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Adsorption of methane-mercaptane mixtures in carbon nanopores[1] M. GOLEBIOWSKA, L. FIRLEJ, U. Montpellier 2, B. KUCHTA, M. ROTH, U. N Iowa, C. WEXLER, U. Missouri — Natural gas is a widely-available but underutilized fuel, in particular for vehicular applications. An attractive alternative to compression is to store methane by physisorption into a suitable substrate (adsorbed natural gas, ANG). Currently there exists several materials that store methane efficiently at room temperature even at moderate pressures, e.g., nanoporous carbon[1]. For easy detection of leaks low concentrations of thiols (mercaptans) are utilized since their threshold for detection by humans is in the PPB. Whereas pure methane adsorption has been extensively studied, understanding of adsorption of methane-mercaptane mixtures is required for the development of ANG systems. Here we present results of Molecular Dynamics simulations of the adsorption of methane-methylmercaptan and methane-ethylmercaptan mixtures carbon. We discuss thiols trajectories during adsorption-desorption cycle and reversibility of their adsorption in the presence of methane. Adsorption is simulated directly in a two-phase system (gas phase remains in equilibrium with the adsorbed phase). [1] P. Pfeifer, et al., Mater. Res. Soc. Symp. Proc. 1041, R02-02 (2008).

[1]California Energy Commission: 500-08-022

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