



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

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**10:00 AM Tuesday**  
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**301 Steidle Bldg.**

### **Structure of Free Volume in Polymers of Intrinsic Microporosity: X-ray Scattering with Insight from Molecular Dynamics Simulations**

Polymers of intrinsic microporosity (PIMs) are high- $T_g$ , amorphous materials combining rigid aromatic segments with sites of contortion. Solution-cast membranes exhibit a large internal surface area and high gas permeability arising from a network of pores smaller than 2 nm. Pore sizes can be measured by several experimental techniques as well as simulations, but results vary due to the assumptions necessary to interpret data as well as the sensitivity of PIMs to sample history. Pore sizes calculated from scattering data would be independent of assumptions regarding, for example, adsorbate-surface interactions. Although broad  $q$  range X-ray scattering patterns include a shoulder at the size scale corresponding to pore sizes, the development of an appropriate model is complicated by the superimposition of several amorphous halos on top of this shoulder as well as the presence of a high concentration of pores of poorly defined geometry. Comparison with scattering patterns calculated from molecular dynamics simulations, including partial structure factors, yields some insight into how these high- $q$  scattering features can be incorporated into a model capable of extracting pore sizes from scattering patterns.