SEMINAR

Friday, March 16, 2007
1:30 PM
MSC 100

Computer Modeling of Solvation and Biopolymers in Aqueous Systems and Diffusion Mechanisms in Ordered Binary Crystals

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Solvation in supercritical water under equilibrium and non-equilibrium conditions is studied via molecular dynamics simulations using both polarizable and non-polarizable water models. The influence of solute charge distributions, solvent density and electrostrictive effect on solvation structure and dynamics is examined with a diatomic probe solute molecule. The validation of the linear response theory is discussed in various densities.

Homology model of Hepatitis B DNA polymerase (HDP) is generated based on the crystal structures of HIV type 1 RT. The modeled structure is refined. The preliminary molecular dynamics simulation of interaction between modeled HDP and ligands in water solution is presented.

Diffusion mechanisms in Ni_3Al of various compositions ($Ni_{73}Al_{27}$, $Ni_{75}Al_{25}$, $Ni_{77}Al_{23}$) at elevated temperatures (1300 ~ 1550 K) are investigated with molecular dynamics/static simulations using both Finnis-Sinclair and EAM type interatomic potentials. It is found that diffusion in all compositions investigated is predominated by Ni diffusion via the intrasublattice mechanism. Ni-Al coupled diffusion effect is observed at off-stoichiometric compositions ($Ni_{73}Al_{27}$, $Ni_{77}Al_{23}$) and explained at atomic level.