

RESOLV: VORTRAGSANKÜNDIGUNG

DONNERSTAG, 27.06.2013

UM 10:00 UHR IN NC 02/99

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"Ionic liquids: from Molecule to System"

Abstract:

The potentials of ionic liquids (ILs) as solvents or catalysts in chemical processes are attracting increasing attentions not only by academic researchers but also industries. In order to design task-specific ILs and develop innovative IL-based processes, it is of significance to understand the nature of ILs with a multi-scale viewpoint from molecular to system. Hence, the multi-scale structure-properties relationship of ILs are studied using the quantum mechanics (QM), molecular dynamics (MD) and computational fluid dynamics (CFD) to bridge the electronic, atomistic/molecular and mesoscopic scales across several orders-of-magnitude in length and time.

The *ab initio* molecular dynamic simulation and coarse-graining molecular simulation were performed and the electronic structures and properties were investigated at an electronic scale. The results showed that the hydrogen-bond networks were extensively existed in almost all the ILs, both conventional and task-specific ionic liquids. The existed hydrogen bonds strongly affect the chemo-physical properties of ILs. On the other hand, at the molecular scale, the force field parameters were determined for a number of ILs, and then the thermodynamic and transport properties of the ILs were predicted by MD. Radial and space distribution functions were used to depict the microscopic structures of the ILs. At the mesoscopic scale, the ionic clusters were simulated and characterized, and the macroscopic effect on the fluid dynamic behavior of gas-IL system, such as bubble size distribution, gas holdup, Sauter diameter and interfacial area are analyzed by a high speed image pick-up system and CFD modeling.

Based on the above fundamental research results, several innovative IL-based processes using ILs as catalysts or solvents, such as cleaner process of Methyl methacrylate (MMA), production of ethylene glycol, lower temperature electrolytic aluminium process and gas purification process, were developed in our group.

Alle Interessenten sind zur Teilnahme am Vortrag herzlich eingeladen.