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Ab Initio Simulations of Silica Alpha Quartz Surfaces and their Interaction with Water[1] YUN-WEN CHEN, HAI-PING CHENG, Quantum Theory Project, Department of Physics, University of Florida — Two types of dry silica alpha quartz (0001) surfaces have been investigated through density functional calculations. One is the dense surface proposed by Rignanese et al.[1] that has 3-fold flower like six-member rings on the top and the three-member rings underneath. The other one is a newfound surface that has zigzag-shape six-member rings on the top and the three-member rings underneath. It is found that the new one is energetically more stable than the dense surface. The interactions of the surfaces with water molecules have also been concerned. Both of the surfaces have the similar hydrophilic properties. We report our results from MD simulations at a temperature of 300K.

[1]. G.-M. Rignanese, Alessandro De Vita, J.-C. Charlier, Roberto Car, Phys. Rev. B **61**, 13250 (2000)

[1]NSF/DMR/ITR-0218957

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