

# Development of Room Temperature Na-S and Na-Se Batteries: What Lessons Learned from Li-S Chemistry

Zeynep Erdol,<sup>1,2</sup> Ali Ata,<sup>2</sup> and Rezan Demir-Cakan<sup>3\*</sup>

<sup>1</sup> Department of Material Science and Technology, Turkish-German University, Istanbul, Turkey

<sup>2</sup> Department of Materials Science and Engineering, Gebze Technical University, Kocaeli, Turkey

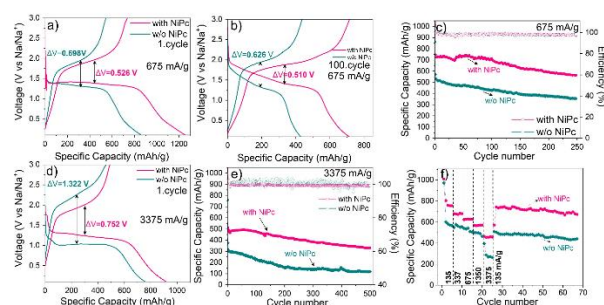
<sup>3</sup> Department of Chemical Engineering, Gebze Technical University, Kocaeli, Turkey

The uncontrolled growth of the world's population and the rapid advancement of technology are leading to ever-increasing energy and environmental problems. In order to find effective solutions to these problems and for a sustainable future, the need for rechargeable batteries with high energy density is increasing day by day. Although most of the work in the literature has focused on sulfur-based batteries, the practical implementation of sulfur-based batteries seems unlikely due to several challenges such as the severe shuttle effect of polysulfides, the low electrical conductivity of sulfur, and significant volume changes during discharge and charge cycles leading to low coulombic efficiency, deteriorated cycle stability and safety issues. On the other hand, selenium-based batteries have attracted significant research interest in recent years and have been recognized as one of the most promising candidates for next-generation energy storage systems due to their characteristics such as higher conductivity under ambient conditions, higher density and comparable volumetric capacity (3253 mAh·cm<sup>-3</sup>) compared to their sulfur-based counterparts.

When it is compared with the sulfur-based batteries, the discharge-charge behaviors differ depending on the type of electrolyte solvent, namely carbonate- or ether-based. While the working principle of Se cathode in ether-based electrolyte demonstrates a stepwise conversion from long to short-chain polyselenide formation, a single-step conversion from Se to the least Se reduction species (i.e., Na<sub>2</sub>Se or Li<sub>2</sub>Se) is observed in the carbonate-based electrolyte without generation of dissolved polyselenide intermediates [1,2]. However, Se-based batteries are still plagued with several challenges related to the end-products. For instance, regarding Na-Se batteries, the low density of Na<sub>2</sub>Se (2.62 g·cm<sup>-3</sup>) leads to drastic volume expansion during complete sodiation (~ 336 %), which deteriorates the structural integrity of the Se cathode during repeated cycles. Another issue raises from the low electronic conductivity of Na<sub>2</sub>Se, resulting in low active material utilization and sluggish redox kinetics [3].

Herein, we will discuss potential electrocatalyst (i.e. tetraiodo nickel phthalocyanine (NiPc), Mn<sub>2</sub>O<sub>3</sub>) to improve the electrochemical performance of Na-Se batteries. It will be

demonstrated that the presence of even a small amount of electrocatalyst improves the electrocatalytic conversion of Na<sub>2</sub>Se by lowering the decomposition energy barrier of Na<sub>2</sub>Se. The improved cell performances are verified by the decrease in reaction polarization, Tafel slope values, and the measured internal resistance of Na-Se cells in addition to the DFT calculations. Consequently, the Na-Se cell with the electrocatalyst exhibited outstanding rate capability, which is one of the most promising rate performance characteristics demonstrated in the literature (Figure 1).



**Figure 1.** Comparison of the galvanostatic charge/discharge profiles of cathodes with and without NiPc electrocatalyst at 675 mA·g<sup>-1</sup> for a) 1.cycle and b) 100.cycle, c) Cycling performance of cathodes with and without NiPc electrocatalyst at 675 mA·g<sup>-1</sup> current density, d) Comparison of the galvanostatic charge/discharge profiles of cathodes with and without NiPc electrocatalyst at 3375 mA·g<sup>-1</sup> for 1.cycle, e) Cycling performance of cathodes with and without NiPc electrocatalyst at 3375 mA·g<sup>-1</sup> current density, and e) Rate performance of the two cathodes at varied current densities. (1 C = 675 mA·g<sup>-1</sup>)

## References

- [1] Z. Erdol, A. Ata, R. Demir-Cakan, ChemElectroChem, 2022, 9 (15), e202200465
- [2] Z. Erdol, A. C. Yüzer, N. Kılıç, M. Ince, A. Ata, R. Demir-Cakan, Journal of Power Sources, 2023, 579, 233297
- [3] Z. Erdol, A. Ata, R. Demir-Cakan, 2023, submitted.



Rezan Demir-Cakan completed her bachelor and master degree from Yildiz Technical University at the Chemical Engineering Department. She received her Ph.D. degree at the Max Planck Institute of Colloids and Interfaces Interfaces, in Germany (2009), under the supervision of Markus Antonietti working on the synthesis, characterization and applications of hydrothermal carbon materials. Then she moved to France, the group of Jean-Marie-Tarascon, focusing on the rechargeable lithium batteries, more specifically on lithium-sulphur batteries between 2009-2012. Currently she has been working as a Professor at the Chemical Engineering Department of Gebze Technical University. Her research interests include the synthesis of nanostructured energy materials and their application in the field of rechargeable batteries.  
e-mail: demir-cakan@gtu.edu.tr tel: +90 262 605 2125