



The Electrochemical Society – Detroit Section

Seminar Notice: Wednesday, January 16th, 2008

COMPUTATIONAL DESIGN OF ELECTRODE MATERIALS

Dr. Anton Van der Ven

Department of Materials Science and Engineering
University of Michigan, Ann Arbor, MI, USA

The last decade has seen the emergence of a field in computational materials science that allows us to predict materials properties without any experimental input. These first-principles tools, which start from the basic laws of physics, have played a pivotal role in the development and optimization of new electrode chemistries for Li-ion batteries. Electrode chemistries are now routinely screened based on predicted voltages, phase stability, and transport properties before ever being synthesized in the lab.

Without going into the technical details, I will describe how these tools have been used to design and predict properties of electrode materials for Li-ion batteries and Ni-metal hydride batteries. As examples, I will focus on Li_xCoO_2 , $\text{Ni}(\text{OH})_2$, LiFePO_2 , LiMn_2O_4 and the mixed transition metal oxides such as $\text{Li}_x(\text{Ni}_{0.5}\text{Mn}_{0.5})\text{O}_2$ as well as carbon-based electrodes. I will also highlight major challenges and opportunities in first-principles modeling of electrode materials, including exciting developments in the understanding and prediction of kinetic properties of electrodes, which play a crucial role in determining rate capabilities and cycle life-times.

Speaker bio:

Dr. Van der Ven received his PhD in Materials Science at MIT in 2000. He continued as a post-doctoral researcher at MIT until 2004, after which he joined the faculty in the Department of Materials Science and Engineering at the University of Michigan in 2005. Van der Ven's research focuses on fundamental studies of thermodynamic and kinetic properties of intercalation compounds for Li-ion batteries and alloys for structural applications.

Date: *Wednesday, January 16th, 2008*

Location: Lawrence Technological University
21000 West Ten Mile Road
Southfield, MI 48075

Building #5 (Taubman Welcome Center), 4th Floor, Room 406
Use Parking Lot A, C or D (Lots C & D are accessed off NW Highway)

Time: 5:30 pm Reception / 6:30 pm Dinner / 7:30 pm Speaker

Price: \$20 Members / \$22 Guests / \$15 Students

Payment: Cash or Check

RSVP by: Wednesday, January 9th, 2008 to Chad Kotarba
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