Abstract Submitted
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Accuracy of Density Functional Theory to Predict Vapor-Liquid Equilibria[1] NEERAJ RAI, HIMANSHU GOEL, ZACHARY WINDOM, CHARLES BUTLER, AMBER JACKSON, ANNA TACONI, BREANNA ELLIS, Mississippi State University — Sorption and phase equilibria is central to numerous separation processes such as ammonia production, acid gas removal from flue gases, and petroleum refining. However, a fundamental understanding of these processes is severely lacking due to our inability to probe these systems at the molecular scale to elucidate sorption mechanism. Recent developments and implementation of novel Monte Carlo algorithms in CP2K software suite allow one to combine first principles approach to compute the system energies, and Gibbs ensemble Monte Carlo technique to model sorption and phase equilibria. Here, we use density functional theory at different levels of approximations to calculate vapor liquid equilibria of weakly interacting systems that are dominated by dispersion interactions. Our results indicate that use of dispersion correction scheme (D3) with GGA functionals perform better than rVV10 nonlocal density functional.

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