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Gas Adsorption Characterization of Rigid and Amorphous Polymers GREGORY LARSEN, Penn State University, FLOR SIPERSTEIN, PETER BUDD, The University of Manchester, CORAY COLINA, Penn State University — Nanostructured materials have unusual mechanical, electrical and optical properties and are becoming increasingly important for energy storage. A variety of materials, such as zeolites, metal organic frameworks, covalent organic frameworks, activated carbons, and hypercrosslinked polymers, have recently been explored for energy storage. Polymers of Intrisic Microporosisity (PIMs) are macromolecules that form nanoporous materials (effective pore size <2 nm) that are rigid at a nanometer length scale due to the structure of the selected monomers, but can be flexible at a macroscopic scale and show swelling properties due to their polymeric nature. PIMs offer an interesting alternative to the materials mentioned above, as the functionality can be directly embedded in the material framework, allowing for intrinsic control in adsorptive properties by the PIM and flexibility in alternate adsorption applications such as CO2 sequestration. In this work, we present our recent efforts to study PIMs by MC simulations, and demonstrate the effects of box size and chain length on simulated measurements including pore size distribution and surface area.

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