Complex Hydrides-Multifunctional Materials for Energy storage and Conversion

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Clean, abundant, and sustainable energy is undoubtedly one of the greatest challenges in the 21^{st} century. Fossil fuels that account for more than 80% of the world's current energy needs are limited and harmful to the environment. While renewable energy sources such as solar and hydrogen together can meet our energy need, considerable material challenges remain before they can replace fossil fuels. I will outline some of these challenges in energy storage and conversion with particular emphasis on hydrogen storage [1], Li-ion batteries [2-4], and perovskite-based solar cells [5] and discuss how complex hydrides may provide a possible solution. At the outset these three classes of materials do not appear to have anything in common. However, a closer look reveals that all these materials are ionically bonded systems composed of multi-component negative ions mimicking the chemistry of halogens. This class of negative ions known as "superhalogens" has been an active research field for some time. I will demonstrate how understanding gained from their studies in the gas phase can help in the design and synthesis of halogen-free electrolytes in metal-ion batteries as well as address some of the fundamental problems associated with the stability of organic hybrid perovskites solar cells exposed to moisture and ways in which their band gaps can be tuned for photovoltaic applications [5]. If time permits, I will also discuss issues with irreversibility [6] and safety of complex borohydrides [7] for hydrogen storage. Experimental evidence will be provided to establish the predictive capability of our theory.

- 1. P. Jena: "Materials for Hydrogen Storage: Past, Present, and Future", J. Phys. Chem. Letters 2, 206 (2011).
- 2. S. Giri, S. Behera, and P. Jena: "Superhalogens as Building Blocks of Halogen-free Electrolytes in Li-ion Batteries", *Angew. Chem. Int. Ed.* **53**, 13916 (2014).
- 3. H. Zhao, J. Zhou, and P. Jena: "Stability of B₁₂(CN)₁₂²⁻ and its implication for Li/Mg ion batteries", *Angew. Chem. Int. Ed. (VIP)* DOI 10.1002/anie.201600275
- 4. P. Jena, "Superhalogens: A Bridge between Complex Metal Hydrides and Li-ion Batteries". J. Phys. Chem. Letters 6, 1119 (2015).
- 5. H. Fang, and P. Jena, "Super-ion Inspired Colorful Hybrid Perovskite Solar Cells", *J. Mat. Chem. A* DOI 101.1039/c5ta09646d
- 6. Y. Liu, S. Giri, J. Zhou, and P. Jena: "Intermediate phases during decomposition of metal borohydrides, M(BH₄)_n (M=Na, Mg, Y)", *J. Phys. Chem. C* **118**, 28456 (2014)
- D. A. Knight, R., Zidan, R. Lascola, R. Mohtadi, C. Ling, P. K. Sivasubramaniam, J. A. Kaduk, S. -J., Hwang, D. Samanta, and P. Jena.: "Stabilization of Hydrogen rich, yet highly pyrophoric Al(BH₄)₃ via the synthesis of the hypersalt K[Al(BH₄)₄]", J. Phys. Chem. C 117, 19905 (2013)



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