Molecular basis of tetrahydrofuran-induced enclathration

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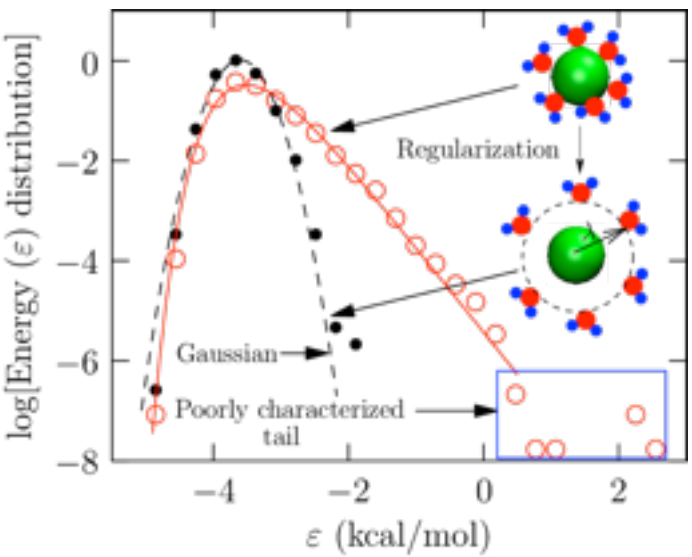
In investigating the molecular basis of tetrahydrofuran-induced enclathration of methane, we need to model how solutes partition into complex liquid mixtures. In this quest, we recognized the need for theory and simulation approaches that are sensitive to the chemistry of solute-solvent interaction.

We have developed a new approach — one that sidesteps the current dominant computational paradigm based on alchemically changing solutes — to calculate free energies based on regularizing the binding energy of the solute with the solvent. In essence, by introducing suitable external constraints, we deal with short-range, chemically specific solute-solvent interactions differently from the long-range, non-specific contributions. Our approach is readily applicable to systems modeled by *ab initio* potentials or molecularly complex organics or macromolecules.



- The grant from PRF helped in training one doctoral student (now at Intel [Portland]), and partially supported the current student.
- It has so far resulted in eight (8) peer-reviewed publications and one more is in preparation.
  - 2 of the 8 were recognized by the Journal of Chemical Physics as top monthly-downloaded articles.