223d Adsorption of Nitrogen and Methane in Ets-4

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Nitrogen-methane separation are acquiring importance in separation of landfill gases, or natural gas reservoires that contain a large content of nitrogen. Despite the fact that nitrogen methane separations are considered far more expensive than nitrogen-carbon dioxide separations, ETS-4 seems to be a good candidate for this type of separation. In this work we study the behavior of nitrogen, methane and their mixtures in different models of ETS-4 to understand the peculiarities of these materials that make them useful for this separation. We use grand canonical Monte Carlo simulations to calculate the adsorption isotherms, and simple models for the adsorbed gases: Lennard-Jones model for methane, and 2-center Lennard-Jones model for nitrogen. We observed that nitrogen is preferentially adsorbed in materials dehydrated at high temperature at high loadings, and that the low coverage selectivity is little affected by the sample dehydration temperature.