

Joint CQSE and CASTS Seminar

Weekly Seminar
May 23, 2014 (Friday)

TIME May 23, 14:30 ~ 15:30
TITLE Meeting Industrial Challenges for Fluid Property Prediction via First Principle Calculations
SPEAKER Prof. Shiang-Tai Lin
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Abstract

The knowledge of thermodynamic properties of a fluid is critical for the design, development, and optimization of relevant chemical processes. However, the collection of such data via experimental approaches can be very time-consuming or even impractical in some areas, such as drug discovery where properties of thousands to millions of chemicals are investigated. Recent advances in the quantum physical and quantum chemical theories open up possibilities to obtain these important properties without resorting to any experimental measurement. However, there are challenges remain such as the need for overwhelming computational resources for industrial problems and the insufficient chemical accuracy for phase equilibrium predictions. In this talk, we present approximate methods for fluid property predictions that utilize results from quantum chemical solvation calculations. The method we have developed is general and can be used to determine all aspects of properties of a chemical or a mixture of chemicals under almost any conditions. More importantly the property predictions can be made within seconds on a modern personal computer even for very complex systems. These appealing features allow for the screen of a large volume of molecular candidates of diversified chemical structures within a reasonable time, making it a particle tool for material and process developments.

