Connecting observations and simulations of the silica-water interface

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IR/Raman, NMR, XPS, SFG, SHG and RAXR have all been used to study the silica-water interface. Each technique provides significant information about the structure and dynamics of this nanoscale region, but none of them shows a complete picture of the chemistry of this important system. This talk will review recent experimental studies of silica-water interfaces and discuss efforts using computational chemistry to descrie the various observations made. DFT and classical simulations are applied to model various aspects of the experimental data. Implications for understanding the pH behavior of silica-water interfaces are also discussed. This work focuses on comparisons of the quartz (101)-water and amorphous silica-water models with regard to protonation of bridging O atoms that can lead to hydrolysis and dissolution.