Abstract Submitted
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Dynamics Simulations of Adsorption of Natural Gas Mixtures in Graphene Nanocells DREW LEMKE, ALEXANDER ST. JOHN, Unversity of Missouri, Physics Department, MICHAEL ROTH, Northern Kentucky University, Physics Department, CARLOS WEXLER, Unversity of Missouri, Physics Department — adsorption of natural gas (NG) in graphene nanocells is of significant interest for its potential use for energy storage. In most studies NG is assumed to be comprised of pure methane, its main component. However, this neglects that 10-30 percent of NG is made-up of as ethane, propane or heavier gases which may preferentially adsorb eventually reducing the storage capacity. In this studies we seek to understand the adsorption of NG mixtures by performing Molecular Dynamics (MD) simulations. Whereas most adsorption simulations are done with the computationally more efficient Grand Canonical Monte Carlo (GCMC) methods, MD offers advantages for the study of larger molecules where internal configurations changes are important. In addition, MD permits studying time-dependent processes such as diffusion, which can help determine the reversibility of irreversibility of the adsorption of the heavier molecules [1].

Drew Lemke
Unversity of Missouri, Physics Department

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