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A Density Functional Theory-based Force Field for Modelling Silica-Water Interfaces

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The silica-water interface is well studied given its ubiquity in geochemical environments. Many force fields have been developed for both silica and water independently, however, little attention has been given to interaction parameters developed specifically for the interface. As a consequence, simulations continue to use traditional "mixing rules"to calculate silica-water Lennard-Jones interaction parameters. This study bridges this gap by developing a force field explicitly optimized for silica-water interfaces beyond mixing rules. Silica-DDEC, a recently developed force field with electrostatics matched to density functional theory (DFT) is used as the starting point. Lennard-Jones parameters are developed by benchmarking against DFT-derived interaction energies. The results reveal that traditional mixing rules overestimate water binding energies while the new parameters correct this error for β-cristobalite and amorphous silica surfaces. The parameters are also transferrable to other silica interfaces such as α-quartz. The performance of the new parameters is further investigated for its effect on the structural and dynamic properties of water in silica slit pores. The improved parameters lead to faster dynamics due to the elimination of the overbinding effect. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

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References

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