



~~~~ Polymer Physics Seminar ~~~~

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10:00 AM Tuesday

August 23rd, 2011

301 Steidle Bldg.

Characterizing the Structure and Porosity of Organic Molecules of Intrinsic Microporosity by Molecular Simulations and X-ray Scattering

Organic molecules of intrinsic microporosity (OMIMs) are amorphous, glassy solids that contain pores of sizes smaller than 2 nm, which are of interest for gas storage and separations applications. The philosophy behind OMIMs is similar to that of polymers of intrinsic microporosity (PIMs): rigid, awkwardly shaped molecules frustrate packing and form low density materials with intrinsically porous structures. OMIMs are designed by connecting rigid core and end-group structures to produce concave geometries that allow for the formation of micropores by hindering efficient packing. An atomistic simulation procedure has been developed for OMIMs to study the effect of structure on packing behavior by systematic variation of the core and end-group geometries. The porosity of the simulated samples was characterized by geometric surface areas and pore volumes, which were in qualitative agreement with available experimental data. In addition, simulated structure factors were compared to experimental WAXS data, agreeing well in both peak positions and relative intensities. Further analysis of the simulations aided the interpretation of scattering patterns through assignment of peaks to characteristic distances within the structures.