Is it possible to predict excess properties of mixed solvents by *ab initio* molecular simulation?: Effective fragment potential version 2 – Molecular dynamics (EFP2-MD) Simulation study

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Effective fragment potential version 2 - molecular dynamics (EFP2-MD) simulations, where the EFP2 is a polarizable force field based on ab initio electronic structure calculations were applied to water-methanol binary mixture. Comparing EFP2s defined with (aug-)cc-pVXZ (X = D,T) basis sets, it was found that large sets are necessary to generate sufficiently accurate EFP2 for predicting mixture properties. It was shown that EFP2-MD could predict the excess molar volume. Since the computational cost of EFP2-MD are far less than ab initio MD, the results presented herein demonstrate that EFP2-MD is promising for predicting physicochemical properties of novel mixed solvents.

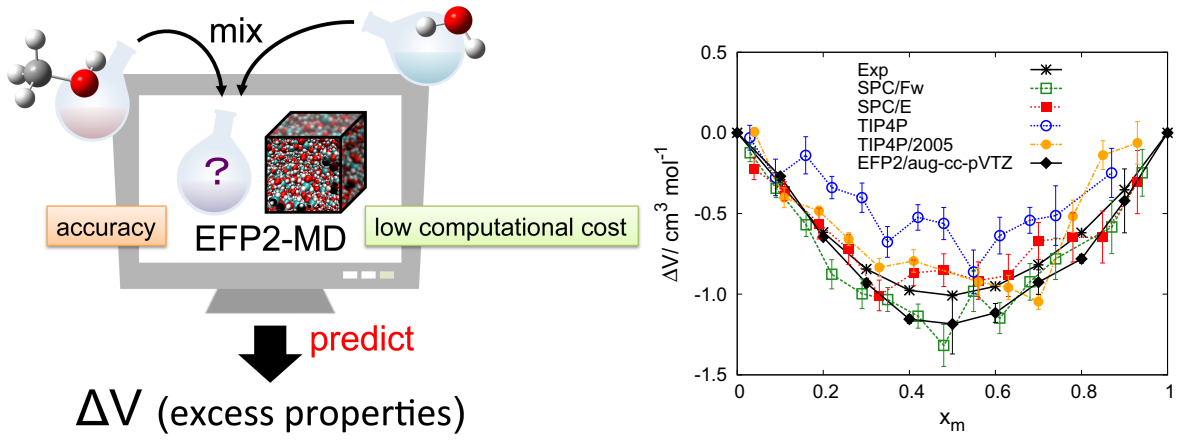

Figure 1: Excess molar volume (ΔV) of a water-methanol mixture at ambient conditions (1 atm, 300 K) simulated by EFP2/aug-cc-pVTZ-MD. For references, experimental and classical MD simulation results are also shown.

References

1. N. Kuroki and H. Mori, *Chem. Phys. Lett.* **694** (2018) 82–85. (selected as Frontiers Article)