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An atomistic model of layered double hydroxides (LDHs), an important class of nanoporous materials, is presented. 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 and other anions in a positively-charged brucite-like layer. Water and various anions are distributed in the interlayer space for charge compensation. A modified form of the consistent-valence force field, together with energy minimization and molecular dynamics (MD) simulations, is utilized for developing an atomistic model of the materials. To test the accuracy of the model, we compare the vibrational frequencies, X-ray diffraction patterns, and the basal spacing of the material, computed using the atomistic model, with our experimental data over a wide range of temperature. The Diffusivities for in the LDHs structure were computed and estimated by calculating mean square displacements. Also, the particle insertion method is used to simulate the adsorption isotherm for . The agreement between the computed and measured results ranges from very good to excellent.

To develop a more accurate model of LDH materials, we have been developing atomistic models of LDH materials in polycrystalline form, and studying atomistic modeling of diffusion and adsorption in them. In addition, the simulation for adsorption of arsenic (As) in a solution containing LDH is being studied, to solve a problem which is very important to purification of water.