Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

**Ab Initio Electrochemical Capacitance Studies of Supercapacitor Materials in Aqueous and Non-Aqueous Electrolytes** CHRISTINE UMBRIGHT, KENDRA LETCHWORTH-WEAVER, T.A. ARIAS, Department of Physics, Cornell University, Ithaca, NY 14853 — Novel electrical energy storage devices are becoming increasingly necessary as technological advances demand higher energy capacity and more efficient methods of charging. *Ab initio* Joint Density-Functional Theory (JDFT) allows for the simultaneous study of electrodes, electrolytes, and their interactions in a uniform, comprehensive way. In this work, JDFT is utilized to study the energy storage capabilities of supercapacitor materials, such as graphene. The unique electronic structure of graphene results in a heightened influence of fluid capacitance on the total capacitance of the electrode. Confinement effects on capacitance are also investigated, as JDFT allows for prediction of ion structuring within the fluid. This research hopes to further the understanding of electrochemical systems for use in future energy storage solutions.

Christine Umbright
Department of Physics, Cornell University, Ithaca, NY 14853

Date submitted: 14 Nov 2014 Electronic form version 1.4