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Thema
Kommission I: Bodenphysik und Bodenhydrologie

Bodenphysik und Bodenmineralogie - Sensorik und neue Analysemethoden von Phasenwechselwirkungen und Systemeigenschaften in Böden

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Titel
Hydration and the true water content of swellable clay minerals

Abstract
Water affects biological, chemical and transportation processes as well as mechanical properties of soils. Thereby, clay mineral content determines the moisture balance of soils. In-situ moisture measurements depend on reliable calibration based on the true water content. Drying the soil at 105 °C is the most common procedure to determine the water content although it is known, swellable clay minerals retain hydration water up to much higher temperatures.
The amplified water uptake and retention by swellable clay minerals results from hydration of interlayer cations. Thereby, the water binding mechanisms are complex due to structural heterogeneity and are determined by layer charge density and location of substitutions. While several experimental studies deal with the maximum water uptake of selected smectites and heating conditions for full dehydration a comprehensive understanding of the relation between the structure of smectites and water uptake/release is still missing.
The Na-saturated smectite / water interface for the montmorillonite-beidellite series is investigated in the present work within the density functional theory (DFT). Layer charge is varied between 0.125 and 0.5 per formula unit [$O_{10}(OH)_2$] by substitution of Al^{3+} by Mg^{2+} in the octahedral sheet (montmorillonites) and by substitution of Si^{4+} by Al^{3+} in the tetrahedral sheets (beidellites). Starting from the water free supercells (with integer molar ratios), the number of water molecules is increased discretely. Stable hydration states (1H to 3H) do not necessarily correspond to the formation of water layers (1W to 3W) in the interlayer, which is deduced from the development of the basal spaces during hydration. With the help of ab initio thermodynamics, the energy states are related to temperature, and partial pressure of H_2O and the resulting phase diagrams revealed hydration state in dependence of relative humidity (RH) as well as necessary temperatures for full dehydration to determine the true water content. Thereby it was shown that 2:1 layer silicates with a layer charge of 0.125 are swellable but reach only the 1H state even at 100% RH, but the removal of water molecules from the interlayer requires temperatures >110 °C and partial pressures of water $<10^{0}$ Pa. In contrast water uptake of smectites with layer charge 0.375 requires RH of >11% at room temperature, but dehydration occurs at moderate heating.