Advancing Chemical Potential Calculations of Large Polymers: *Introducing the Effect of Conformational Change*

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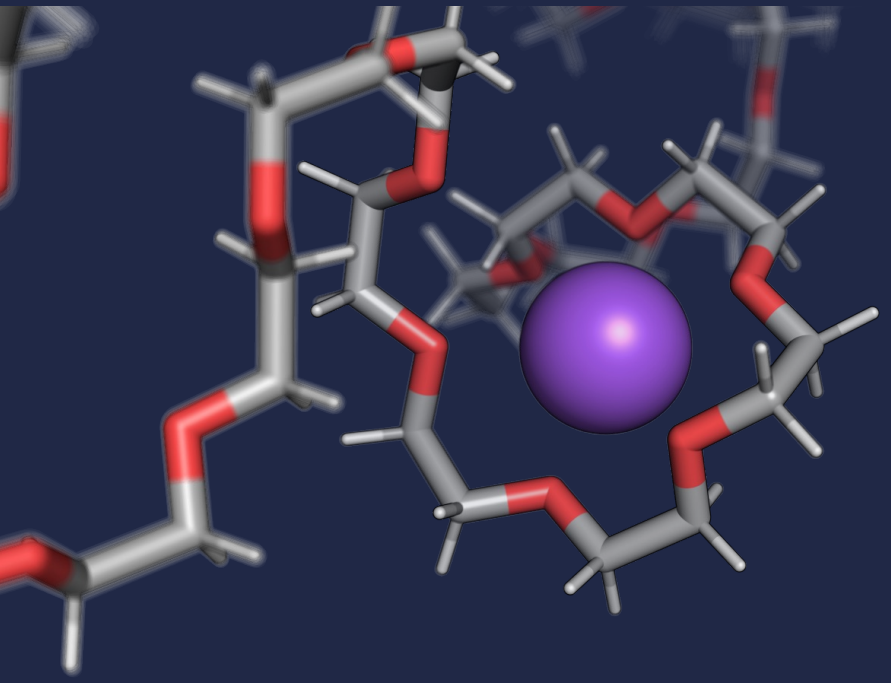
Background

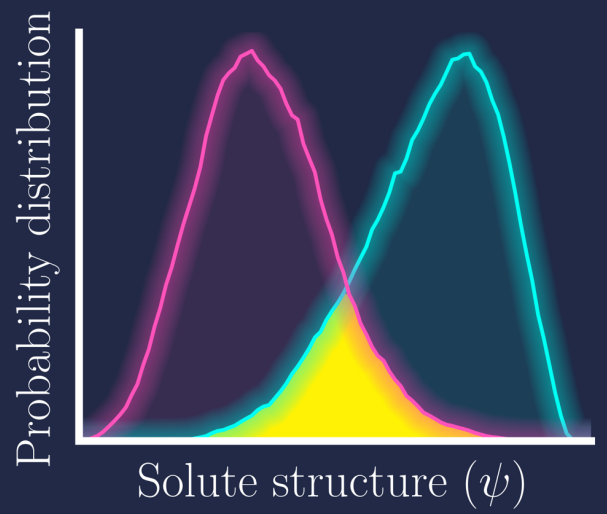
Structural changes in soft matter like polymers affect their thermodynamics.

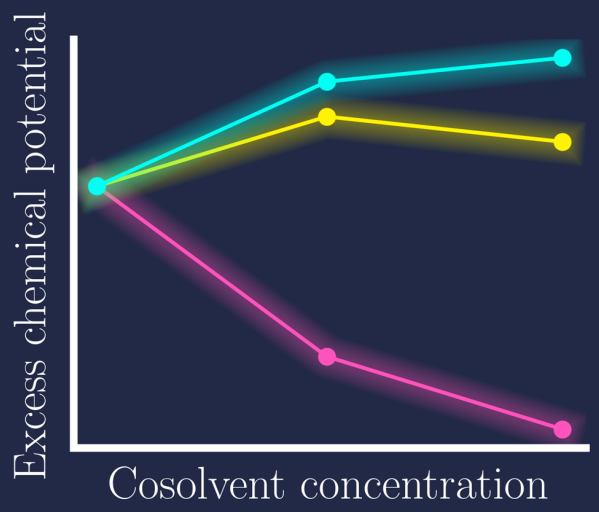


Results & Methodology

Development of new BAR-like method to account for changes in conformational ensemble due to co-solvent

$$\sum_{\psi \in A} \mathcal{F}\left(\Delta\mu^{\mathrm{solv}}(\psi) - \Delta\mu^{\mathrm{ex}}\right) = \sum_{\psi \in B} \mathcal{F}\left(-\Delta\mu^{\mathrm{solv}}(\psi) + \Delta\mu^{\mathrm{ex}}\right)$$





Conclusions

Our method correctly captures the physics of PEG solvation in water, Urea, and NaCl can capture