31 May 2017, 2pm (Ingram Lecture Theatre)	Piero Canepa (Bath)	**Overcoming limitations of Li-ion batteries with Multivalent Cathode Materials**

Overcoming limitations of Li-ion batteries with Multivalent Cathode Materials

Pieremanuele Canepa,[a,b,c] Gopalakrishnan S. Gautam,[a, b, c, d] and Gerbrand Ceder[a, b, c, d]

[a]Materials Science Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, pcanepa@lbl.gov

[b]Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139

[c]Joint Center for Energy Storage Research, Argonne National Laboratory, Lemont, IL 60439, United States

[d]Department of Materials Science and Engineering, University of California Berkeley, Berkeley, CA 94720

Abstract: Multi-valent (MV) ion intercalation batteries that replace Li^+ ions with MV cations such as Mg^{2+} constitute a promising approach to meet the high energy density requirements of the next generation of electrical devices. One of the most pressing challenges in achieving high energy density MV-ion systems is to develop suitable cathode materials with a high enough voltage and diffusivity of the MV cation. To date, there have been limited examples demonstrating the feasibility of rechargeable multivalent batteries, and among them, most of the focus has been on Mg technology. From the limited experimental studies performed to date, the feasibility of a battery technology based on multivalent intercalation is not yet clear. The cathode represents a critical component of this technology; hence it is important to assess the feasibility of multivalent insertion cathodes. In this work, we will present a detailed analysis, based on first-principles DFT calculations, of multivalent ion intercalation in various promising candidates such as the spinel AB_2O_4 (A = Multivalent ions such as Mg, Zn, Ca or Al and B = Transition metal) and various layered vanadium pentoxide (V_2O_5) polymorphs under various hydration conditions [**1-6**]. The results will demonstrate that computational materials science is a powerful tool to pave the successful development and optimization of new materials for energy dense multivalent batteries. The work is entirely supported by the Joint Center for Energy Storage Research (JCESR).

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