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Structural Characterization of a Polymer of Intrinsic Microporosity: X-ray Scattering With Insight From Molecular Dynamics Simulations[1] AMANDA G. MCDERMOTT, GREGORY S. LARSEN, Penn State University, PETER M. BUDD, University of Manchester, CORAY M. COLINA, JAMES RUNT, Penn State University — Polymers of intrinsic microporosity (PIMs) are high-T_g, amorphous materials exhibiting high gas permeability and a large concentration of pores smaller than 2 nm, arising from a combination of rigid segments and sites of contortion. Structures generated by molecular dynamics simulations accurately reproduce characteristic scattering features from PIM-1 at high q, allowing us to investigate their origin by examining partial structure factors. Unlike scattering patterns typical of nonporous amorphous polymers, broad q range PIM scattering patterns include a shoulder at the size scale corresponding to pore sizes measured by other techniques. We discuss the development of a model for extracting pore sizes from scattering patterns.

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