140b Atomistic Simulation of Nanoporous Layered Double Hydroxide Materials and Their Properties

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An atomistic model of layered double hydroxides (LDHs), an important class of nanoporous materials, is presented. Since they have a well-defined layered structure with nanometer (0.3 ~ 3 nm) interlayer distances and contain certain important functional groups. These materials have wide applications, ranging from adsorbents for gases and liquid ions to nanoporous membranes and catalysts. They consist of two types of metallic cations that are accommodated by a close-packed configuration of OH^- and other anions in a positively-charged brucite-like layer. Water and various anions are distributed in the interlayer space for charge compensation.

We develop molecular models of these materials using energy minimization and molecular dynamics(MD) simulation.

The effect of CO_3^{2-} concentration gradient is examined by changing the number of CO_3^{2-} in the interlayer region of the LDHs. We use MD simulation to estimate the diffusivity of CO_3^{2-} for a variety of CO_3^{2-} concentration gradient for each system. The diffusivities decrease as the concentration of CO_3^{2-} in the unit cell increases.

It is difficult to evaluate of characterization of the intra-crystalline region by experimental method, because the size of the intra-crystalline region is generally very small and its state, position and direction of this region is varied. To simulate the intra-crystalline region of the LDHs, the distance between layers is expanded to 30 Å thick(meso-pore). At the beginning of MD simulation, carbon dioxide molecules are distributed in the intra-crystalline region. Then, their diffusion coefficient and potential adsorption to the surface are recorded during the simulation.

The results of this study and their implications for the use of such materials as adsorbents, catalysts and membranes are discussed.