

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

**Characterizing the Structure and Porosity of Organic Molecules
of Intrinsic Microporosity by Molecular Simulations and Experiment¹**

LAUREN J. ABBOTT, AMANDA G. MCDERMOTT, Penn State University, AN-
NALAURA DEL REGNO, University of Manchester, KADHUM J. MSAYIB, MAR-
IOLINO CARTA, RUPERT TAYLOR, NEIL B. MCKEOWN, Cardiff University,
FLOR R. SIPERSTEIN, University of Manchester, JAMES RUNT, CORAY M.
COLINA, Penn State University — Organic molecules of intrinsic microporosity
(OMIMs) are amorphous, glassy solids that contain interconnected pores of sizes
smaller than 2 nm. The philosophy behind OMIMs is similar to that of polymers of
intrinsic microporosity (PIMs); rigid, awkwardly shaped molecules frustrate pack-
ing and form low density materials with intrinsically porous structures. Atomistic
simulations were performed on OMIMs using our recently developed packing and
compression procedure to study the effect of structure on packing behavior. The
structure and porosity of the simulated samples were characterized, such as by
surface areas and structure factors, and compared to experimental results. The
presented computational procedure will further understanding of structure-property
relationships and aid in the design of novel materials with high surface areas.

¹Supported by NSF/Materials World Network/EPSC.

Lauren J. Abbott
Penn State University

Date submitted: 08 Dec 2010

Electronic form version 1.4