

Abstract Submitted  
for the MAR11 Meeting of  
The American Physical Society

**First-Principles Studies of Functionalized Si(111) in Air and in Water**<sup>1</sup> YAN LI, Brookhaven National Laboratory, GIULIA GALLI, University of California, Davis — We have investigated structural, electronic and vibrational properties of hydrogen and methyl-terminated Si(111) surfaces both in air and in contact with water, by combining density functional theory and many-body perturbation theory within the GW approximations. The computed surface dipole moments for both H-Si(111) and CH<sub>3</sub>-Si(111) surfaces were found to be consistent with measured electron affinities (EAs), and can be explain by simple electronegative trends. While GW self-energy corrections greatly improve the absolute values of EAs, the EA difference of the two surfaces remains overestimated by about 0.3 eV. The variations in CH<sub>3</sub> frequencies, e.g. the umbrella mode and CH stretching mode, for the surface in air and water are also well reproduced by our calculations. The influence exerted by the adsorption of water molecules on the hydrophobic H-Si(111) and CH<sub>3</sub>-(111) surfaces, in particular, on the EAs and the surface vibrational frequencies will be discussed and compared with recent experiments.

- [1] A. Aliano, Y. Li, G. Cicero and G. Galli, J. Phys. Chem. C 114, 11898 (2010).  
[2] Y. Li and G. Galli, Phys. Rev. B 82, 045321 (2010).

<sup>1</sup>This work was funded by NSF under Grant No. CHE-0802907.

Yan Li  
Brookhaven National Laboratory

Date submitted: 16 Nov 2010

Electronic form version 1.4