INTERFACE-INDUCED IONIC CONDUCTIVITY IN LITHIUM AND SODIUM-BASED METAL HYDRIDE NANOCOMPOSITES

Laura de Kort, Petra de Jongh, Peter Ngene

Materials Chemistry and Catalysis, Debye Institute for Nanomaterials Science, Utrecht University

e-mail: l.m.dekort@uu.nl

The development of improved energy storage devices, such as rechargeable batteries, is crucial for the transition to a sustainable energy supply. All-solid-state batteries, in which the common liquid organic electrolyte is replaced by a solid-state electrolyte, could potentially lead to safer batteries with increased energy density.^[1] Recently, metal hydrides (e.g. LiBH₄ and LiCB₁₁H₁₂) have gained attention as promising solid electrolytes due to their electrochemical and thermal stability, low density and high ionic conductivity at elevated temperatures. However, for successful incorporation of metal hydride electrolytes in all-solid-state batteries, sufficient ionic conductivity at room temperature is a prerequisite. Therefore, strategies that enhance the room temperature conductivity in complex hydrides (10-8 S cm-1 for LiBH₄) are of major importance.

In this contribution, we will show that the formation of a nanocomposite with a non-conducting mesoporous oxide is an effective approach to design highly conductive metal hydride-based solid electrolytes. Using nanocomposites based on LiBH₄, Li(BH₄)_x(NH₂)_{1-x}, NaBH₄ and NaNH₂ as examples, we will demonstrate that this versatile approach can generally enhance the lithium and sodium ionic conductivities by several orders of magnitude, e.g. from 10⁻⁸ S cm⁻¹ to 10⁻³ at 30 °C for the Li-based systems. [2-4]

The origin of this profound increase in ionic conductivity by nanocomposite formation will be discussed using the results of several characterization techniques, including solid state NMR, DRIFTS and X-ray Raman scattering (XRS). These results reveal that a conductive interfacial layer is formed at the metal hydride-metal oxide interface, both for the Li- as well as the Na-based metal hydrides. Interestingly, the nature of this interface, and correspondingly the conductivity of the nanocomposite, depends strongly on the physical and chemical properties of the metal oxide used. We will discuss the relationship between the strength of the metal hydride-oxide interface reactions and the ionic conductivity of the nanocomposites. Finally, we will highlight how the interface interaction could be tuned to rationally design highly conductive Na and Li ion conductors based on complex hydrides.

References

- [1] Janek, Jürgen, and Zeier, Wolfgang G., Nature Energy 1.9 (2016): 1-4.
- [2] de Kort, Laura M., et al., Journal of Alloys and Compounds (2021): 163474.
- [3] de Kort, Laura M., et al. *Journal of Materials Chemistry A* 8.39 (2020): 20687-20697.
- [4] Blanchard, Didier, et al., Advanced Functional Materials 25.2 (2015): 184-192.



In 2018, Laura concluded her master research in Nanomaterials Science at Utrecht University during which she studied the activity of zeolite Y extrudate catalysts for bio oil conversion. After an internship at Holst Centre/TNO, she started her PhD research at Utrecht University in the group of Petra de Jongh and Peter Ngene. In her research she works on the development of novel metal hydride-based solid electrolytes, in which she specifically studies the impact of nanocomposite formation on the metal hydride conductivity.