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Adsorption-induced Pore Expansion and Contraction in Activated Carbon MATTHEW CONNOLLY, CARLOS WEXLER, University of Missouri Physics Department — Adsorbent materials such as activated carbon and Metal-Organic Frameworks (MOFs) have received significant attention as a potential storage material for hydrogen and natural gas.1 Typically the adsorbent material is assumed to consist of rigid slit- or cylindrical-shaped pores. Recent work has revealed the importance of the mechanical response of the adsorbent in the presence of an adsorbate. Here, we first demonstrate the flexibility of pore walls in activated carbon and the effect this has on the pore structure of the bulk samples. The interaction is modeled as a competition between Van der Waals interactions between neighboring walls and a resistance to bending due to the rigidity of graphene. Minimal energy configurations were calculated analytically for a simplified potential and numerically for a more realistic potential. The pore structures are discussed in the context of pore measurements on activated carbon samples. Following recent work by Cole and Neimark, large pressures due to an adsorbed film are predicted in the narrow pores of activated carbon. The coverage-dependent nature of adsorbed-film pressure, indicating a pressure-variant pore structure, is discussed in terms of adsorption isotherms.

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