Electronic Supplementary Information

for

Understanding Methane/Carbon Dioxide Partitioning in Clay Nano- and Meso-Pores with Constant Reservoir Composition Molecular Dynamics Modeling

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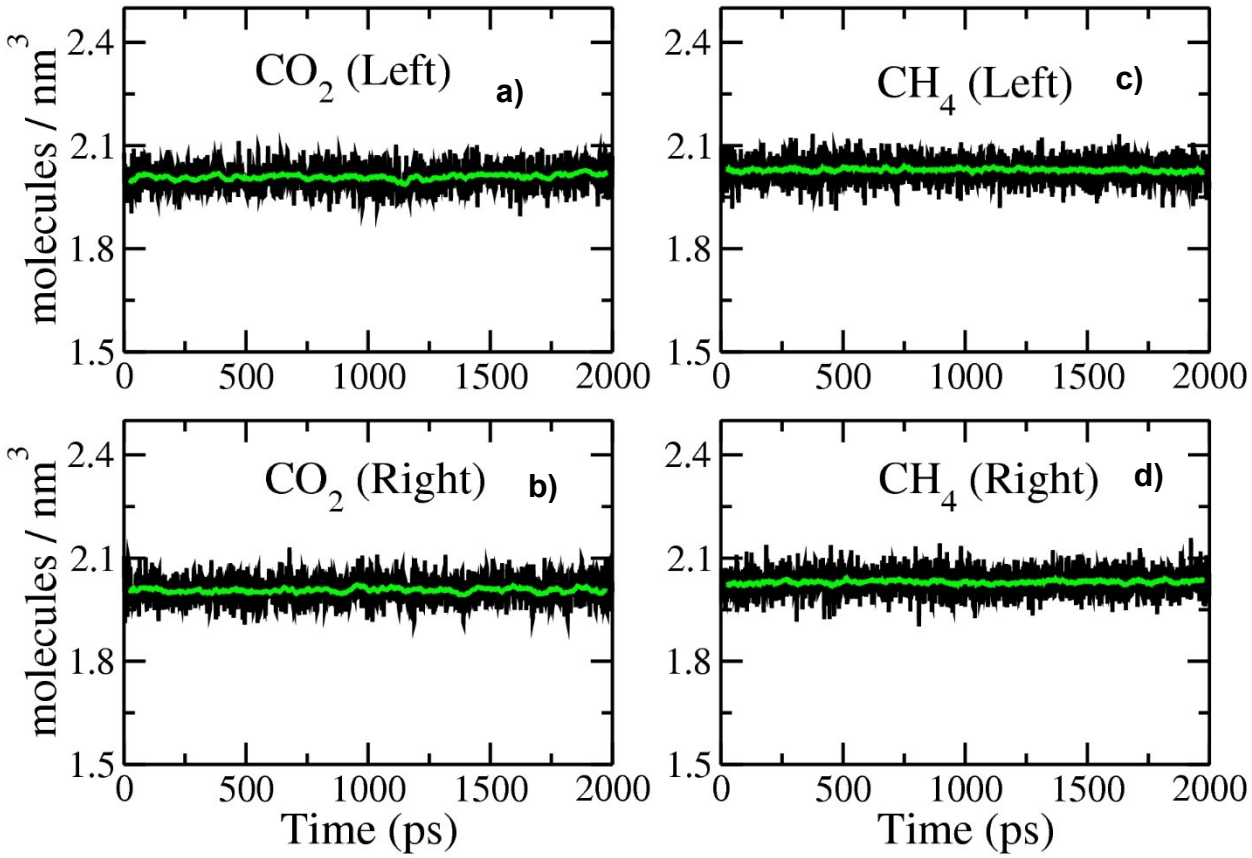

Figure S1. Concentration variation in the left and right control regions for CO_2 (a and b) and CH_4 (c and d) as a function of simulation time during the production run in the system with a pore thickness of 43.0 Å. The target densities for both molecules were set to 2 molecules/nm^3. The concentration variation in systems with other pore thicknesses is comparably small. Black lines represent the instantaneous concentration values, and the green lines the average values with block sizes of 50.