

Abstract Submitted  
for the MAR11 Meeting of  
The American Physical Society

**Water-Thin-Film Adsorption on Alpha-Quartz (0001) Surface<sup>1</sup>**

YUN-WEN CHEN, YAN WANG, HAI-PING CHENG, Department of Physics and Quantum Theory Project, University of Florida — We investigated thin water films adsorbed on quartz (0001) surfaces using first-principles density functional theory calculations. Interfacial structure and energetics were studied through a layer-by-layer deposition. From monolayer to multilayer, the low energy state configurations and adsorption sites show a transition due to formation of a highly stable bilayer membranelike structure. The water adsorption energy on a quartz surface coated by this membrane is of typical hydrogen bond strength for both dry and fully hydroxylated surfaces. The interactions between the surface and the water films are short-ranged due to shielding of the bilayer.

<sup>1</sup>This work is supported by the NSF under Grant No. DMR-0804407.

Yun-Wen Chen  
Department of Physics and Quantum Theory Project, University of Florida

Date submitted: 19 Nov 2010

Electronic form version 1.4