Contribution ID: **19** Type: **Oral Presentation**

On the calculation of solvation free energy from Kirkwood-Buff integrals: A large scale molecular dynamics study

Friday, 13 July 2012 11:00 (20 minutes)

Abstract content
   (Max 300 words)

Solvation of (bio)molecules in water is severely affected by the presence of cosolvent within the hydration shell of the solute structure. Furthermore, since solute molecules can range from small molecules, such as methane, to a large protein structure, it is imperative to understand the detailed structure-function relationship on the microscopic level. In this context, Kirkwood-Buff (KB) theory, which connects the microscopic pair-wise molecular distributions to global thermodynamic properties, provides a widely accepted framework. In this talk, we present a molecular dynamics simulation approach to calculate the solvation free energies within the framework of KB theory of solutions. As initial test cases, we study the solvation of methane, ethanol, and propanol in aqueous methanol mixtures. Our results are in good agreement with the existing experimental data. The approach presented here can also be used to study conformational transitions of large (bio)macromolecules.

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 consider for a student
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Yes

Level for award
 (Hons, MSc,
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Main supervisor (name and email)
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Session Classification: Biophysics

Track Classification: Track A - Division for Condensed Matter Physics and Materials