



## ~~~~ Polymer Physics Seminar ~~~~

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**10:00 AM Tuesday**  
**November 2<sup>nd</sup>, 2010**  
**301 Steidle Bldg.**

### **Simulated Adsorption and Characterization of Novel Nanoporous Polymers**

Polymers of intrinsic microporosity (PIMs) are a new class of porous polymer based on the simple design principle of combining monomers that are both rigid and non-planar or non-linear. These structural conditions inhibit space efficient packing and give the polymers their microporosity, but put no limitation on the chemical structure of the monomers. The potential for a wide variety of chemistries combined with the high surface areas make PIMs a novel material to address a variety of issues such as gas storage, separations, purification, and catalysis. To date, a variety of PIMs have been synthesized in both networked and non networked forms. The aim of our research is to develop a thorough understanding of the adsorption process in PIMs and aid in the rational design of novel PIMs. In this work, the effect of simple modifications along the backbone and spirocenter of the basic PIM-1 structure are investigated via simulations. By careful parameterization and calculation of charges from ab initio methods, a molecular dynamics relaxation process is used to develop highly realistic simulation samples of each PIM. Characterization of surface areas and pore size distributions highlight structural differences produced by each functional change. Combined with grand canonical Monte Carlo adsorption simulations of methane and several other gases, the adsorptive behavior of each PIM is predicted for comparison to future experimental work.