

Dehydroxylation of smectites from Nudged Elastic Band and Born-Oppenheimer Molecular Dynamics simulations

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Streszczenie

High-temperature treatment of smectite minerals leads to the dehydroxylation process. One of the consequences of this process is the loss of sorption ability, which is an interesting, but not fully understood, phenomenon. A combination of static and dynamic quantum-chemical methods was used to analyze structural changes associated with the dehydroxylation of smectite layers. The work aims in the determination of multi-path reaction mechanism. The Nudged Elastic Band (NEB) method allowed for the recognition of intermediate structures, transition states and activation energies in the studied reaction mechanisms. Born-Oppenheimer Molecular Dynamics (BOMD) was used to investigate the interatomic distances time-evolution of atoms involved in the dehydroxylation process at different temperatures. The simulations were carried out in the crystalline phase, for which the computational model was prepared based on the dioctahedral structure of smectites with the chemical formula: $\text{Ca}_2\text{Al}_4\text{Si}_8\text{O}_{22}(\text{OH})_2$. It was found, that the process requires a proton transfer to the oxygen atom of the hydroxyl group located in the octahedral sheet, which results in the release of water molecule from the layer. In addition, it has been shown that the process of a water molecule formation on the surface is also possible. The process occurring inside the layer is more energetically favoured than that on the surface. However, high activation energies were obtained in both cases, what proves that the dehydroxylation reaction takes place only at a relatively high temperatures. It has also been demonstrated that this process can follow several different mechanisms.

Słowa kluczowe

Smectites, Dehydroxylation, Reaction mechanism, Activation energy, NEB, BOMD

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