Carbon Dioxide Adsorption in Novel Amorphous Polymers: A Computational Study

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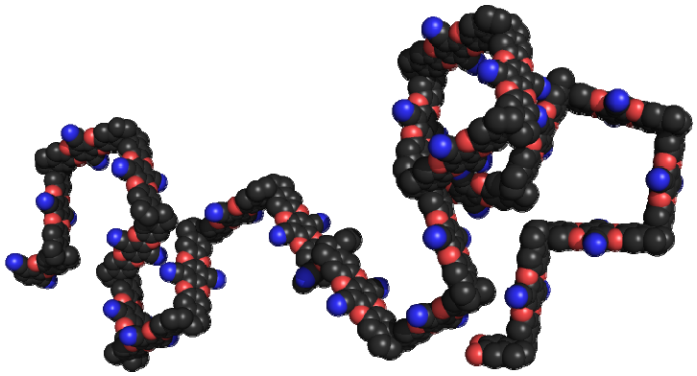
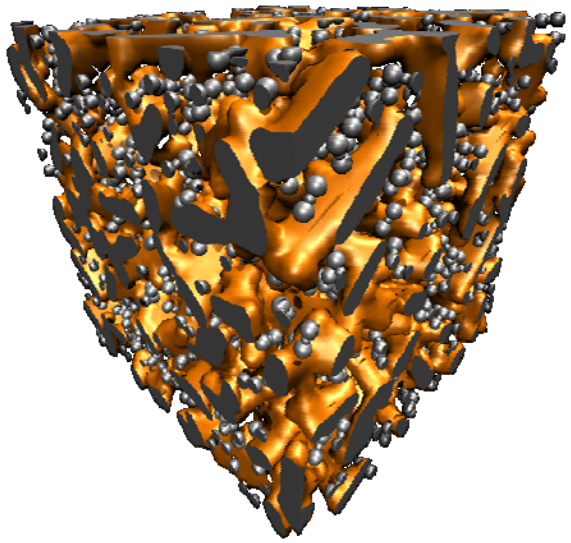
We are developing computational procedures for optimizing the structure of polymers for use in adsorption-based separations, and hence to generate a polymer-based porous material with significantly higher selectivity and capacity for carbon dioxide adsorption than materials currently available. Development of realistic models of complex polymeric systems is a challenging task, because efficient packing at high densities requires sophisticated computational methods.

As a first approximation we have generated the structure of PIM-1 under the assumption that the framework is rigid due to the sequence of connected aromatic rings. Via grand canonical Monte Carlo (GCMC) simulations, adsorption isotherms and heats of adsorption were calculated. Despite the complexity of PIM-1, the simulation results demonstrate the effectiveness of our model when compared to experimental data.



PIM-1 monomer structure



CO_2 adsorbed on PIM-1, 50 A simulation box