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From clusters to bulk systems: Water-silica interactions YAO HE, CHAO CAO, YIN-XIA WAN, HAI-PING CHENG, University of Florida — We present our computational investigations on the energetics of clusters that consist of H_2O and SiO_2 using first-principles Born-Oppenheimer molecular dynamics method. Cohesive energy and hydration energy of both pure (or dry) and hydroxylated (or wet) ring-structured clusters have been investigated as functions of system size. We have found clear trends of energy as the cluster size increases. Energetics of a small silica nano-rod that contains 108 atoms is also obtained as a middle reference point for size evolution. Results from cluster and nano-rod calculations are compared with values from bulk quartz and cristobalite calculations using various theoretical treatments.

Yao He
Dept of Physics, University of Florida

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