Other

Theory and Computation for Understanding the Li-air Battery

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Tureaud Hall 206
October 11, 2012 - 01:30 pm

Abstract:

With increasing emphasis on vehicle electrification and on distributed energy generation from renewable resources, the Li-air battery has attracted substantial research interest due to its high specific energy of 12 kWh/kg of Li whereas state-of-the-art Li-ion rechargeable batteries have theoretical specific energies around 0.16 kWh/kg of battery. Realistic estimates of the energy storage capacity that include battery components reduce this amount to ~1.7kWh/kg of battery, which is equivalent to gasoline. A serious challenge with Li-Air batteries is the sizable overpotential and sluggish rates associated with the oxygen reduction reaction by (Li-ORR) at the carbon cathode. A possible solution is to use electrocatalysts to reduce the overpotential and enhance the reaction rates, as is practiced for hydrogen fuel cells, which operate on oxygen reduction reaction by hydrogen (H-ORR). In this presentation I will go over some of the experimental findings along with simulated results where we find the trends for the intrinsic activity of Au, Ag, Pt, Pd, Ir, and Ru for the Li-ORR with respect to the adsorption of energy of oxygen.

Speaker's Bio:

Dr. Shelton is currently the Associate Director of EMSL—the Environmental Molecular Sciences Laboratory at Pacific Northwest National Laboratory. His primary responsibility is to lead integration experimental capabilities with computation including both numerical and data intensive computing. He received his Ph.D. in 1989 in theoretical condensed matter physics from the University of Cincinnati. Following his Ph.D. he was a National Academy of Sciences/National Research Council Postdoctoral fellow in the Complex Systems Theory Group at the Naval Research Laboratory. He then joined Oak Ridge National Laboratory as a staff scientist in 1992. Dr. Shelton was a group leader of the Computational Condensed Matter Physics group until 2001 and a Distinguished Senior Research Staff member of the Computational Chemical Sciences group prior to coming to EMSL in September 2010. The main body of his work is in the general area of disorder systems, alloy theory and surface science where he has worked on incorporating magnetic and chemical disorder including point defects, such as vacancies and antisites in both materials and chemistry.

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