A Robust Method to Calculate the Solubility Limit of Solids by Molecular Simulation

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Despite the development of sophisticated methods to study vapor-liquid equilibrium, the development of methodologies to study solid-liquid equilibrium has received much less attention due to inherent complexity involved with calculation of free energy of solids. In this talk, we will demonstrate a robust method to calculate the solubility limit of solids in different solvents. The method combines pseudo-supercritical path integration for free energy calculations of the solid and a recently developed transition matrix Monte Carlo method for phase equilibria calculations. We will validate the method by computing the solubility limits of sodium chloride in water. We will further show the applicability of the method to solutes of complex topology and crystals that exist as polymorphs.