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Water-Silica Interactions from Quantum Calculations and Non-Markovian Meta-Dynamics[1] YINGXIA WAN, HAIPING CHENG, University of Florida — The interaction of silica clusters and water molecules has been investigated using first-principles Born-Oppenheimer molecular dynamics (BOMD) method. A small silica nano-rod that contains 108 atoms is chosen to illustrate the effects of external stress. Our results show clearly that the hydration energy between the nano-rod and water increases as a function of strain, which suggests that the water is more reactive under stress. Further simulations have been performed in which the nano-rod is twisted or squashed. We have also implemented a meta-dynamics based on the ideas of the extended Lagrangian and coarse-grained Non-Markovian dynamics. Hopefully, the method can be used to explore free energy barriers of chemical reactions.

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