MATERIALS CHEM SEMINAR

Date: Thursday, Feb. 14th

Time: 12:15 pm, 1315 Chemistry

Prof. Andrew Gewirth

University of Illinois

Battery Interfaces: Spectroscopic and Spectrometric Studies of Li-Ion and Li-O_2

Surface processes on battery electrodes are responsible for aspects of battery capacity, charge and discharge rate, and durability. In this talk we will discuss application of surface electrochemical techniques to Li-ion battery anodes and Li-O_2 battery cathodes. For the former, we examine how crystal face and doping level changes Li insertion energetics for the case of Si and Ge. We also examine the solid electrolyte interphase (SEI) formed on battery anodes, and particularly show that the SEI is associated with formation of a high molecular weight oligomer at the interface, the properties of which control potential-dependent strain evolution at the interface. The majority of oligomer formation occurs only after bulk deposition of Li, consistent with the radical-initiated polymerization mechanism predicted from density functional theory (DFT) calculations of cyclic solvent molecules.

We also examine Li-O_2 battery cathodes and use electrochemical, mass spectrometric, and NMR spectroscopic measurements to examine the products and activity of different solvents and catalysts for these electrodes. Regardless of the catalyst employed, the amount of O_2 measured upon charge is significantly less than that expected for complete Li_2O_2 formation and decomposition, in agreement with the rapidly fading capacity observed during battery cycling. Detailed NMR studies, including ^{6}Li and ^{13}C, confirm the presence of degradation products regardless of solvent or catalyst.