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From cluster to bulk: Size dependent energetics of silica and silica-water interaction YAO HE, CHAO CAO, YIN-XIA WAN, HAI-PING CHENG, Department of Physics and Quantum Theory Project, University of Florida
— We present our computational studies on the energetics of clusters that consist of H2O and SiO2 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 are investigated as functions of system size. We have found clear trends in both energy values as the cluster size increases. Energetics of a small silica rod that contains 108 atoms is also obtained as a middle reference point for size evolution. The interaction of the nano-rod with water molecular has been investigated thoroughly at various sites. Results from cluster calculations are compared with one from bulk quartz and cristobalite calculations. (Acknowledgement: This work is supported by NSF/ITR grant).

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