Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

The role of hydrogen bonding in water-metal interactions[1]
ADRIEN POISSIER, SRIRAM GANESHAN, MARIVI FERNANDEZ-SERRA, Stony Brook University — The hydrogen bond interaction between water molecules adsorbed on a Pd-$\langle 111 \rangle$ surface, a well known nucleator of two dimensional bilayers of ice at low temperatures, is studied using density functional theory calculations. The role of the exchange and correlation potential in the characterization of both the hydrogen bond and the water-metal interaction is analyzed in detail. We conclude that the choice of this potential is critical in determining the cohesive energy of water-metal complexes. The crucial factor nonetheless is not the description of the metal screening, even if this screening represents an important ingredient for the water-metal interaction. The different characterization of the hydrogen bonds between water molecules and the *pseudo hydrogen bonds* established between the water and the surface is at the heart of the large disparity we observe in our calculations. These results put in evidence the urgent need for an accurate characterization of the hydrogen bond interaction with density functional theory.

[1]The work is supported by DOE grant DE-FG02-09ER16052

Marivi Fernandez-Serra
Stony Brook University

Date submitted: 20 Nov 2009 Electronic form version 1.4