
Physics Colloquium

University of Missouri-Kansas City

Department of Physics

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Modeling of adsorption in pores with strongly heterogeneous walls: Grand Canonical Monte Carlo study.

Phenomenon of adsorption is not easy to model. At the same time, various applications of adsorption in catalysis and in the porous materials characterization require a model of the mechanism of adsorption. Existing theoretical models (Langmuir, BET, ...) have been based on relatively simple and usually not very realistic assumption. The main drawback is the lack of the lateral intermolecular interactions. Additionally, in porous materials, intricate structures of the pores make each situation very unique and impossible to include in any general theoretical model. So, it is not a surprise that the main theoretical tools to study adsorption phenomena are computer simulations.

In the talk, we will present grand canonical Monte Carlo simulations of adsorption in a model porous material with cylindrical pores. We compare an adsorption mechanism in ideal smooth wall pores with more realistic heterogeneous situation. A lattice-site type approach is proposed to model adsorption site distribution on a heterogeneous wall of the pore. It is characterized by a random distribution of adsorption sites on the surface. Each site is defined by structural and energetic amplitude. An influence of those parameters on the adsorption mechanism and the resulting form of adsorption isotherms will be discussed. Finally, we verify the lattice-site approach by comparing it with a realistic all atoms model where the pore walls are built directly from a disordered lattice of atoms.

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****Coffee at 3:10: Colloquium at 3:30 in Room 310****