

Abstract Submitted
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Multi-scale Simulations of SiO₂ Systems I: Classical and Hybrid Simulations¹ CHAO CAO, YAO HE, HAI-PING CHENG, University of Florida — Classical MD simulations show that bulk and nano-wire silica glass exhibit completely different stress-strain curves. A typical bulk sample breaks almost instantaneously while a nano-wire sample usually breaks “gradually.” A further simulation on nano-wire sample surrounded by water molecule shows that the stress-strain curve is not affected very much by the presence of water molecules. However, from previous quantum calculations (by Du et. al), one would believe that the water molecules do affect the fracture of silica a lot. Therefore, multi-scale simulations on a simple model SiO₂ chain are performed and compared with classical simulations on the same system to investigate mechanisms underlying the inconsistency. The multi-scale simulation is also compared with a full quantum calculation in our second talk.

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