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Carbon Molecular Sieves: Reconstruction of Atomistic Structural Models with Experimental Constraints

***Kowalczyk, P.*[1]**, Terzyk, A.P.[2], Gauden, P.A.[2], Furmaniak, S.[2], Wisniewski, M.[2], Burian, A.[3], Hawelek, L.[4], Kaneko, K.[5], and Neimark, A.V.[6]

piotr.kowalczyk@curtin.edu.au

[1] *Curtin University, Perth, Australia*
[2] *Nicolaus Copernicus University, Torun, Poland*
[3] *Silesia University, Katowice, Poland*
[4] *Institute of Non-Ferrous Metals, Gliwice, Poland*
[5] *Shinshu University, Nagano, Japan*
[6] *Rutgers, New Jersey, United States*

Carbon molecular sieves (CMs) attracted recently a considerable attention owing to their remarkable separation properties. CMs are expected to pay an important role in the development of novel energy-efficient membranes for separation of gas mixtures composed of light particles (e.g., CH_4, CO_2, H_2, He, N_2, O_2, H_2S, SO_2, etc.). Although experimental manifestations of the impact of internal nanopore structure on the sieving properties of CMs have been known for a long time, an experimentally informed structural model of CMs has been recently developed. From our original reconstruction methodology, we found that carbon molecular sieve film (CMS-F) synthetized in our laboratory posses a disordered matrix enriched with bended carbon chains (sp-hybridized orbitals) and various carbon clusters as opposed to the turbostratic carbon or graphite-like microcrystals (as proposed by Franklin, Jenkins and Kawamura, and Shiraishi). The pore structure of CMS-F has defected lamellar morphology of one-dimensional periodicity with narrow (~0.4 nm) ultramicropores. The model is applied to study adsorption properties of CMS-F with respect to adsorbates of practical interest, such as N_2, H_2, CO, and C_6H_6. Special attention is paid to the phase transformations in the course of adsorption. In particular, we show theoretically and confirm experimentally that N_2 solidifies within CMS-F pores at 77 K upon adsorption of 5 mmol/g, and its further adsorption is associated with the adsorbed phase compression induced by strong surface forces.