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

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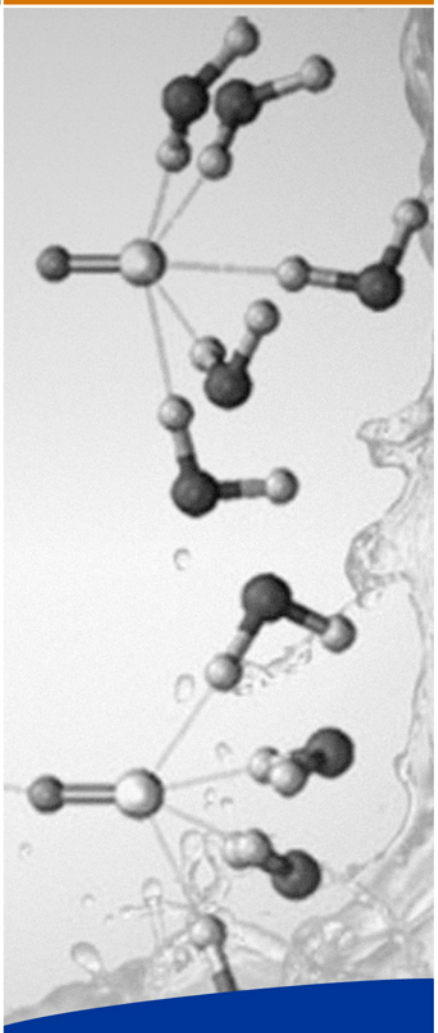

Presented by…

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Abstract

Direct dynamics have made the application of classical chemical dynamics simulations possible for a broad range of problems. However, since classical dynamics is approximate it is important to understand when the use of classical dynamics is appropriate. In this talk the following will be addressed: (1) the methodology of direct dynamics simulations; (2) accuracy of classical dynamics simulations, with emphasis on unimolecular and intramolecular dynamics; (3) post-transition state dynamics; and (4) gas-phase SN2 reaction dynamics. The VENUS/NWChem software package is used for the simulations and access to high-performance computing is critical for the research.

More info?

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

http://www.depts.ttu.edu/chemistry/Faculty/hase/

Date: November 6

Location: BSF Crick

Time: 10:00 am