

# Joint CQSE and CASTS Seminar

Weekly Seminar  
Dec. 25, 2015 (Friday)

TIME Dec. 25, 2015, 14:30 ~ 15:30  
TITLE Estimate Phase Behaviors of Engineering Fluids from  
First-Principles Calculations  
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## Abstract

In the field of chemical engineering, thermophysical properties of pure fluids and phase behaviors of mixtures are crucial for the design and optimization of purification processes for two reasons. The first reason is that the major operating cost in the chemical industries is the separations and purifications processes, especially in manufacturing fine chemicals, speciality chemicals, and pharmaceuticals. The other one is that these separation and purification processes are largely designed on the basis of phase equilibrium. For examples, the distillation processes and crystallization processes are designed with information of vapor-liquid equilibrium and that of solid-fluid equilibrium, respectively. The most reliable way to obtain the required information is experimental measurements, but a reliable thermodynamic model can significantly reduce the time, cost, and risk for problems involving extreme operation conditions and/or toxic chemicals. Therefore, both approaches are equally important to obtain such data. In past decades, several research groups are devoted to develop reliable thermodynamic models. Some benchmarked thermodynamic models are briefly summarized in this presentation, including those utilizing results from first-principles calculations.

