Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Advances in a Joint Density-Functional Theory for Electronic Systems in Contact with Liquid Water: A New Form of Density Functional for Water JOHANNES LISCHNER, TOMAS ARIAS, Cornell University
— We present a framework for studying complex electronic systems, such as biological molecules or electrochemical interfaces, that are dissolved in liquid water. The key ingredient, that renders calculations possible, is the usage of an approximate, yet accurate "classical" density-functional theory of water, while the electronic system is described by traditional Kohn-Sham theory. The electronic system (e.g. biosolute) is then coupled to the aqueous environment via molecular pseudopotentials. Here, we present a new form of "classical" density functional for water which is the first to properly account for the structure of the molecule in an exact way. We accomplish this by writing the free energy in terms of three effective potentials, one for the oxygen and one for each hydrogen atom, in which fictitious non-interacting water molecules move. In this talk, we will show that the resulting functional correctly reproduces the following properties of water: the linear and *nonlinear* dielectric response, the site-site correlation functions, the surface tension, the bulk modulus of the liquid and its variation with pressure, the density of the liquid and the vapor phases, and their coexistance.

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Date submitted: 07 Dec 2008 Electronic form version 1.4