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Vapor liquid equilibria of hydrofluorocarbons via first principles Monte Carlo simulations[1] NEERAJ RAI, HIMANSHU GOEL, Mississippi State Univ — The Kohn-Sham density functional theory (DFT) is a popular approach to compute condensed phase properties. In Kohn-Sham DFT, the local or semi local density functionals do not capture van der Waals interactions accurately. An accurate description of van der Waals interactions is essential in determing thermodyanmic properties of molecules. The development of fully non local van der Waals density functional adequatey describe dispersion interactions. In this work, we present first principles Monte Carlo simulations to obtain vapor liquid coexistence curves for hydrofluorocarbons by using Becke-Lee-Yang-Parr (BLYP) functional, dispersion corrected functionals, and with rVV10 nonlocal van der Waals density functional.

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Neeraj Rai
Mississippi State Univ

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