



Novel Nanoporous Materials: In Silico Design

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The Pennsylvania State University

Materials Engineering Fall 2014 Seminar Series

Monday, Oct. 6th
3:30 pm Coffee
3:45 pm Seminar
ARMS 1010

The characterization of amorphous materials presents significant challenges due to their irregular and disordered nature. Porous polymers, for example, are commonly characterized experimentally by gas adsorption, from which properties such as surface areas and pore volumes are commonly reported. Molecular simulations are a powerful tool for studying the structure and properties of these amorphous polymeric materials, providing atomic detail that might be unavailable from experimental methods. This work presents a general and predictive simulation methodology for amorphous polymeric materials from only the knowledge of the chemical structure. Validation of this predictive methodology is provided, for a broad range of polymers, by characterization of the simulated structures in comparison to available experimental data, including WAXS, surface areas, BET isotherms and glass transition temperatures. Specifically adsorption of several gases in 'linear high free volume polymers' such as Polymers of Intrinsic Microporosity, as well as in cross-linked systems, such as poly(styrene-co-vinylbenzyl chloride) hypercrosslinked polymers, will be presented. This work demonstrates the potential of molecular simulations for future design of amorphous polymers. The synergism between simulations and experiments allows for improved understanding of the structure and properties of amorphous polymers and their potential for a variety of applications.

Professor Colina obtained her Ph.D. at the North Carolina State University (2004) and her B.S. (1993) and M.Sc. (1994) at Simón Bolívar University. She was a Postdoctoral Research Associate in the Department of Chemistry at the University of North Carolina at Chapel Hill. She was previously a faculty member at Simón Bolívar University and joined the Department of Materials Science and Engineering at The Pennsylvania State University as Associate Professor in January 2007. She currently serves as the vi-chair for the Computational Molecular Science and Engineering Forum, CoMSEF, AIChE, and in the programming committee for the Foundations of Molecular Modeling and Simulation Conference FOMMS 2015: Molecular Modeling and the Materials Genome, among others. She has several national and international collaborations and has presented the results of her research globally in more than 150 national and international conferences. She has published over 70 papers (including conference proceedings). Her current research interests include nanoporous materials for several industrial applications, deep eutectic solvents (ionic liquids analogs) and biomaterials.