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Molecular models for nanoporous amorphous carbons via a novel monte carlo algorithm AMIT KUMAR, RAUL LOBO, NORMAN WAGNER, Center for Mol. & Eng. Thermodynamics, Dept. of Chem. Eng. Univ. of Delaware, Newark, DE 19711 — Nanoporous carbons (NPCs) are interesting amorphous phases of carbon that can exhibit very favorable gas permeation selectivity, which is an area of research. However, computational studies of such amorphous, nonequilibrium phases are hindered by the lack of a robust method to generate candidate molecular structures that validate against the known properties of such materials. A new monte carlo algorithm has been developed to create structural models for amorphous carbons. The simulation method mimics the experimental preparation of nanoporous carbons (NPC) by pyrolysis from polyfurfuryl alcohol as a guideline. The resulting molecular structures exhibits properties that compare favorably to those observed experimentally for real NPCs. These atomistic NPC models are approaching a realistic representation of NPCs used for gas separations and as such, are being used to study the diffusion of small gas molecules in these materials. Comparisons are made to other methods in the literature and possible improvements are discussed.

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