Tailoring selective pores of carbon molecular sieve membranes towards enhanced N_2/CH_4 separation efficiency

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We report the significance of controlling the effective pore size in our newly developed hybrid CMS matrix for enhanced N_2/CH_4 selectivity based on experimental characterizations and density functional theory (DFT) calculations. A new class of CMS membranes with an excellent N_2/CH_4 selectivity is demonstrated by pyrolysis of a homogeneous, hydrogen-bonded blend of a polyimide and ladder-structured polysilsesquioxane. DFT calculations suggest that electron accumulation at SiO_x phases of hybrid CMS membranes strongly hinders the diffusion of CH_4 compared to N_2 due to a larger electron overlap, resulting in a smaller effective pore size. Moreover, elevating the pyrolysis temperatures enhanced the N_2/CH_4 solubility selectivity due to the strong repulsive interaction between newly formed ultramicropores with CH_4. As a result, the hybrid CMS membranes showed an excellent single gas and $N_2/CH_4/C_2H_6$ (20/76/4) mixed gas N_2/CH_4 selectivity (28 and 16, respectively).