Theoretical study on the adsorptive separation of ethane/ethylene in DUT-8 metal-organic frameworks

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Separation of C_2H_6/C_2H_4 mixture is still a challenging issue due to their similar physicochemical properties. Among several methods, an adsorbent-based gas separation has been considered as an alternative to replace inefficient separation process. Rigid metal-organic framework DUT-8(M) (M = Cu and Ni), which consists of paddle-wheel metal node and 2,6-naphthalene dicarboxylic acid (NDCA) linkers, is good candidate as C_2H_6-selective adsorbent. In this study, to understand the gas adsorption characteristic of the rigid DUT-8(M), we applied grand canonical Monte Carlo (GCMC) simulations and density functional theory (DFT) calculations. GCMC simulations provided well-fitted curves of C_2H_6/C_2H_4 adsorption isotherms with experimental results up to 1 bar at 273 K. The adsorption occurred predominantly near the corners of the square-shaped pore of DUT-8(M), where the gases could interact with two adjacent NDCAs. Furthermore, binding energy of C_2H_6 obtained from DFT calculation was about 4 kJ/mol higher than that of C_2H_4 because of the C-H$\cdots\pi$ interaction near the linkers. Through this study, it was proven that rigid DUT-8 is the effective adsorbent for C_2H_6/C_2H_4 separation.