Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Multiscale Simulation of SiO2 II: Quantum Simulations[1] YAO HE, CHAO CAO, HAI-PING CHENG, University of Florida — To investigate effects of external stress and the influence of water molecules on the energetic stability of low dimension silica systems, we have performed ab initio molecular-dynamics simulations as well as hybrid classical/quantum simulations of SiO2 chains. These silica chains are formed by edge-sharing two-rings. We present strain dependent interactions of silica-water systems at room temperature. Our investigations provide qualitative and quantitative descriptions of the reaction processes. We have also compared these ab initio results with results obtained from our multiscale simulations method, in which the quantum region is embedded in a classical region.

[1]NSF/ITR grant number: DMR-0325553

Yao He
University of Florida

Date submitted: 29 Nov 2005 Electronic form version 1.4