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Hydration forces between calcium carbonate surfaces under nanoconfinement conditions

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Calcium carbonate is an abundant material in the earth's crust, and is the main building block in shells and bones and other cementing materials. Hydration forces play an important role during the growth and dissolution of these minerals.

Solvation forces (hydration forces when water is the solvent), arise from the ordering of molecules confined between two surfaces at nanometer separation [1]. The ordering of the confined liquid depends on the surface properties such as hydrophobicity. Even though the origin of solvation forces is well understood, their experimental measurement is difficult [2,3]. A good understanding of solvation forces is important to explain crystal growth and dissolution initiated at the atomic scale, it is also highly relevant to understand biomineralization [2,4,5]. In this work, molecular dynamics simulations of hydration forces and the free energy of solvation of the two common calcium carbonate polymorphs, calcite and aragonite, in water is performed.

Density profiles and orientational order parameters of the confined liquid were computed. The solvation force depends strongly on the type of surface considered; the (001) surface of aragonite, with orhorombic symmetry , and the $(10\bar{1}4)$ of calcite with hexagonal symmetry, leads to very different water adsorption patterns. However, solvation forces at short separations (< 1 nm) are dominated by the presence of two water layers that adsorb strongly on the calcium carbonate surfaces. Since the solvation force is dependent on the ordering of the liquid induced by the substrate, the forces also depend on the degree of surface-to-surface epitaxy. Surfaces in registry promote a higher level of ordering, which implies a longer ranged solvation force, decaying over > 3 nm for calcite.

References

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