Molecular basis of tetrahydrofuran-induced enclathration

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Clathrate hydrates are an important potential source of energy. They are also promising materials to sequester CO_2 or store H_2. In investigating the molecular mechanism of how tetrahydrofuran promotes the enclathration of methane, we are developing theory and simulation tools to probe how additives change the hydration thermodynamics of the solute of interest.

We have developed a new approach — one that sidesteps the current dominant paradigm based on alchemically changing solutes — to calculating free energies based on regularizing the binding energy of the solute with the solvent. We seek to identify and exploit the different energies with which a solute interacts with a solvent at different spatial scales. This approach leads to a transparent accounting of the hydration thermodynamics and is readily applicable to systems modeled by *ab initio* potentials or molecularly complex solutes such as organics or even macromolecules.