Silica Surface States and their Wetting Characteristics

Scientific Achievement

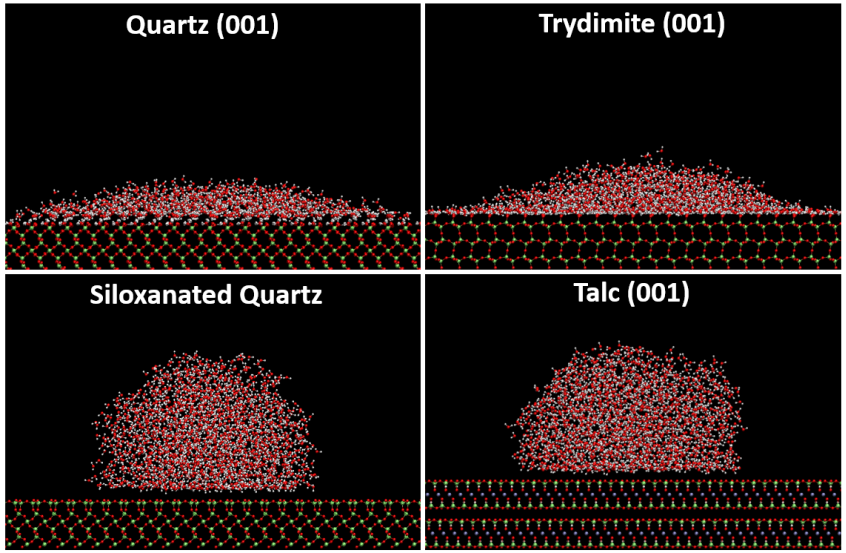
Classic molecular dynamics and ab-initio simulations have been used to determine nanodrop behavior at the nonpolar siloxane surfaces and polar silica surfaces.

Significance and Impact

Wetting of silica surfaces (talc (001), siloxanated quartz, trydimite (001) and quartz (001)) depends on surface polarity and extent of hydroxylation, of particular significance in the analysis of fluid flow in geo-architected nanoporous silica structures, the surface states of which may be defined by sintering temperature.

Research Details

- The nonpolar siloxane surfaces are characterized by a water contact angle of 80 degrees, an MD "water exclusion zone" about 3 Å, a relaxed interfacial water orientation, an inertness to hydroxylation, and a minimal hydration energy.
- The polar silica surfaces can be wetted by water and have a more ordered interfacial water structure. Silanol groups form at the polar silica surface during hydroxylation reactions, and the calculated hydration energy for such silanolated silica surfaces varies from -1.2 to -1.6 eV.



MD simulation results for water sessile drops (7nm diameter) at selected silica surfaces after 1ns. Color codes for atoms: green, N; lime, Si; blue, Mg; red, O; white, H.

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