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A quantum mechanical study of quartz (101) interfacial boundaries

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Density functional theory (DFT) calculations were performed on periodic and molecular models to explore the energetics of bonding modes at quartz-quartz interfaces – common grain contacts in sandstones. Four interface types were modeled: H_2O-mediated, silanol H-bond mediated, O-O peroxide bonds, and siloxane bonds. Each type of interface may exist in the subsurface of the Earth depending upon water activity, temperature, and pressure as the interfacial structures are stable within DFT molecular dynamics simulations up to 473 K. The results predict interfacial energies SiOSi > SiOOSi > SiOH-$6H_2O$ > 2SiOH, as expected based on similar bond strengths in other systems. The proposed SiOOSi interface is not generally accounted for in chemo-mechanical models but could be important in sandstones at depth in the Earth. Energies of fracturing SiOSi and SiOOSi interfaces are compared. The implications for inter-grain fracturing and H_2 generation are discussed.

