Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

The Interplay of Short- and Long-Ranged Forces in Simulations of Confined Water using Local Molecular Field Theory JOCELYN RODGERS, JOHN WEEKS, University of Maryland, College Park — A molecular model of water confined between walls is studied using local molecular field (LMF) theory. LMF theory splits the long-ranged Coulomb $1/r$ potential between charge sites into a short-ranged core potential and a long-ranged, slowly-varying potential ideal for mean-field averaging. The core potential may be treated explicitly by simulations using the minimum image convention with a renormalized external field defined by mean field averaging of the longer-ranged potentials. Here we apply local molecular field theory to molecular dynamics simulations of molecular water confined between walls, with and without an electric field. This is a geometry where short-ranged spherical truncations of Coulomb interactions can fail spectacularly, but in tandem with the effective external field defined by LMF theory such truncations correctly predict structural and electrostatic properties of water. Further the concepts behind LMF theory elucidate the varying contributions of hydrogen-bonding and dipolar interactions in determining the structure of water at surfaces.

Jocelyn Rodgers
University of Maryland, College Park

Date submitted: 27 Nov 2007 Electronic form version 1.4