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Regularizing binding energy distributions and thermodynamics of hydration. Application to water modeled with classical and ab initio simulations

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The high-energy tail of the distribution of solute-solvent interaction energies is poorly characterized for condensed systems, but this tail region is of principal interest in determining the excess free energy of the solute. We introduce external fields centered on the solute to modulate the short-range repulsive interaction between the solute and solvent. This regularizes the binding energy distribution and makes it easy to calculate the free energy of the solute with the field. Together with the work done to apply the field in the presence and absence of the solute, we calculate the excess chemical potential of the solute. We present the formal development of this idea and apply it to study liquid water.

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