

# Physical Chemistry Student Seminar

## “First-Principles Study of Kinetic Properties in Lithium Amides and Alanates”

The pursuit of developing competitive alternatives to the combustion of fossil fuels for energy production has led to not one silver bullet, but a great variety of new problem specific solutions. In particular, future development of passenger vehicles hinges on novel developments in electrochemical energy storage and production. To meet the current vehicular standards the system needs to provide a range of 400km [1], and be compact and relatively light, as well as safe and affordable. Adapting current vehicles to a proton exchange membrane (PEM) fuel cell powered source is an attractive option, as their high chemical density allows them to meet current standards.

The possible methods to adopt as a standard system of on-board hydrogen storage for vehicles powered by (PEM) fuel cells, are cryogenic liquid, compressed gas, chemical hydrogen storage sorbents and solid metal hydride[2,3]. Particularly favorable are metal hydrides, which are low-cost, lightweight materials that exhibit high volumetric and gravimetric densities, possibility for on-board recharging, and high cycling. However, some of the challenges facing the development of these types of systems are poor thermodynamics or kinetics. Therefore the underlying mechanisms, and the limiting processes for the decomposition of these materials need to be understood.

From experimental work on the decomposition of hydrogen storage materials, it has been suggested that bulk diffusion of metal species is the bottleneck for hydrogen release. The two systems investigated in our work are lightweight lithium-aluminum hydrides and lithium-amides. Both systems release a considerable amount of hydrogen at moderate temperatures. The amide system is found to reversibly store hydrogen as the  $\text{LiNH}_2\text{—LiH}$  composite (7.0 wt %), and the alanate decomposes as  $\text{LiAlH}_4 \rightarrow \text{LiAlH}_6$  (5.3 wt %).

Using first-principles density functional theory we found the defects facilitating mass transport by calculating individual formation energies, highest concentrations, and activation barriers for defect mobility. The results are used to further our understanding of the fundamental mechanism of mass transport and evaluate the possibility of kinetics as the limiting process for these two hydrogen storage reactions.

[1] L. Schlapbach and A. Züttel, “Hydrogen-storage materials for mobile applications,” *Nature*, vol. 414, pp. 353–358, Jan 2001.

[2] M. Winter and R.J. Brodd, “What Are Batteries, Fuel Cells, and Supercapacitors?” *Chem. Rev.* 2004, 104, 4245–4269

[3] S. Litster, and G. McLean “PEM fuel cell electrodes”, *Journal of Power Sources* 130 (2004) 61–76

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