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The study of adsorption of monomolecular water layer on the calcium carbonate methods of the density functional theory

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Abstract

A mechanism is investigated in this paper. geometric and energy characteristics of the process of moisture sorption on the calcite surface (110), which is one of the most widespread crystalline modifications of calcium carbonate, in particular being the main constituent of such a mineral as chalk.

Calculations of a cluster $(CaCO_3)_{20}$ with a fixed structure corresponding to the crystal structure of calcite and having a developed surface of the (110) type are calculated. The surface area (110) was 147.5 Å^2.

Sorption of 5 and 6 water molecules on a cluster $(CaCO_3)_{20}$ was studied. The geometry of the cluster was fixed, the position of the water molecules was optimized.

The following calculation methods were used: semi-empirical PM7 method for primary calculations, pure DFT methods with PBE functional for calculating system geometry, DFT with B3LYP5 hybrid functional and 6-31G (d, p) full-electron basis for calculating the geometry and energy of the system. When calculating the adsorption energy, the BSSE correction was taken into account.

The accuracy of calculating the geometry of the system for fast methods (semi-empirical PM7 and pure DFT methods with different bases) is compared with DFT/B3LYP5/6-31G(d,p).

As a result of the study, the configuration of the active centers of the calcite surface (110), involved in the adsorption of water molecules and the energy of water sorption for various configurations of interaction with the active center, was determined.

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