

Abstract Submitted
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Effects of water on the reactivity and stability of SiO₂ nanostructure.¹ YAO HE, CHAO CAO, HAI-PING CHENG, University of Florida — To investigate effects of water on the reactivity and stability of SiO₂ nanostructure, we have performed first-principles molecular dynamics simulations of SiO₂ nano-chain and nano-rod. The SiO₂ nanostructures, which have stimulated many current research endeavors, can react with water strongly under internal or external stress. In our study, water monolayer films that cover the entire system are used to study the collective motion of protons. Structure, charge separation, stress dependent bond breaking and formation, and proton conduction are discussed based on results obtained at room temperature. Finally, we extend our effort to carbon nanotubes.

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