Computer simulations of quartz (101)-water interface over a range of pH values

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The original force field for clay materials (ClayFF) developed by Cygan el al. (J. Phys. Chem. B 2004, 108, 1255) is modified to describe negative charging of the (101) quartz surface above its point of zero charge (pH ~ 2.0-4.5).The modified force field adopts the scaled NBO charges derived by the quantum mechanical calculations which are used to obtain the desired surface charge density and to determine the delocalization of the charge after deprotonation of surface silanol groups. Classical molecular dynamics simulations (CMD) of the (101) surface of α-quartz with different surface charge densities (0, -0.03, -0.06 and 0.12 $C.m^{-2}$) are performed to evaluate the influence of the negative surface charge on interfacial water and adsorption of Na+, Rb+, and Sr2+ ions. The CMD results are compared with ab initio calculations, X-ray experiment and triple-layer model. The modified force field can be easily implemented into common molecular dynamics packages and used for simulations of interactions between quartz surfaces and various (bio)molecules over a wide range of pH values.

We will also present results for interaction of quartz with organic matter, small organic molecules representing basic building blocks of larger biomolecules and functional groups of organic matter – e.g. benzoic acid, phenol, o-salicylic acid and their conjugated bases.

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