

## Influence of Solvent-Solvent and Solute-Solvent Interaction Properties on Solvent-Mediated Potential

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**Abstract:** A recently proposed universal calculational recipe for solvent-mediated potential is applied to calculate excess potential of mean force between two large Lennard-Jones (LJ) or hard core attractive Yukawa particles immersed in small LJ solvent bath at supercritical state. Comparison between the present prediction with a hypernetted chain approximation adopted for solute-solute correlation at infinitely dilute limit and existing simulation data shows high accuracy for the region with large separation, and qualitative reliability for the solute particle contact region. The calculational simplicity of the present recipe allows for a detailed investigation on the effect of the solute-solvent and solvent-solvent interaction details on the excess potential of mean force. The resultant conclusion is that gathering of solvent particles near a solute particle leads to repulsive excess PMF, while depletion of solvent particles away from the solute particle leads to attractive excess PMF, and minor change of the solvent-solvent interaction range has large influence on the excess PMF.

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