First-pinciples study of α-quartz (0001) surface and its interaction with water layers

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α-quartz (0001) surface reconstruction is studied with combined classical molecular dynamics and density function theory methods. Five reconstruction patterns are identified to be stable under DFT calculation, including three (2×1) patterns and two (1×1) patterns. The energetically most stable surface structure is found to be a (2×1) reconstruction pattern. The experimentally observed (2×2) pattern[1] could be explained by the combined surface patterns, and the calculated energy barrier is in good agreement with the α-β phase transition temperature as measured experimentally. Ordered water layers are found to form ice-like structure adsorbed on the α-quartz (0001) surfaces. The multi-scale technique will be applied on this system to handle the ice-water transition[2].

[1] W. Steurer, A. Apfolter, M. Koch, T. Sarlat, E. Sondergard, W.E. Ernst, B. Holst, Surf. Sci. **601**, 4407 (2007).

[2] V. Ostroverkhov, G.A. Waychunas, Y.R. Shen, Chem. Phys. Lett. **386**, 144 (2004)