

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

First-principles modeling of Li-air battery materials MAXWELL RADIN, Mechanical Engineering Department, University of Michigan, DONALD SIEGEL, Department of Physics, University of Michigan — Of the many possible battery chemistries, the so-called “Li-air” system is noteworthy in that its theoretical capacity (~ 5 kWh/kg, including mass of oxygen) exceeds that of any electrochemical system. Perhaps more importantly, the simplified composition of its air cathode – involving only the inlet of oxygen from the atmosphere – has the potential to provide cost benefits in comparison to the Li-ion systems of today. Although the first rechargeable Li-air battery was demonstrated by Abraham and Jiang 14 years ago, its performance in many dimensions remains poor, and relatively little computational work has been done to elucidate performance-limiting phenomena. This talk will introduce the basic properties and main performance issues associated with Li-air batteries. Opportunities for first-principles modeling to assist in overcoming these obstacles will be highlighted.

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Date submitted: 09 Dec 2010

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