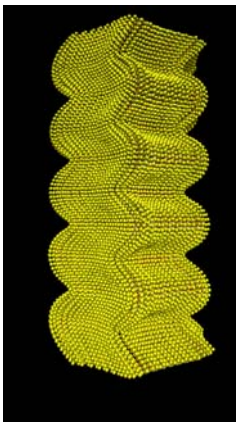
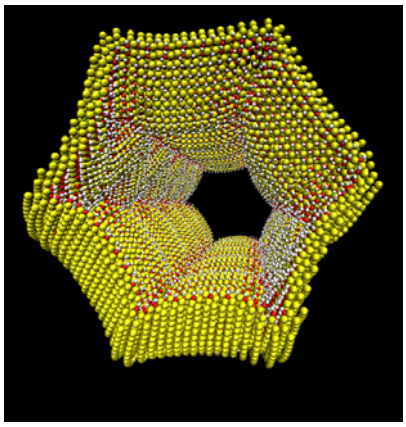
Proton Diffusion through Porous materials, Molecular Simulation Approach

Bharat Kolan[†], Scott Gold[†] and Pedro A. Derosa[†‡]
[†]Louisiana Tech University, [‡]Grambling State University

Abstract

The aim of this wok is to study the proton diffusion and diffusion times through porous materials. The proton diffusion is studied by Molecular Dynamics (MD) simulations using NAMD (not another molecular dynamics) simulation software. A tube-like structure is used and to give this the property of a pore, the outer shell of Si atoms is not allowed to move. First a pore with silicon as its outer structure and oxygen bonded to the silicon and hydrogen as its inner structure is built using the GAUSSVIEW and DLPOLY visualization tools. Next a gold substrate is built in the same manner as the pore and placed at one end of the pore to introduce the electric field in the pore. Input files for the simulation are built from the CONFIG file (contains Cartesian co-ordinates of the structures) using a C-language code developed in the group. We simulated three different structures to check the proton diffusion. 1) We ran MD simulation by placing the gold substrate (negatively charged) at one end and a proton at the other end of a straight pore, the proton is observed to diffuse in 21ps through the 30-nm-long pore and 48 ps through a 61-nm-long pore. 2) Kinks were introduced to the pore and the simulation was run, the proton did not penetrate the pore. 3) We filled the hexagonal pore with water molecules and simulated then the proton is attracted to the nearest oxygen atom of the water molecule and not moving from it. The result of this theoretical study will be presented and connection with actual experiment will be described. This work is part of a synergistic collaboration between simulation and experiment.