

## **Finding stable $\alpha$ -quartz (0001) surface structures via simulations**

Yun-Wen Chen, Chao Cao, and Hai-Ping Cheng

*Department of Physics and Quantum Theory Project,*

*University of Florida, Gainesville, FL 32611, U.S.A.*

Reconstruction of  $\alpha$ -quartz (0001) surfaces is studied using combined classical molecular dynamics and density functional theory. Five reconstruction patterns are identified, including three  $(2 \times 1)$  patterns and two  $(1 \times 1)$  patterns. The energetically most stable surface structure is found to be a  $(2 \times 1)$  reconstruction pattern, and several patterns can co-exist in a large scale surface. A combination of structures can explain the experimentally observed  $(2 \times 2)$  diffraction pattern.

Acknowledgement: this work is supported by the NSF under Grant No. DMR/ITR-0218957 and DMR-0804407.