Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Ab-Initio Physics of Electrochemistry KENDRA LETCHWORTH WEAVER, TOMÁS ARIAS, Cornell University — We present a Joint Density Functional Theory (JDFT)[1,2] capturing the key electrostatic interactions between electronic systems and a fluid environment. This novel theory is relevant to the study of electrochemical systems and includes the dielectric properties of the fluid and charge screening due to the presence of ions in solution. We also demonstrate how DFT calculations can address the fundamental physical issues underlying electrochemistry, including the definition of a consistent reference potential, the treatment of charged surfaces under periodic boundary conditions, and the study of the solid-electrolyte interface as a function of the applied potential. Results for interfacial capacitances and potentials of zero charge calculated using these techniques will be compared to experimental values. Our theory allows simulation of a variety of materials, such as intermetallics and complex oxides, in contact with an ionic liquid environment. This method has a wide range of potential applications including catalysis in fuel cells, batteries, and photoelectrochemical cells.

[1]S. A. Petrosyan, A. A. Rigos, and T. A. Arias, J. Phys. Chem. B, 109, 15436-15444 (2005).
[2]J. Lischner and T. A. Arias, Phys. Rev. Lett. 101, 216401 (2008).

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Date submitted: 28 Nov 2009 Electronic form version 1.4