Computational modelling and design of materials for post-lithium and organic metal ion batteries: practical design strategies and methodological issues

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I will give a quick overview of my research program in computational materials modeling and design and then focus on recent work on ab initio modelling and design of materials for next generation metal ion batteries, specifically active electrode materials for post-lithium and organic batteries which hold the promise of sustainability and scalability. I will present key results of comparative studies of intercalation of ions differing by ion size (e.g. Li vs Na vs K) and valence (e.g. Li vs Mg vs Al) in different phases (including amorphous) of several prospective active electrode materials including carbon, Si, Sn, TiO_2 and vanadium oxides. I will show how ab initio modelling can help develop efficient strategies to improve voltages or enable electrochemical activity for post-lithium storage. I will highlight our recent advances in computational design of organic electrodes, including MOF-like materials, vdW crystals, and polymers. I will highlight conceptual and methodology issues one has to deal with when modelling battery materials such as the use of oxidation states for rationalization of the mechanism, treatment of vdW interactions or deficiencies of functionals or construction of amorphous phases.

About the speaker

Sergei Manzhos is Assistant Professor at the Department of Mechanical Engineering, National University of Singapore. He works on computational materials modelling and design, specifically for applications in advanced electrochemical batteries, focusing on post-lithium and organic batteries, and advanced solar cells, focusing in charge transport materials for perovskite solar cells. Dr. Manzhos is also active in method development in the areas of quantum dynamics (computational vibrational spectroscopy and potential energy surfaces) and large-scale ab initio methods (Orbital-free DFT). He hold PhD in chemistry from Queen's University, Canada (2005) and prior to NUS worked as NSERC Postdoctoral Fellow at the University of Montreal, Canada (2005-2008) and Project Assistant Professor at the University of Tokyo, Japan (2008-2012).