Aqueous Solvation in Extreme Conditions: Accurate Calculations when Accurate Measurements are not Possible

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Frontiers in Chemical Physics and Analysis Seminar Series

Presented by…

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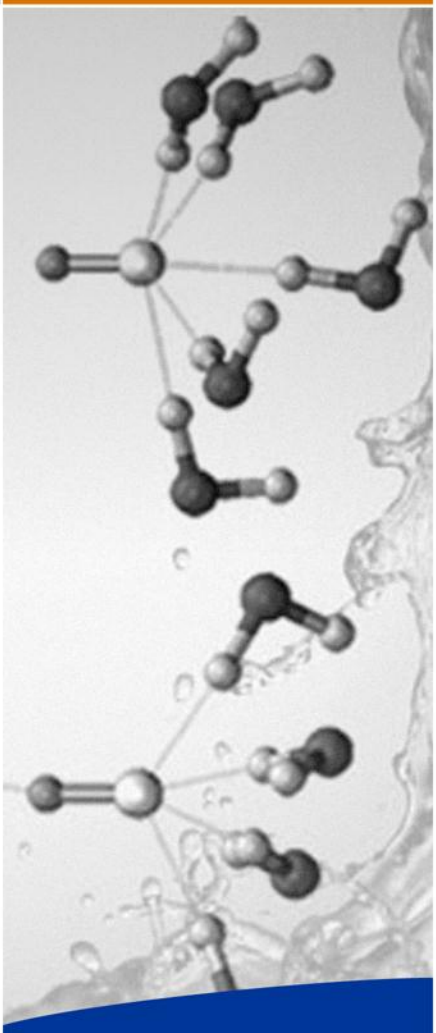
Abstract

High temperature aqueous solutions are central to many natural and industrial processes but their properties can only be measured accurately over a limited range of temperature and density. I will describe a computational approach that allows simulations of thermodynamic properties of such systems from first principles. This approach is a QM/MM method that combines configurational averaging from molecular dynamics or Monte Carlo simulations with accurate quantum chemistry calculations of energies. The method was initially developed for understanding solvation in high temperature water, and it is especially efficient in such systems. Applications to supercritical water and solvation of sodium chloride at high temperatures will be described, followed by more recent work on low-temperature aqueous aerosols. Several comparisons to experiment as well as internal validation methods confirm the reliability of the approach. In conditions where accurate experimental measurements are not possible, this computational method provides a new source of reliable data.



Date: May 17

Location: EMSL Auditorium

Time: 10:00 am

More info?

See http://www.pnl.gov/cmsd/seminars/

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