**4g Molecular Simulation of Nanostructured Materials and Their Use in Storage/Separation of Hydrogen, Hydrocarbons, Aromatics, and Biomolecules**

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The work presented here is a part of my ongoing research in the area of molecular simulation of nanostructured materials [1-4]. Micro- and meso- porous materials SBA-15, CMK-5 and RMM are considered to be promising for storage/separation of gases, biomolecules materials and catalyst supports. These materials have high surface area (SBA-15: 800 m2/g, CMK-5: 2500 m2/g), uniform pore structure, easy to tune pore size (1.5-30 nm), and the surface properties are easy to modify through incorporating heteroatoms or through their use as a host for complex metal catalysts. SBA-15 consists of uniform size mesopores (> 6.5 nm) arranged parallel to each other with micropores interconnecting adjacent mesopores. CMK-5 are carbonaceous materials made using SBA-15 as a template. RMM have pore structure similar to SBA-15 except that the walls are made up of ZSM-5. My experience in molecular simulation has been multi-scale, consisting of Monte Carlo, Molecular Dynamics and ab initio methodologies specifically applied to the structure and properties of nanoporous materials, clusters and alloys. I have used both series and parallel (MPI) programming techniques on supercomputers to study physical, interfacial and reactive properties from Angstrom to nanometer scales.

On a nanometer scale, I have used Molecular Dynamics/Monte Carlo simulation tools to study SBA-15, CMK-5 and RMM. The unoptimized structure has regular arrangement of atoms in a unit cell with dummy atoms representing micelles-like structure. Before optimizing and equilibration, it is subjected a series of modifications to incorporate available characterization data such as micropore size and volume, mesopore size and arrangement of mesopores, surface hydroxyl concentration surface and bulk deformations. The simulated WAXS, SAXS as well as accessible area of the final structure were found to be close to the experimental values. The models were later used to simulate several chemical as well as biochemical engineering applications such as adsorption/separation of Hydrogen (CMK-5), light hydrocarbons and aromatics (SBA-15 and CMK-5), Lysozyme and vitamin E and tethering organometallic catalysts. It was found that the adsorption capacity of hydrogen in CMK-5 is about 10 times higher than some of the single wall carbon nanotubes (SWCN) or activated carbon fibers. The adsorption isotherm of aromatics and light hydrocarbons on SBA-15 matches closely with the experimental data reported in the literature. The RMM's have higher methane adsorption capacity as compared to SBA-15 mainly due to adsorption of methane in the pores of ZSM-5 present in the walls. I have used Monte Carlo simulations to study the tethering of organometallic catalysts inside the SBA-15 and CMK-5.

On a molecular scale, I have used ab initio methods such as Configuration Interaction (QC) and Coupled Cluster (CC) to examine energetics associated with hydrogen diffusion through palladium alloys. The work involves use of activation energy for estimating kinetic rate constant which will be used for studying the Monte Carlo simulation of hydrogen diffusion in Pd-alloys.

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