First-principles calculation of configurations of water molecule on the brucite surface

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In order to clarify the interaction between a mineral surface and a fluid molecule, we calculate stable configuration of the water (H2O) molecule on the mineral surface by first-principles electronic structure calculations. In this study, as the mineral model surface, the (0001) surface of brucite (Mg(OH)2) is employed. Brucite is one of prototypes of hydrous layer mineral. The (0001) surface of brucite is the same as the (111) surface of MgO terminated by hydrogen.

In this study, the first principle electronic structure calculation based on the density functional theory is executed. Troullier-Martins type norm-conserving pseudopotential is adapted for the effective core potential. Electron density is expressed by the plane wave basis set. The surface is modeled by extending the interlayer distance of the 2x2x1 supercell along the c direction.

By the total energy minimization. we find interesting configurations. One of them is that the water molecule locates as its hydrogen points to Mg ion in brucite with three equivalent hydrogen bonds. This is different from the traditional image of the water configuration on the hydrophilic surface, but it corresponds to the interlayer bonding in brucite.