International Center for Quantum Materials

北京大学量子材料科学中心

Computational Studies of Aqueous and Ionic Liquids Interfaces

Dr. Liem X. Dang
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时间：10月4日 16：00

地点：理科五号楼 630

This seminar will present some of Dr. Liem X. Dang's recent work on molecular simulations of aqueous and ionic liquids interfaces using polarizable potential models. The magnitude of the polarization effects on the thermodynamics and structural properties in aqueous and ionic liquids is evaluated and compared to the corresponding experimental measurements. The equilibrium properties of liquid-vapor and liquid-liquid interfaces (i.e., density profiles, surface tension, electrostatic properties, etc.) will be presented and discussed. With the use of the constrained molecular dynamics, the potential of mean force and the transport mechanism of molecules across the interface are investigated.

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