Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Classical Density Functional Theory of Inhomogeneous Polar Molecular Liquids JOHANNES LISCHNER, T.A. ARIAS, Cornell University — We show how free energy functionals for classical assemblies of interacting rigid molecules, composed of an arbitrary number of atoms, can be constructed, such that the entropy of the noninteracting assembly, the thermodynamic properties and the microscopic order of the uniform phase and the dielectric properties in both weak and strong electrostatic fields are reproduced. We use our approach to predict density profiles of liquid hydrogen choride in a parallel plate capacitor with different wall potentials and varying external fields. We show that our theory can easily be coupled to electronic structure calculations within the Joint Density Functional approach and will comment on potential application to water.

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Date submitted: 27 Nov 2007 Electronic form version 1.4