Abstract Submitted
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A Scattering Model for Amorphous, Intrinsically Microporous Polymers[1] AMANDA G. MCDERMOTT, Penn State University, PETER M. BUDD, University of Manchester, NEIL B. MCKEOWN, Cardiff University, CORAY M. COLINA, JAMES RUNT, Penn State University — We discuss the development of a scattering model for glassy, porous polymers in which porosity is equivalent to free volume, deriving significant insight from molecular dynamics simulations. Polymers of intrinsic microporosity (PIMs) exhibit high gas permeability and a large concentration of pores smaller than 1 nm; their porosity arises from an unusual chain structure combining rigid segments with sites of contortion, rather than from any templating effect. Although for many porous materials, useful information such as pore sizes and specific surface areas can be extracted from scattering patterns, a successful scattering model for PIMs must account for several unusual features. Simulated structures that reproduce characteristic scattering features are used to test model assumptions, with the ultimate goal of increasing the utility of scattering for studying microporous polymeric membrane processing and physical aging.

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