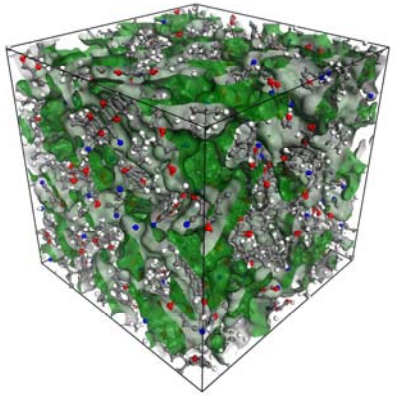
Carbon Dioxide Adsorption in Novel Amorphous Polymers: A Computational Study

Coray M. Colina (Penn State), ACS PRF# 48570-AC7

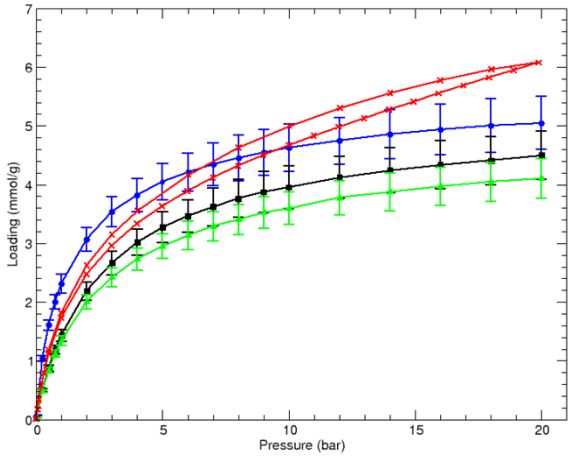


Simulated PIM-1 structure
21-step MD scheme

Polymers of Intrinsic Microporosity (PIMs) are a novel class of porous polymer with potential application in storage, separations, and purification. Development of realistic models of complex polymeric systems is a challenging task, as efficient packing at high densities requires sophisticated computational methods.

We developed a new 21-step MD compression and relaxation scheme, which provides a virtual amorphous sample comparable to experimental samples.

Adsorption isotherms via GCMC simulations facilitated the understanding of the morphological and dynamical properties of PIM-1, and PIM-1 like structures. Despite the complexity of PIM-1 the simulation results demonstrate the effectiveness of the model when compared to experimental data. The simulations predict CO_2 uptake in qualitatively agreement with experimental results. The results of this project were presented at several national and international conferences (8), as well as published (5) in recognized journals in the field.



CO_2 adsorbed on PIM-1