Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Molecular Dynamics Simulations of Water Evaporation CHENGYUAN WEN[1], Virginia Tech, GARY GREST[2], Sandia National Laboratories, SHENGFENG CHENG[3], Virginia Tech — The evaporation of water from the liquid/vapor interface is studied via large-scale molecular dynamics simulations for systems of more than a million atoms at 550K and 600K. The TIP4P-2005 water model whose liquid/vapor surface tension is in excellent agreement with experiments is used. Evaporative cooling at the interface is observed from temperature profiles determined from both translational and rotational kinetic energy. During evaporation, the density of water is slightly enhanced near the liquid-vapor interface. The velocity distribution of water molecules in the vapor phase during evaporation at various distances relative to the interface fit a Maxwell-Boltzmann distribution. While our results indicate an imbalance between evaporating and condensing water molecules, local thermal equilibrium is found to hold in addition to mechanical equilibrium.

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Date submitted: 13 Nov 2014 Electronic form version 1.4