Special Guest Lectures

Atomistic Simulation of Nanoporous Layered Double Hydroxide Materials and Transport and Adsorption of Gas Mixture and Fluids in Them

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Johnston Hall 338
August 01, 2008 - 01:30 pm

Abstract:
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 OH- and other anions in a positively-charged brucite-like layer. Water and various anions are distributed in the interlayer space for charge compensation. As the first step, an atomistic model for a single crystal of these materials was developed. A modified form of the consistent-valence force field, together with energy minimization and molecular dynamics (MD) simulation, 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 diffusivity for CO2 and other gases in the LDHs structure are computed and estimated by molecular dynamics simulations. The agreement between the computed and measured results ranges from very good to excellent. To develop a more accurate model of LDH materials, atomistic models of LDH materials in polycrystalline form has been developed, and studying atomistic modeling of diffusion and adsorption in them. In addition, adsorption of arsenic (As) in a solution containing LDH has been simulated, a problem which is very important to purification of water.

Speaker's Bio:
Nayong Kim achieved his BS in Mathematics from Kyungwon University in Sungnam, Korea. He studied for his masters at Syracuse University and got a degree in Computer Engineering. He got his Ph.D. in Computer Science from Indiana University. .

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