160e Development and Application of the Trappe Force Field

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This presentation will describe the extension of the transferable potentials for phase equilibria (TraPPE) force field to ammonia, to amine, nitro, nitrile and amide functionalities, and to aromatic heterocycles. In many cases, the same parameters for a functional group are used for both united-atom and explicit-hydrogen representations of alkyl tails. Following the TraPPE philosophy, the non-bonded interaction parameters were fitted to the vapor--liquid coexistence curves for selected one-component systems. Applications to fluid phase equilibria of neat and binary systems consisting of low-molecular-weight organic molecules and to crystalline phases of pharmaceutical molecules will be presented.