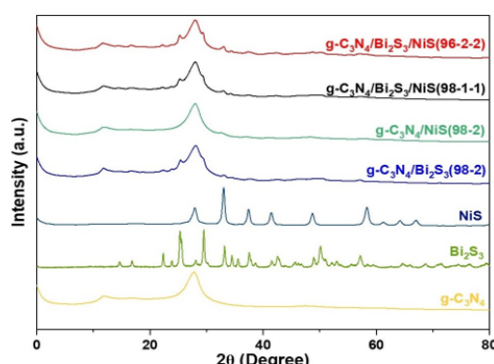


Figure 1. XRD patterns of the prepared samples.

### Acknowledgments

This research was funded by the Science Committee of the Ministry of Education and Science of the Republic of Kazakhstan (Grant No. AP13068426).

### References

- [1] W. Zhao., Z. Chen, X. Yang, X. Qian, C. Liu, D. Zhou, Ok. Y.S. *Renew Sustain Energy Rev*, 132 (2020), 110040.
- [2] Y. Lei, X. Wu Li S., J. Huang, K. H. Ng, & Y. Lai. *J Clean Prod*, 322 (2021) 12901



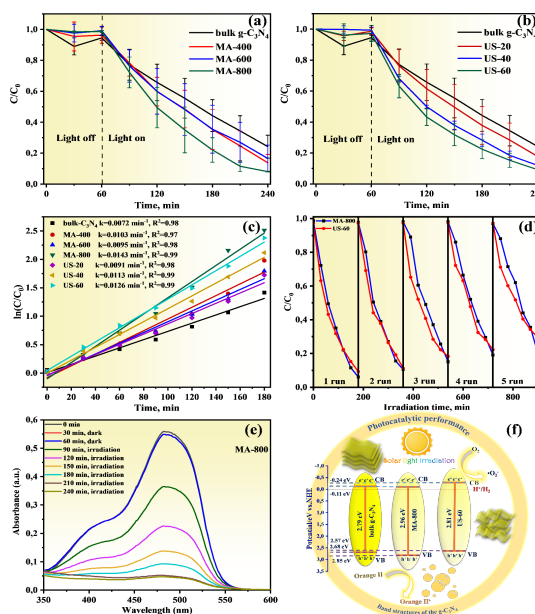
## Enhancement of the photocatalytic activity of g-C<sub>3</sub>N<sub>4</sub> via ball milling exfoliation

Saparbek Tugelbay<sup>1\*</sup>, Batukhan Tatykayev<sup>1</sup>, Almagul Mentbayeva<sup>1</sup>, and Zhandos Shalabayev<sup>1</sup>

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Herein, a sustainable and scalable planetary ball milling technique was applied for grinding and exfoliation of graphitic carbon nitride (g-C<sub>3</sub>N<sub>4</sub>) in order to enhance its photocatalytic activity [1]. Milling parameters such as rotation speed, time, and ball-to-powder ratio were optimized. The superiority of the ball milling technique was compared with the already successfully proven ultrasonic exfoliation method. The efficiency of exfoliation of the mechanically activated g-C<sub>3</sub>N<sub>4</sub> samples was assessed (varied) by their photocatalytic activity, namely the photocatalytic decomposition of the organic dye Orange II under visible light irradiation. The photocatalytic activity of g-C<sub>3</sub>N<sub>4</sub> exfoliated in a ball mill at 800 rpm for 10 min was found to be higher than that of g-C<sub>3</sub>N<sub>4</sub> exfoliated by ultrasonic method and two times higher than that of bulk g-C<sub>3</sub>N<sub>4</sub>. The ball mill-exfoliated g-C<sub>3</sub>N<sub>4</sub> showed highly photocatalytic hydrogen evolution performance with HER equal to 4117.86  $\mu\text{molh}^{-1}\text{g}^{-1}$ , which was more than 7 times superior to the bulk g-C<sub>3</sub>N<sub>4</sub> material. The mechanical activation technique should receive more attention, as all samples processed by this method showed higher photocatalytic performance compare to other methods.



**Figure 1.** Results of photocatalytic activity of processed g-C<sub>3</sub>N<sub>4</sub> (a) mechanical activation, (b) ultrasound, (c) calculation of reaction rate using the Langmuir-Hinshelwood (L-H) formula, (d) results of photocatalytic stability of MA-800 and US-60 samples, result from photocatalytic activity of MA-800(e) and band structures of g-C<sub>3</sub>N<sub>4</sub>(f).

### Acknowledgments

This research was funded by the Science Committee of the Ministry of Education and Science of the Republic of Kazakhstan (Grant No. AP13068426).

### References

[1] Zhu K., Wang W., Meng A., Zhao M., Wang J., Zhao M., Zhang D., Jia Y., Xu C., Li Z. Mechanically exfoliated gC 3 N 4 thin nanosheets by ball milling as high performance photocatalysts // RSC Advances. – 2015. – T. 5, № 69. – C. 56239-56243.



## Evolution of the structure of magnesium-based powder compositions depending on mechanofusion parameters

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Today, work in the field of hydrogen technology is rapidly developing. This trend is typical for most countries of the world. The transition to hydrogen energy involves a significant change in the existing structure of the fuel and energy complex and is associated with the gradual replacement of carbon-containing energy carriers with hydrogen, which is associated with achieving carbon neutrality by 2050. Being an energy-intensive, environmentally friendly and technologically clean energy carrier, hydrogen at the same time poses significant inconveniences, related to its storage and transportation. In this regard, solid-state storage systems based on metal hydrides are currently a relevant method for storing and transporting hydrogen. Metal hydride systems are characterized by high compactness, safety and multiply reversible sorption properties for hydrogen storage, and one of the promising materials is magnesium (Mg)-based compounds [1].

An effective approach to improving the properties of magnesium-based compounds is to reduce the particle size and control the structural and phase composition while maintaining the nanosize of the precipitated phases during consolidation. Research confirms that particle size plays a key role in determining the hydrogen capacity and thermodynamic properties during the hydrogenation and hydrogen dehydrogenation of magnesium-based materials [2]. In nanostructured materials, the large specific surface area and high-density crystalline boundaries significantly destabilize the binding energy between magnesium and hydrogen. This leads to a decrease in the desorption temperature of MgH<sub>2</sub> and an improvement in the kinetics of hydrogen accumulation. Therefore, the kinetics and thermodynamics of dehydrogenation of magnesium-based alloys significantly depend on their microstructure, especially when the alloy particle size is reduced to the nanometer scale [3].

The use of a planetary ball mill activates solids by grinding in impact, impact-attrition or attrition modes. This leads to the accumulation of structural defects, an increase in curvature and surface area, phase transformations and even amorphization of crystals, which in turn affects their chemical activity. The machining process can influence the quality of the final material. Currently, significant experimental experience has been accumulated in machining processes. However, little attention has been paid to such an important process parameter as the ratio of grinding balls to processed powder and its combination with the acceleration and duration of the process [4].

Taking into account the above, the combination of mechanical processing parameters and the selection of optimal process modes can significantly influence the kinetics of hydrogen accumulation and the thermodynamics of magnesium-based alloys, especially when the alloy particle size is reduced to the nanometer scale, which leads to improved kinetics and thermodynamics of dehydrogenation, which can be used to further study intermetallic compounds as hydrogen transport materials.

### Acknowledgements

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### References

- [1] I. Arto, I. Capellán-Pérez, R. Lago, G. Bueno, R. Bermejo. The energy requirements of a developed world. *Energy Sustain Dev*, 33 (2016), pp. 1-13, 10.1016/j.esd.2016.04.001.
- [2] D. Wiedenhofer, M. Lenzen, J.K. Steinberger. Energy requirements of consumption: Urban form, climatic and socio-economic factors, rebounds and their policy implications. *Energy Policy*, 63 (2013), pp. 696-707, 10.1016/j.enpol.2013.07.035.
- [3] P. Mesarić, S. Krajcar. Home demand side management integrated with electric vehicles and renewable energy sources. *Energy Build*, 108 (2015), pp. 1-9, 10.1016/j.enbuild.2015.09.001.



[4] M.Z. Jacobson. Review of solutions to global warming, air pollution, and energy security. *Energy Environ Sci*, 2 (2009), pp. 148-173, 10.1039/b809990c

## From Waste to Energy: Creating Good-Performance TENGs from PVC/ZnO Nanofibers

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**Keywords:** electrospinning, triboelectric nanogenerators, PVC nanofibers, ZnO nanoparticles, energy harvesting, recycling.

The growing demand for sustainable energy solutions has driven the exploration of innovative methods for harvesting energy from ambient sources. This study presents the development of triboelectric nanogenerators (TENGs), a cutting-edge technology that converts ambient mechanical energy into electricity through triboelectrification and electrostatic induction, facilitating the operation of self-powered microelectronic devices. TENGs provide new opportunities for efficiently harnessing mechanical energy for both power generation and sensing applications. Despite the high charge transfer and capture capabilities of various polymer materials used in TENGs, challenges such as relatively low output performance and environmental problems remain.

To address the dual issues of enhancing the triboelectric performance of TENGs and mitigating environmental impact, our research focuses on the innovative recycling of waste polyvinyl chloride (PVC) pipe polymers, doped with zinc oxide (ZnO) nanoparticles. PVC, the second most widely used yet environmentally detrimental polymer due to its non-biodegradability, offers high tribonegativity, making it an excellent candidate for TENG applications through the recycling of waste materials. The addition of ZnO nanoparticles aims to improve electrical performance by enhancing charge transfer capabilities. This combination is processed into a nanofiber morphology to maximize output efficiency. These nanofibers are designed to harvest energy from human motion and contact-separation, effectively capturing low-frequency mechanical energy.

Two types of nanofibers, pure PVC nanofibers and PVC/ZnO nanofibers, have been synthesized. Waste PVC pipes were collected and processed into a 14 wt% polymer solution, identified as the optimal concentration for the pure PVC nanofibers. For the second sample, to enhance triboelectric performance, ZnO nanoparticles were incorporated into the PVC nanofibers at varying weight percentages, with 0.5 wt% of PVC identified as the optimal concentration. The resulting mixture was electrospun into nanofibers to optimize the surface area for enhanced triboelectric interaction. Detailed characterization of the nanofibers was performed to evaluate their properties and effectiveness.

X-ray photoelectron spectroscopy (XPS) analysis provided insights into the chemical composition and surface characteristics of the PVC nanofibers, highlighting the presence of C, and Cl bonds, and confirming the integration of ZnO (Z-O) nanoparticles. Scanning electron microscopy (SEM) revealed a uniform filamentous morphology of the nanofibers, which is important factor for consistent our triboelectric performance. Fourier-transform infrared spectroscopy (FTIR) confirmed the chemical bonds of the pur PVC, and PVC/ZnO nanofibers.

The results demonstrate that, the incorporation of ZnO nanoparticles significantly increased the current and voltage output of recycled PVC-based TENGs, with nanofiber structures providing a larger contact area for charge transfer (see Figure 1). This enhancement is due to the high tribonegativity of PVC and the piezoelectric properties of ZnO nanoparticles. Recycling waste PVC reduces non-biodegradable waste, contributing to environmental sustainability and making them good candidate for energy harvest material like TENGs.



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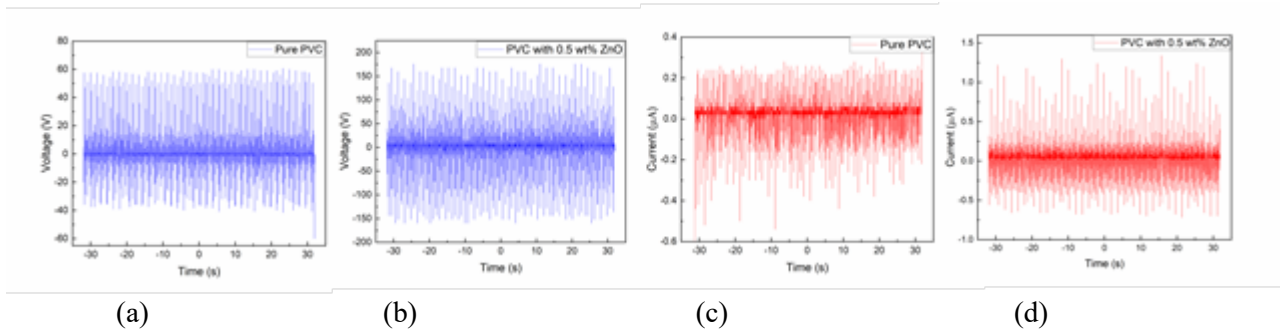


Figure 1. Voltage and current output of TENGs tested for pure PVC and PVC/ZnO composites. The voltage output for (a) pure PVC and (b) PVC/ZnO, and the current output for (c) pure PVC and (d) PVC/ZnO.

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## Plastic relaxation in nanocrystalline Al with Cu segregated at grain boundaries: atomistic investigation, machine learning and continuum modeling

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The study included an atomistic study, generalization of atomistic study data using an artificial neural network (ANN), and continual modeling of the macrovolume dynamics of a substance using the smoothed particle method, which describes the elastic-plastic response of a substance using the constructed ANN. Low-angle  $\Sigma 99a(110)Al$  boundaries and high-angle  $\Sigma 9(110)Al$  boundaries were studied. The performed molecular dynamics (MD) study showed that the mechanisms of the elastoplastic transition in nanocrystalline aluminum substantially depend on the concentration of copper atoms segregated on GBs. For a small-angle GB  $\Sigma 99a(110)Al$ , a successive change in the mechanisms of activation of plastic flow is observed: GB migration, rotation of grains, emission of dislocations from GB. In the case of a high-angle GB of  $\Sigma 9(110)Al$  type, the initial GB migration is replaced by grain rotation. The change in the mechanisms of activation of plastic flow with an increase in the concentration of segregated copper atoms is accompanied by a nonmonotonic change in the critical stress of the elastic-plastic transition. The maximum of this dependence for both studied boundaries is reached at a concentration of copper atoms of 7.2–7.6 at.%. For GB  $\Sigma 99a(110)Al$  type, the maximum stress was about 3 GPa, for GB  $\Sigma 9(110)Al$  type - about 2 GPa.

An artificial neural network (ANN) is used to approximate the mechanical response and plastic deformation mechanisms to describe the behavior of GBs, which in a complex way depends on the concentration of copper on the GBs and the previous history of deformation. The proposed ANN describes the values of elastic and plastic deformation, the number of defect atoms, and the grain rotation angle. Comparison of ANN results with MD data not used in ANN training demonstrates good quantitative agreement between strain-stress relationships and adequately reflects the mechanisms of plastic deformation. The use of ANN makes it possible to obtain, in a short time, continuous dependences on the concentration of copper atoms for the strain-stress curves, the proportion of defect atoms, and the plastic deformation provided by grain rotation. With the help of ANN, the boundaries of copper concentration regions were established, in which plastic relaxation occurs mainly due to the rotation of grains, reducing the number of defects in the bulk of grains, which suggests an increased resistance of such nanocrystalline samples to long-term deformation. For a  $\Sigma 99a(110)Al$  type small-angle grain boundary, the range of preferential grain rotation corresponds to concentrations of segregated copper atoms of 1.5–3.6 at.% and 7.2–8.7 at.%.

To describe the mechanical properties of macrovolumes of nanocrystalline aluminum with copper atoms segregated on GBs, a trained ANN is used to describe the elastic-plastic properties of a substance in the smoothed particle method. The solution of the equations of continuum mechanics using this technique made it possible to simulate the plastic deformation of micropillars of a substance formed from nanocrystalline aluminum.

### Acknowledgments

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## ZnO-based gas CO sensor: A DFT Study

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This study investigates the crystal lattice parameters and adsorption characteristics of carbon monoxide (CO) on a zinc oxide (ZnO) (100) surface using density functional theory (DFT) calculations. The ZnO (100) surface's structural parameters were evaluated, revealing lattice constants of  $a = 3.263 \text{ \AA}$  and  $c = 5.235 \text{ \AA}$ , with a volume of  $48.30 \text{ \AA}^3$ , slightly deviating from Mohamed Achehboune et al. (2022) values. The adsorption energy for CO on the ZnO surface was  $-0.84 \text{ eV}$ , indicating a favorable interaction.[2] The bond length between carbon (C) and zinc (Zn) increased from  $2.02 \text{ \AA}$  to  $2.1434 \text{ \AA}$ , while the bond length between oxygen (O) in CO and carbon decreased from  $1.3 \text{ \AA}$  to  $1.14 \text{ \AA}$ , with a bond order of one post-relaxation.

The study's findings align with experimental results by Quanzi Yuan et al. (2009), especially regarding bond length, angle adjustments, and the band gap energy increase upon CO adsorption[1]. The band gap modification was quantified using the sensitivity factor  $S = 10.18$ . This work provides critical insights into the adsorption mechanism of CO on ZnO surfaces, impacting the design and optimization of ZnO-based gas sensors. The analysis of adsorption energy, bond length alterations, and structural parameters offers a comprehensive understanding of interaction dynamics at the molecular level, crucial for advancing sensor technology in monitoring air quality and detecting hazardous gases.

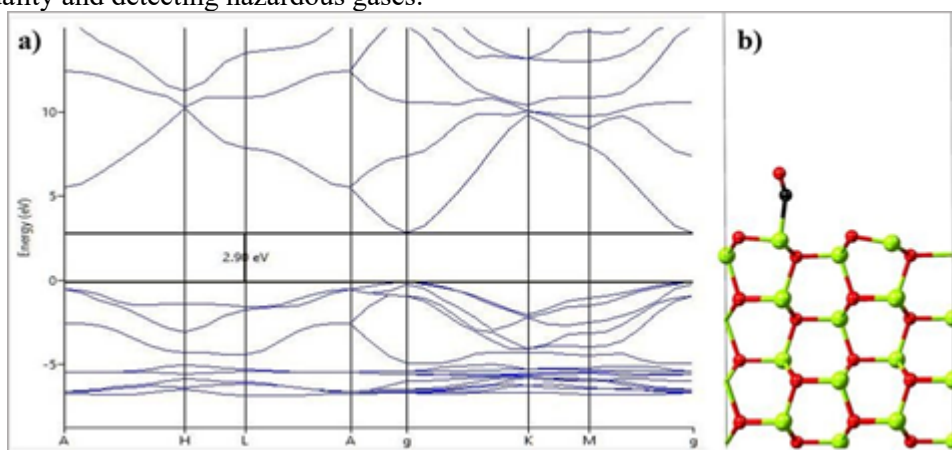


Figure 1. a)ZnO 100 surface band gap and b) CO gas adsorption on ZnO 100 surface

### References

[1] Yuan, Q.; Zhao, Y.-P.; Li, L.; Wang, T. *Journal of Physical Chemistry. C./Journal of Physical Chemistry. C* **2009**, *113* (15), 6107–6113.

[2] Achehboune, M.; Khenfouch, M.; Boukhoubza, I.; Derkaoui, I.; Mothudi, B. M.; Zorkani, I.; Jorio, A. *Computational Condensed Matter* **2022**, *31*, e00627.



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## Development of centrifuge-assisted method for powder bed compaction in additive manufacturing

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**Keywords:** Additive manufacturing, Powder bed fusion, Artificial gravity, Discrete element method, Packing density.

The laser powder-bed fusion (L-PBF) process is one of the promising Additive Manufacturing (AM) techniques due to its efficient way to produce complex shapes and fine 3D components. There are a lot of experimental and numerical studies on particle compaction in AM, but most of these studies focus on conventional methods of powder compaction and distribution. Traditional methods typically involve a blade/roller to reduce the surface roughness of the powder bed, which causes particle segregation, resulting in a non-uniform powder bed. Nevertheless, there were some studies that focused on the compaction of powder through centrifugal force, indicating its advantages, such as improved packing structure compared to traditional processes. In this work, both experimental and numerical analyses were conducted to investigate the effect of artificial gravity on the compaction of metal powder. The packing density of the powder bed is analyzed experimentally and numerically under various artificial gravity (G). The results show enhanced packed powder compaction with increasing gravity in comparison to the powder bed compaction using conventional methods. This research work contributes to a better understanding of the developed method for powder bed packing, which significantly affects the quality of the final product in additive manufacturing. As artificial gravity and its impact on the packing behavior of powder bed in AM was not investigated before, this method presents a potential application of gravitational acceleration to improve powder compaction and distribution.

## Ionic conductivity and a deuterium kinetic isotope effect in chitosan films

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Chitosan (CS) is a hydrophilic and biodegradable polysaccharide made of glucosamine and N-acetylglucosamine residues. Chitosan is widely used in anion exchange membranes in fuel cells due to its flexibility for modification and thermal/chemical stability [1]. Besides these features, this biopolymer is well-known as a highly proton-conductive material [2]. All this makes chitosan an excellent platform for versatile applications. Proton conductivity and high-water affinity of CS arise from its molecular structure that has three different polar functional groups, which are hydroxyl (–OH), primary amine (–NH<sub>2</sub>), and C–O–C groups [3]. Intermolecular solid hydrogen bonds between glucosamine monomers' amino and hydroxyl groups create a rigid crystalline structure [4]. At the same time, CS can dissolve in acidic aqueous solutions because of D-glucosamine residues that can be protonated [5]. According to Pemble et al. [6], the intramolecular and intermolecular hydrogen bonding in chitosan dissolved in acidic media forms a noncovalently bound network. When deuterium replaces protic hydrogen in a chemical bond due to the deuteration, the stretching vibrational frequencies of the bond are affected directly. Since deuterium has a greater mass, the vibrational frequencies are reduced. As a result, this leads to a change in the polymer's properties, including its conductivity. The main objective of this paper is to shed light on the proton conduction features of chitosan by investigating the kinetic isotope effect in protonic conductivity and the sheet resistivity between the protonated and deuterated chitosan. This study obtained and characterised the protonated and partially deuterated CS films via FTIR, XRD, and UV-vis spectroscopic analysis. The results revealed that the CS films are deuterated because of the appearance of the absorption signals from C–D and O–D/N–D peaks on the FTIR spectra. XRD patterns of CS films align with previous works: pure chitosan exhibits broad peaks at  $2\theta=10^\circ$  and  $20^\circ$ , revealing the semi-crystalline nature of the protonated CS film [7-8]. As noted, a deuteration only affects the intensity of signals. Based on the UV absorption peaks at around 234-281 nm arising due to the  $\pi\rightarrow\pi$  bond transition in the CS molecule, it might be





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suggested that the optical band gap (as well as the electronic band gap as predicted) is of high value as for insulators. Chronoamperometry has demonstrated a typical current pattern for ionic conductors with a predominant role of ionic species in charge transfer based on the transference number measurements. The 4-probe measurements of the sheet resistance and the charge mobility also confirm that the contribution of electrons to the charge transfer is low. Besides this, there is a constant change in the electrical/electrochemical response of protonated and partially deuterated CS films, most likely due to a deuteration known as the kinetic isotope effect. The kinetic isotope effect in chitosan provides insight into the ionic conduction process in hydrated chitosan and the understanding of the ionic conductivity differences between protonated and deuterated chitosan from the microscopic viewpoint. These results are helpful for research on the application of biopolymer chitosan, an environmentally friendly material, as a fuel cell electrolyte and for the potential functionality of chitosan for creating new products.

### References

- [1] V. Vijayakumar, S.Y. Nam. *Membranes*, 12(2022) 1265-1276.
- [2] G. Zhao, Y. Chen, X.-F. Li, S. Zhang, Y. Situ. *Green Chemistry*, 22(2020) 2426–2433.
- [3] N. Adiera, H. Rosli, K.S. Loh, W.Y. Wong, R.M. Yunus, T.K. Lee, A. Ahmad, S.T. Chong. *Molecular Sciences*, 21(2020) 632- 684.
- [4] X.Y. Kong, X.Y. Li, X.H. Wang, T.T. Liu, Y.C. Gu, G. Guo, F. Luo, X. Zhao, Y.Q. Wei, Z. Y. Qian. *Carbohydrate Polymers*, 79(2010) 170–175.
- [5] M.R. Leedy, H.J. Martin, P.A. Norowski, J.A. Jennings, W.O. Haggard, J.D. Bumgardner. *Chitosan for Biomaterials II*, Springer, 2020 129–165.
- [6] O.J. Pemble, M. Bardosova, I.M. Povey, M.E. Pemble, Z. Papageorgiou. *Polymers*, 13(2021) 1566-1579.
- [7] I. Ishmaturrahmi, R. Rahmi, I. Mustafa. *IOP Conf. Ser.: Mater. Sci. Eng.*, 523(2019) 012020.
- [8] S. Kumar, J. Koh. *Int. J. Mol. Sci.*, 13(2012) 6102–6116.

## Formation of doped poly-Si nanolayers via spin-on doping and magnetron sputtering safe methods for TOPC on Si solar cells

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Silicon solar cells continue to dominate the renewable energy industry due to the abundance of silicon on Earth, its accessibility, stability, and relatively low cost. Nowadays, various technological concepts have been implemented to improve the efficiency of solar cells. Tunnel Oxide Passivated Contact (TOPCon) silicon solar cell developed at Fraunhofer ISE have high potential for commercialization. The main feature of this structure is the presence of a tunnel layer of silicon oxide between the doped poly-Si layer and the c-Si substrate. The silicon oxide nanolayer can significantly increase the lifetime of minority charge carriers  $\tau_{eff}$  and as a result achieve high efficiency. For instance, one of best efficiency for Si solar cell reaching of 25.7% was achieved by TOPCon structure [1], while the calculated theoretical maximum reaches 28% [2]. Conventional technologies for producing TOPCon solar cells involve the transportation, storage, and use of highly toxic and explosive gases. Therefore, developing alternative methods is essential to safely manufacture high-efficiency solar cells.

In this work, ultrathin SiO<sub>2</sub> tunnel layer (~1.5 nm) was formed by the immersion of silicon wafer in nitric acid at a high temperature and/or by rapid thermal oxidation (RTO) method. Thin layer of a-Si with a thickness of ~50 nm was deposited via sputtering method using a MAGNA-TM 200 installation. Boron and phosphorus containing solutions of our own production were deposited on the surface of the resulting films by spin coating method. Subsequently, the simultaneous diffusion of boron and phosphorus, along with the crystallization of the silicon layer, was performed in a quartz tube furnace and/or by the rapid thermal annealing (RTA) method at temperatures ranging from 850 to 950°C. To reduce reflection from the surface indium tin oxide (ITO) layers were deposited on both surfaces of the wafers. As a result, a basic method for fabrication of TOPCon solar cells using safe synthesis methods was developed. To study the characteristics of the resulting structures, the spectra



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of X-ray reflectometry (XRR) and X-ray diffraction (XRD), the lifetime of minority charge carriers ( $\tau_{\text{eff}}$ ), sheet resistance, current-voltage characteristics etc. was measured.

### References

- [1] A. Richter, J. Benick, F. Feldmann, A. Fell, M. Hermle and S. Glunz, *Sol. Energy Mater. Sol. Cells*, 173 (2017) 96-105.
- [2] R. Peibst, M. Rienacker, Y. Larionova, N. Folchert, F. Haase, C. Hollemann, S. Wolter, J. Krügener, P. Bayerl, J. Bayer, M. Dzinnik, R. Haug и R. Brendel, *Solar Energy Materials & Solar Cells*, 238 (2022) 111560.

## Improving dye sensitized solar cell performance through optimized *N*-alkyl carbazole - PEDOT co-polymer counter electrodes

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In dye-sensitized solar cells (DSCs), the counter electrode plays a crucial role in facilitating electron transport, completing the electrical circuit, and ensuring long-term performance stability. However, the traditionally used platinum counter electrode is associated with cost constraints. Therefore, conductive polymer materials have emerged as promising alternatives. Polycarbazole and its derivatives exhibit versatile electronic properties that promise advances in optoelectronic devices, sensors, and flexible electronics, offering higher efficiency, functionality, and reliability. Despite its favorable electrical properties, polycarbazole struggles with degradation issues when exposed to iodine-containing electrolytes used in DSCs. To take advantage of its beneficial properties, we have synthesized novel copolymer-based counter electrodes by electrochemical copolymerization of three carbazole derivatives with PEDOT. The results are PEDOT-PCz4, PEDOT-PCz6 and PEDOT-PCz8 electrodes. The characterization of the newly prepared electrodes showed superior catalytic activity compared to Pt and PEDOT electrodes. Under a simulated solar irradiation of 100 mW cm<sup>-2</sup>, the copolymer-based electrodes exhibited lower charge transfer resistance (RCT') and higher short-circuit current density (JSC) values. In particular, the PEDOT-PCz8, PEDOT-PCz6 and PEDOT-PCz4 electrodes exhibited RCT' values of 14.00 Ω, 16.71 Ω and 17.55 Ω and JSC values of 16.65 mA/cm<sup>2</sup>, 16.31 mA/cm<sup>2</sup>, and 16.24 mA/cm<sup>2</sup>, respectively. Moreover, the power conversion efficiency (PCE) of the DSCs containing these copolymer-based electrodes surpassed those with traditional Pt and PEDOT electrodes. Specifically, PCE values of 8.9%, 8.5% and 8.0% were achieved with PEDOT-PCz8, PEDOT-PCz6 and PEDOT-PCz4 electrodes, exceeding the efficiencies of 7.90% and 7.56% obtained with PEDOT and Pt electrodes, respectively. These results underline the potential of copolymer-based counter electrodes as cost-effective and efficient alternatives to improve the performance of DSCs and pave the way for advances in renewable energy technology.



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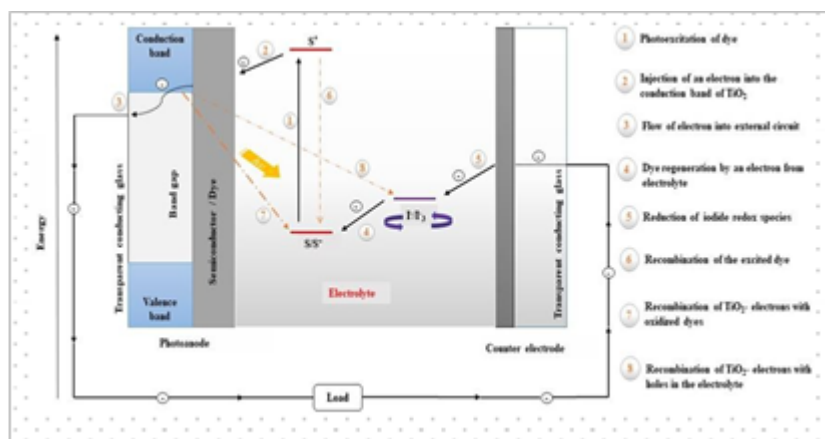


Figure 1. Basic working mechanism of the DSC.

## References

- [1] M. Grätzel. *Chemistry Letters*, 34 (2005) 8–13.  
 [2] B. C. O'Regan, M. Grätzel. *Nature*, 353 (1991) 737–740.  
 [3] J. Gong, K. Sumathy, Q. Qiao, Z. Zhou. *Renewable & Sustainable Energy Reviews*, 68 (2017) 234–246.

## Pt-free and efficient counter electrode with $\text{FeCo}_2\text{S}_4$ nanowires for dye-sensitized solar cells

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The population's growing demand for energy has made the development of alternative and renewable energy sources one of the most urgent and important problems of recent years. Dye-sensitized solar cells (DSSCs), originally introduced by Grätzel and O'Regan, represent a third generation of photovoltaic devices that offer unique advantages over silicon solar cells, including low material cost, ease of fabrication, and environmental friendliness. The development of an alternative counter electrode for dye-sensitized solar cells with a simple and straightforward method is an ad hoc research direction for solving problems used with an expensive Pt-based counter electrode.

In this work, a  $\text{FeCo}_2\text{S}_4$  counter electrode was developed directly on a fluorine-doped titania (FTO) coated glass substrate using a three-step solvothermal method: Preparation of precursor, preparation of cobalt iron oxide and sulfurization process. The  $\text{FeCo}_2\text{S}_4$ @FTO counter electrode was characterized by various spectroscopic and microscopic methods and incorporated into a DSSC device to evaluate the performance of the electrode.

The DSSC with the  $\text{FeCo}_2\text{S}_4$  counter electrode achieved an efficiency of 95 %, which is comparable to the Pt-based electrode. This shows that the  $\text{FeCo}_2\text{S}_4$  counter electrode is suitable as an alternative counter electrode as it can be produced at a lower cost and has an almost similar photovoltaic efficiency to the reference electrode.



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## Enhancing dye-sensitized solar cells efficiency and stability with Ti-MOF-based quasi-solid-state electrolytes

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Metal organic frameworks (MOFs) are three-dimensional compounds consisting of organic ligands and metal ions/clusters as secondary building blocks. MOFs are promising photoactive materials for artificial photosynthesis and photocatalysis due to their highly conjugated frameworks, tunable electronic properties, large surface area, exceptional light and thermal stability, simple and relatively inexpensive synthesis, and structural versatility. These properties make them ideal for use in photovoltaics. MOFs are successfully used as hole- or electron-conducting materials, photoanodic materials or solid-state sensitizers in dye-sensitized solar cells (DSSCs).

For the first time, quasi-solid-state electrolytes based on Ti-MOF are prepared for highly effective quasi-solid-state electrolytes (QSE) for DSSCs.  $\text{Ti}^{4+}$  and benzene-1,4-dicarboxylic acid coordinate to form Ti-MOF, which can absorb electrolyte components and largely retains the properties of a liquid electrolyte. Meanwhile, the Ti-MOF-based QSE can effectively penetrate the photoanode film to ensure good interfacial contact. Due to the increased content of  $\text{I}^-/\text{I}_3^-$  redox couples, the short-circuit current density ( $J_{sc}$ ) of the QSE cells gradually improves while the open-circuit voltage ( $V_{oc}$ ) first increases before decreasing. The change in  $V_{oc}$  can be attributed to the synergistic function of cations (such as  $\text{Ti}^{4+}$ ,  $\text{Li}^+$ , etc.) and tert-butylpyridine (TBP), which can cause a shift in the conduction band (CB) of the  $\text{TiO}_2$  photoanode and influence electron recombination. A high conversion efficiency of over 10.51% can be achieved by adjusting the QSE and is higher than the reference liquid electrolyte (LE) 9.14%. For indoor application, the QSE is 11.10% at 1000 lux, 20.24% at 3000 lux and 25.9% at 6000 lux, while the LE is 7.87%, 14.47% and 16.94%, respectively. This work will pave the way for the high-efficiency fabrication of quasi-solid-state electrolytes in DSSCs.

## Impact of Mild Mechanical Stresses on Device Physics of Slot-Die Coated Flexible Perovskite Solar Cells

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Halide perovskites represent a promising class of novel photoactive materials, with potential applications in flexible and printed photovoltaic devices [1,2]. It is crucial to consider the tolerance and stability of devices to various mechanical stresses, as these factors are vital for the effective and long-term operation of this technology. In typical flexible perovskite solar cells (FPSCs) manufactured on plastic substrates (e.g., polyethylene terephthalate (PET)) with a conductive transparent oxide layer (e.g., indium-doped tin oxide (ITO)), the ITO and perovskite layers are the ones that are prone to cracking upon moderate bending of devices. While the formation of cracks in the ITO layer can be characterised by studying the changes in device series resistance, the formation of cracks in the perovskite layer may not be as straightforward to characterise. From a microscopic perspective, the cracking of the perovskite layer can be indicative of an increase in the density of bulk and surface defects, which subsequently leads to an increase in the density of trap states within the layer [3,4]. This subsequently enhances the loss of photo-generated charge carriers via trap-assisted carrier recombination processes. Nevertheless, in order to gain a more comprehensive understanding of the impact of applied mild mechanical stresses on the properties and behaviour of devices, it is necessary to undertake a complex analysis of the charge carrier generation, recombination, and extraction processes in devices both before and after the application of mild mechanical stresses [5].



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In this connection, this study demonstrates the fabrication and characterisation of FPSCs on flexible PET/ITO substrates. The main device functional layer, comprising ETL, perovskite, and HTL, is deposited using the slot-die coating method (see Figure 1). The devices were fabricated on both ITO/PET substrates with applied mild mechanical stresses before depositing functional layers and on fresh ITO/PET substrates. It was found that applying mild mechanical stresses only to ITO/PET substrates resulted in a decrease in photovoltaic performance of up to 30%, while applying mild mechanical stresses to the complete devices resulted in a deterioration of their performance by up to 50%. Through an exhaustive quantitative analysis of the generation, recombination, and extraction processes within the solar cells, it has been determined that the reduction in photovoltaic performance resulting from mild mechanical stresses is primarily attributed to a considerable increase in recombination losses originating from bulk and surface traps. The findings of this study offer valuable insights into the impact of mild mechanical stresses on the performance and behaviour of FPSCs. The acquired knowledge can be leveraged to develop novel strategies and measures to mitigate the deterioration in flexible PSCs performance due to various mechanical stresses.

### Acknowledgment

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### References

- [1] M. S. Kiani, H. P. Parkhomenko, M. Mangrulkar, S. Aigarayeva, A. Akhanuly, E. O. Shalenov, A. Ng, A. N. Jumabekov, ACS Omega 2023, 8, 21212.
- [2] H.P. Parkhomenko, E.O. Shalenov, Z. Umatova, K.N. Dzhumagulova, A.N. Jumabekov. Energies 2022, 15, 3056.
- [3] D. Yang, R. Yang, S. Priya, S. (Frank) Liu, Angewandte Chemie International Edition 2019, 58, 4466.
- [4] S. P. Dunfield, L. Bliss, F. Zhang, J. M. Luther, K. Zhu, M. F. A. M. van Hest, M. O. Reese, J. J. Berry, Advanced Energy Materials 2020, 10, 1904054.
- [5] Z. Liu, S. Li, X. Wang, Y. Cui, Y. Qin, S. Leng, Y. Xu, K. Yao, H. Huang, Nano Energy 2019, 62, 734.

## Semiconductor film $\text{CuBi}_2\text{O}_4/\text{Pt}$ for photoelectrochemical water splitting

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Hydrogen is one of the most attractive and most efficient energy sources, which can effectively solve the problem of environmental pollution and energy shortages. The main problem holding back the large-scale use of hydrogen as a fuel source is the complexity of its production.

The modern commercial method for producing hydrogen from water by electrolysis attracts more attention due to its simplicity [1]. Moreover, such a process for producing hydrogen can be considered environmentally friendly and renewable only if the energy for electrolysis is obtained from renewable sources (water, wind, etc.) [2].

Semiconductor FTO/ $\text{CuBi}_2\text{O}_4$  films were obtained by electrochemical deposition in a potentiostatic mode from nitric acid solutions containing copper and bismuth salts and thermally oxidized in a muffle furnace.

A method has been developed for the chemical deposition of platinum nanoparticles on the surface of a semiconductor compound  $\text{CuBi}_2\text{O}_4$  by immersion coating from an aqueous solution of platinum-hydrochloric acid followed by heating in air. From 1 to 3 cycles of deposition of platinum nanoparticles were carried out, after each of which the elemental composition and photoelectrochemical parameters of the samples were recorded. The results of photoelectrochemical studies have shown that the obtained semiconductor is characterized by p-type conductivity and good photoresponse, which confirms the possibility of further use in photocatalytic systems.



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It was noted that the deposition of Pt nanoparticles promotes an increase in the electrocatalytic activity of CuBi<sub>2</sub>O<sub>4</sub> electrodes in the photoelectrochemical water splitting. The trend towards an increase in the volume of hydrogen evolved is evident: 1 cycle of applying platinum to the surface increases this indicator by 2.2 times, 2 cycles - by 5.8 times, and 3 cycles - by 16.8 times.

Using SEM and microphotographs, it was found that the deposition of Pt nanoparticles does not change the composition and morphology of the initial CuBi<sub>2</sub>O<sub>4</sub> film.

CuBi<sub>2</sub>O<sub>4</sub>/Pt electrodes are possible to be considered as a promising PEC system for use in photoelectrochemical solar cells and devices for photoelectrochemical water splitting due to High values of the quantum efficiency of the photocurrent, a significant increase in the photocatalytic activity and photoelectrochemical stability.

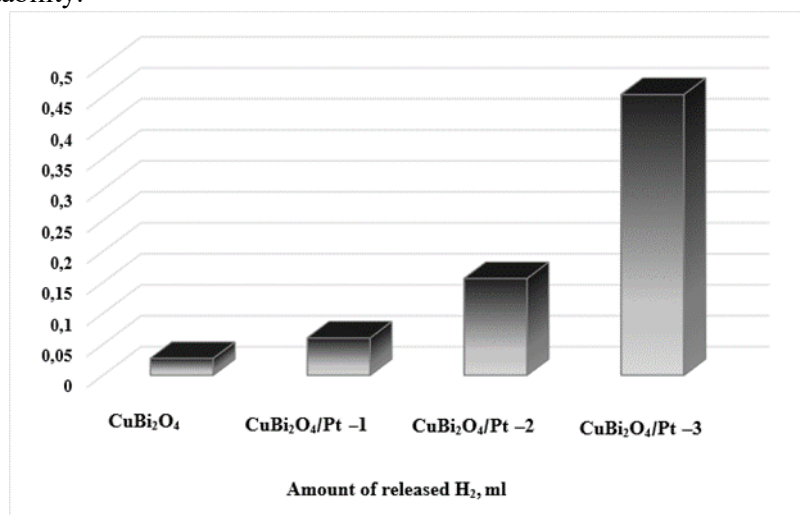


Figure 1. The amount of released hydrogen depending on the number of cycles of deposition of platinum nanoparticles on the surface of CuBi<sub>2</sub>O<sub>4</sub> electrodes

### References

- [1] C.A. Rodriguez, M.A. Modestino, D. Psaltis, C. Moser, *Energy Environ Sci.* (2014) <https://doi.org/10.1039/C4EE01453G>  
[2] K. Wenderich, G. Mul, *Chem Rev.* (2016) <https://doi.org/10.1021/acs.chemrev.6b00327>

## Study of hysteresis effects in printed flexible perovskite solar cells utilizing inorganic and organic electron transport layers

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Flexible perovskite solar cells (FPSCs) fabricated using solution-processed printing techniques have garnered significant attention due to their potential for high efficiency and scalability [1-3]. However, challenges such as cost-effective manufacturing under ambient conditions, control of ion migration in the perovskite layer, and stability under various environmental conditions remain unresolved [3-4]. This study focuses on fabricating printed FPSCs under ambient conditions using the slot-die coating technique and investigates the impact of SnO<sub>2</sub> quantum dot (QD) and (6,6)-Phenyl C61 butyric acid methyl ester (PCBM) based electron transport layers



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(ETLs) on device performance and hysteresis effects. Experimental and theoretical analyses revealed that while SnO<sub>2</sub> QD based devices exhibit superior photovoltaic properties, they also suffer from significant hysteresis compared to PCBM-based devices. The fabricated devices achieved average power conversion efficiencies (PCEs) of 9.3% and 5.2% for SnO<sub>2</sub> QD- and PCBM-based ETLs, respectively, with hysteresis indices (HI) of 0.531 and 0.156. The superior performance of SnO<sub>2</sub> QD-based devices is attributed to better optical transmittance and higher quality perovskite layer formation, as evidenced by XRD and SEM analyses. Additionally, numerical simulations indicated a lower concentration of mobile ions in the perovskite layer of PCBM-based devices. However, the higher HI in SnO<sub>2</sub> QD-based devices is due to more effective ion redistribution during forward and reverse J-V scans. These findings highlight the interplay between ETL choice and perovskite grain morphology on device performance and hysteresis, providing insights for developing high-performance, hysteresis-free printed FPSCs.

### References

- [1] Y. E. Kalay, Y.Kuru, E. Unalan Int. J Hydrogen Energy, 12 (2015) 915–920. H. Kong, W. Sun, H. Zhou, Journal of Semiconductors. 42 (2021) 101605.
- [2] H. Liu, Z. Zhang, Z. Su, et.all, Advanced Science. 9 (2022) 2105739.
- [3] H.P. Parkhomenko, Y. Yerlanuly, V. V. Brus, A.N. Jumabekov, Organic Electronics. 129 (2024) 107049.
- [4] J. Zhang, W. Zhang, H.-M. Cheng, S.R.P. Silva, Materials Today. 39 (2020) 66–88.

## Optimization of MoO<sub>x</sub>-Au-MoO<sub>x</sub> multilayer transparent electrode for monolithic Si/perovskite tandem solar cells

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Tandem solar cells are being widely studied due to their ability to overcome the efficiency limitations of conventional single-junction solar cells. Silicon/perovskite tandem solar cells represent a promising field in photovoltaic technology, leveraging the complementary properties of both materials to achieve higher power conversion efficiencies (PCE). However, despite a number of outstanding achievements and record-breaking PCEs, the scientific community faces the major challenge of scaling up and commercialization of tandem solar cells. One example of a bottleneck hindering the scalability of Si/perovskite tandem solar cell production is the reliance on indium-based transparent conductive oxides (TCO) for top electrode. Although TCO layers offer several compelling advantages (e.g. high transparency, high conductivity, ease of deposition), the shortage of indium makes large-scale production non-viable. Additionally, the elevated sheet resistance of these films poses a challenge in expanding the cell's surface area. Thus, there's a need for alternative transparent conductive films. In addition to TCO layers, various other materials and structures have been reported for transparent electrodes in perovskite top cells within tandem structures. For instance, silver nanowires, graphene, poly(3,4-ethylenedioxythiophene) (PEDOT: PSS) and dielectric-metal-dielectric (DMD) [1,2]. DMD structure exhibits substantial variability in both sheet resistance and transparency, making it a promising candidate for tandem application. This variability can be achieved through adjustments of the metal and dielectric layers thickness. This work optimizes MoO<sub>x</sub>-Au-MoO<sub>x</sub> DMD structures as the top transparent electrode for monolithic Si/Perovskite tandem solar cells. It has been demonstrated that the sheet resistance varies significantly with the thickness of the metal layer. The increase in thickness of gold layer from 6 to 10 nm leads to a decrease in sheet resistance from 55 to 9 Ohm/sq. Additionally, as the thickness of the top MoO<sub>x</sub> layer increases from 30 to 50 nm, there is a significant enhancement in transmittance within the spectrum from 300 to 1100 nm. A comparison



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of DMD structures with a MoOx top layer ranging from 30 to 50 nm reveals that a thicker film boosts the fill factor from 60.72% to 65.23% and the short-circuit current density from 12.29 to 16.65 mA/cm<sup>2</sup>, ultimately enhancing PCE. Thus, this work explores the potential of substituting TCO films with DMD structures, which offer greater variability in optical and electrical characteristics.

### References

- [1] Z. Ren, J. Zhou, Y. Zhang, A. Ng, Q. Shen, S. H. Cheung, H. Shen, K. Li, Z. Zheng, S. K. So, A. B. Djurišić and C. Surya, *Solar Energy Materials and Solar Cells*, 2018, 179, 36–44.
- [2] G. Giuliano, A. Bonasera, G. Arrabito and B. Pignataro, *Solar RRL*, 2021, 5.

## Nb<sub>2</sub>C-Based Flexible Supercapacitor for Wearable Electronics

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Wearable electronics demand robust, flexible, and efficient energy storage solutions. Niobium carbide (Nb<sub>2</sub>C) MXene emerges as a highly promising material for these applications due to its unique properties, including high electrical conductivity, excellent mechanical flexibility, and large surface area.

In order to achieve exact control over its morphology and content and optimize it for optimum electrochemical performance, Nb<sub>2</sub>C MXene is synthesized using selective etching procedures.[1] The study delves into the integration of Nb<sub>2</sub>C MXene into flexible supercapacitors, emphasizing the achieving of high specific capacitance, fast charge-discharge cycles, and long-term cycling stability.[2] Methods for improving the robustness and pliability of MXene electrodes-such as employing flexible substrates and polymer binders-are examined.

The incorporation of these supercapacitors into wearable technology highlights their ability to offer reliable and robust energy storage without sacrificing the comfort or flexibility of the device [3]. The high conductivity and flexibility of Nb<sub>2</sub>C MXene enable seamless conformability to various wearable form factors, facilitating continuous and efficient energy supply.

Challenges such as scalable production, material stability, and device integration are acknowledged, underscoring the need for further research.[1][2] Nonetheless, Nb<sub>2</sub>C MXene-based flexible supercapacitors represent a significant advancement in the field of wearable electronics, promising to enhance the functionality and user experience of future wearable devices.

### References

- [1] Wang G, Yang Z, Nie X, Wang M, Liu X. A flexible supercapacitor based on niobium carbide mxene and sodium anthraquinone-2-sulfonate composite electrode. *Micro machines*. 2023 Jul 28;14(8):1515. doi:10.3390/mi14081515
- [2] Shen B, Hao R, Huang Y, Guo Z, Zhu X. Research progress on mxene-based flexible supercapacitors: A Review. *Crystals*. 2022 Aug 5;12(8):1099. doi:10.3390/cryst12081099
- [3] Nam S, Kim J-N, Oh S, Kim J, Ahn CW, Oh I-K. Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> mxene for wearable energy devices: Supercapacitors and Triboelectric nanogenerators. *APL Materials*. 2020 Nov 1;8(11). doi:10.1063/5.0028628





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## Thin Film of Conducting Polyaniline composite electrode materials for a Supercapacitor via Interfacial Chemical-oxidative polymerization based Approach

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Free-standing thin films of conducting polyaniline composite materials were successfully synthesized via an interfacial chemical-oxidative polymerization approach. The demand for 2D film and 1D fiber structures of conducting polymers, such as polyaniline, for stretchable and flexible electrodes, circuits, and wires is increasing. However, the inherent insolubility and invisibility of polyaniline in common solvents pose challenges in producing films or fibers. To address these limitations, an interfacial oxidative method incorporating a cross-linking agent was employed to create a thin film of polyaniline.

The cross-linker, an aniline derivative with varying hydrocarbon chain lengths derived from O-aminophenol, was utilized to tailor the mechanical properties of polyaniline, resulting in thin, transparent and flexible films. Interfacial oxidative polymerization, a cost-effective and straightforward method for polyaniline production, was utilized in this study. During the process, aniline and a monomer of the cross-linking compound were dissolved in organic solvents like toluene or benzene, while an aqueous solution containing an oxidizing agent and an acidic dopant was gradually introduced to the solution of the monomers. At the interface between the two solutions, polyaniline composite film began to form. During the polymerization process at temperatures lower 0-5°C, high molecular weights may be achieved. Consequently, at 0-5°C, thicker films are produced, whereas at room temperature, thinner ones.

This approach demonstrates a promising method for the synthesis of thin films of conducting polyaniline composite electrodes for a supercapacitor with enhanced mechanical properties. An aqueous symmetric supercapacitor device can be fabricated using the synthesized thin films of polyaniline put on aluminum current collector as both cathode and anode electrodes in 1 M HCl or H<sub>2</sub>SO<sub>4</sub> electrolyte solutions (figure 1).

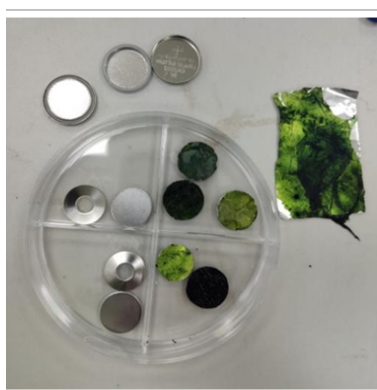


Figure 1. Polyaniline composite film.



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## Synthesis and Characterization of High Entropy Oxide Target (FeCoMnNiCr)<sub>3</sub>O<sub>4</sub> for Supercapacitors Applications

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High entropy oxides (HEOs) have emerged as promising candidates for advanced energy storage applications due to their unique combination of properties [1]. However most of the researchers were focused on the bulk materials [2,3]. In this study, we report the synthesis, characterization, and electrochemical evaluation of a novel (FeCoMnNiCr)<sub>3</sub>O<sub>4</sub> HEO deposited on nickel foam substrate via magnetron sputtering.

The synthesized HEO material is thoroughly characterized using scanning electron microscopy (SEM), for X-ray diffraction (XRD), and inductively coupled plasma (ICP) spectroscopy. SEM analysis revealed the uniform deposition of the HEO film on the nickel foam substrate, while XRD confirmed the formation of the desired (FeCoMnNiCr)<sub>3</sub>O<sub>4</sub> phase after annealing at 700 °C with high crystallinity. ICP analysis provided insights into the elemental composition and stoichiometry of the deposited HEO film.

The electrochemical performance of the (FeCoMnNiCr)<sub>3</sub>O<sub>4</sub> on nickel foam was evaluated using a three-electrode cell configuration, with a calomel electrode and platinum electrode serving as the reference and counter electrodes, respectively. The cyclic voltammetry (CV) and galvanostatic charge-discharge (GCD) measurements were conducted to assess the supercapacitive behavior of the composite material.

Preliminary electrochemical results demonstrate excellent capacitance and rate capability, indicating the potential of the (FeCoMnNiCr)<sub>3</sub>O<sub>4</sub> as a high-performance electrode material for supercapacitor applications. The multifunctional nature of the composite, coupled with its facile synthesis and promising electrochemical properties, makes it a strong contender for next-generation energy storage devices.

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### References

[1] Zhang, D., Xu, S., Li, T., Zhang, M., Qi, J., Wei, F., Meng, Q., Ren, Y., Cao, P., & Sui, Y. (2023). High-Entropy oxides prepared by dealloying method for supercapacitors. *ACS Applied Engineering Materials*, 1(2), 780–789. <https://doi.org/10.1021/acsaenm.2c00198>

[2] Yin, Y., Zhang, W., Zhang, X., Theint, M. M., Yang, J., Yang, Z., Li, J., Liang, S., & Ma, X. (2023). Low-dimensional high entropy oxide (FeCoCrMnNi)<sub>3</sub>O<sub>4</sub> for supercapacitor applications. *Dalton Transactions*, 52(26), 9005–9016. <https://doi.org/10.1039/d3dt00909b>

[3] Talluri, B., Aparna, M., Sreenivasulu, N., Bhattacharya, S., & Thomas, T. (2021). High entropy spinel metal oxide (CoCrFeMnNi)<sub>3</sub>O<sub>4</sub> nanoparticles as a high-performance supercapacitor electrode material. *Journal of Energy Storage*, 42, 103004. <https://doi.org/10.1016/j.est.2021.103004>



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## **Ion Beam Assisted Deposition of LiCoO<sub>2</sub> cathode thin films for lithium-ion batteries**

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Ion Beam Assisted Deposition (IBAD) allows precise control over the surface morphology and microstructure of the thin films [1, 2], which is critical for optimizing the performance of microbattery electrodes. This technique can be tailored the film properties to meet specific requirements of lithium-ion microbatteries, such as improving ionic conductivity and reducing interface resistance between electrode and electrolyte and creating dense, uniform, and highly adhesive films [1, 3] that can withstand the mechanical stresses during battery operation. In this work, IBAD was used to deposit thin films of lithium cobalt oxide (LiCoO<sub>2</sub>), which are commonly used as cathode materials in lithium-ion batteries, paying special attention to the effect of this method on the properties and performance of films. Some sets of deposition conditions were investigated to find optimal conditions for sputtering: substrate with and without laser treatment to modify the surface for better adhesion and the accelerator and ion beam settings including voltage and current and IBAD without heating the substrate and IBAD with heating the substrate to 300°C. Here, the important parameters are the values transmitted to the accelerators and the ion beam to obtain an oriented film, since this is the basis for the operation of the IBAD. X-ray diffraction (XRD) analysis confirmed the formation of a highly oriented LiCoO<sub>2</sub> phase with a predominant (003) orientation. Scanning electron microscopy (SEM) demonstrated that the films possess a dense and uniform surface morphology, crucial for enhanced electrochemical performance. The precise control over thin film properties provided by IBAD makes it a promising technique for the development of scalable materials for microbatteries.

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### **References**

- [1] Hirvonen J.K. (1995). Ion Beam Assisted Thin Film Deposition. In: Pauleau, Y. (eds) Materials and Processes for Surface and Interface Engineering. NATO ASI Series, vol 290. Springer, Dordrecht. [https://doi.org/10.1007/978-94-011-0077-9\\_9](https://doi.org/10.1007/978-94-011-0077-9_9)
- [2] Hughes M. What is Ion Beam Assisted Deposition (IBAD)? June 29, 2022. The Global Source Semicore. <https://www.semicore.com/news/what-is-ion-beam-assisted-deposition-ibad>
- [3] Hubler G.K., Hirvonen J.K. Ion-Beam-Assisted Deposition (1994). Book Chapter. ASM Handbook, Surface Engineering, Volume 5. DOI: <https://doi.org/10.31399/asm.hb.v05.a0001290>



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## Polymer Templated Electrospinning Technique for the Preparation of One Dimensional NCA Cathode Materials

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Lithium-ion batteries (LIBs) are important in portable electronic devices and electric vehicles due to their high capacity and long cycle life. The development of high-performance cathode materials for lithium-ion batteries is a key challenge in energy storage. Because of its greater specific capacity, reduced cost, and improved environmental compatibility, the Ni-high layered NCA cathode material is therefore one of the most competitive options [2]. Also, it has recently been commercialized by Tesla and Panasonic, proving that it is an appropriate candidate for electric vehicles. Still, understanding the synthesis of NCA and how its limits may be addressed by morphological or structural alterations, such as coating or doping, as well as the functionalization of NCA particles, is essential to expanding the use of NCA batteries [3].

This study investigates the fabrication of one-dimensional NCA (nickel cobalt aluminum) cathode materials using the polymer template electrospinning technique. The suggested approach uses electrospinning's advantages as a flexible and scalable method for creating nanofibrous materials [1]. By introducing polymer templates into the electrospinning process, we aim to enhance the structural and electrochemical properties of the resulting NCA cathode materials.

In this study, we systematically investigate how the synthesized 1D-NCA cathode material's morphology, crystallinity and electrochemical performance are affected by several factors, including concentration and processing conditions. To assess structural and electrochemical characteristics, among other characterization techniques, transmission electron microscopy (TEM), X-ray diffraction (XRD), electron scanning microscopy (SEM), and electrochemical testing are utilized. The studies' findings demonstrate uniformly fine fibers with effective pore sizes.

The results of this study are expected to demonstrate the effectiveness of polymer-templated electrospinning techniques for the fabrication of high-performance 1D-NCA cathode materials for lithium-ion batteries, which have a lot of potential applications.

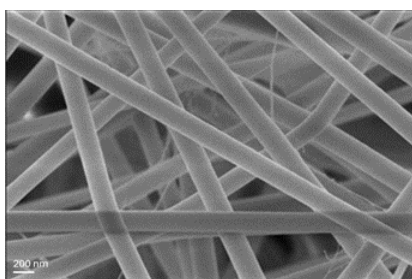


Figure 1. High-resolution SEM images of NCA nanofibers

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### References

- [1] C. Lv, Y. Peng, J. Yang, X. Duan, J. Ma, and T. Wang, *Inorganic Chemistry Frontiers*, 5, 5 (2018)
- [2] J. Wu, H. Zhu, H. Yu, Z. Wang, H. Jiang, and C. Li, *Industrial & engineering chemistry research*, 61, 7 (2022)
- [3] A. Purwanto, C. S. Yudha, U. Ubaidillah, H. Widiyandari, T. Ogi, and H. Haerudin, *Materials Research Express*, 5, 12 (2018)



## Harnessing Gas Sensors for Early Detection of Potato Spoilage in Agricultural Storage

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Potatoes are a vital crop in agriculture, serving as a significant source of nutrition worldwide, including in Kazakhstan. However, the rapid spoilage of potatoes during storage poses a major challenge, leading to economic losses and food waste. Mainly, food spoilage is primarily associated with the growth of microorganisms, which degrade carbohydrates, proteins, and other organic macromolecules in food, leading to the production of various gases and other byproducts. Therefore, monitoring gases and volatile organic compounds (VOCs) holds promise for the early detection of food spoilage, including potato spoilage.

In this study, commercial MQ-3 (SnO<sub>2</sub>-based) gas sensors were used to detect VOCs during potato spoilage development over 13 days in a storage box at room temperature. The sensor was connected to an Arduino UNO microcontroller, along with humidity and temperature sensors. The input and heater voltage supplied to each sensor was 5V DC. To eliminate noise, a preamplifier and amplifier were connected to the sensor. The system operates by changing the analog output voltage, ranging between 0V and 5V, in response to variations in input gas concentrations. Additionally, environmental sensors for humidity and temperature were used, and aerobic microorganisms, coliforms, yeast, and mold were counted daily using specific microbiological petrifilms.

This study showed that the MQ-3 sensor detected a rise in gas emissions after three days of storing potatoes in the storage box, coinciding with an increase in coliform and aerobic microorganisms. Moreover, after six days of incubation, the sensor observed a further rise in gas emissions, which continued to increase until the 13th day. This enhancement in gas emission after six days was mainly correlated with mold and yeast growth in the potatoes. Thus, these results demonstrate that the VOC gas sensor has the potential to detect potato spoilage, offering a promising alternative or complement to traditional microbiological methods and offering a valuable approach to improving storage practices and reducing waste.

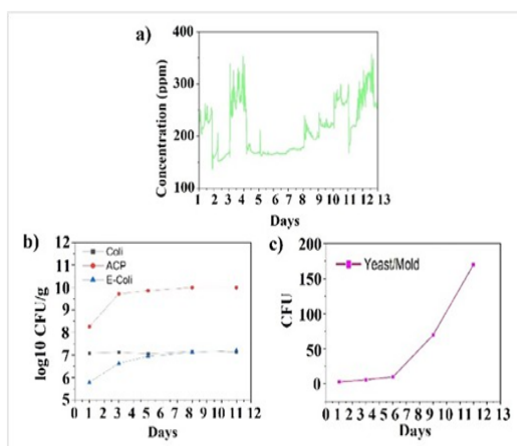


Figure 1. Monitoring potato spoilage using MQ-3 gas sensor system: a) ethanol gas concentration detected by sensor, b) *E. coli/Coliform* and aerobic bacteria and c) yeast/mold populations in potato (g) during the spoilage time. One biological replica. CFU-colony forming unit, g – gram fresh weight of potato



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