



"Soft-Matter Seminar"

Nico van der Vegt

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Title:

Molecular Simulations of intermolecular and surface interactions mediated by water

Abstract:

In my talk I will present atomistically detailed simulations of (1) simple, aqueous electrolyte solutions and (2) short peptides on metal surfaces in water and emphasize the development and validation of molecular models in both systems. Aqueous solutions of alkali halides and alkali acetates have been analysed by means of Kirkwood-Buff theory that relates solution structure to thermodynamic properties such as derivatives of salt activities with concentration. On the basis of this analysis I will present some well-known Hofmeister series and discuss some aspects of ion pairing that play an important role in biological systems. In the second part of my talk, I will discuss a combined quantum-classical modeling approach which we use in order to develop potentials that describe the interaction of organic molecules, amino acids and short peptides to inorganic surfaces in contact with liquid water. As an example, I will discuss classical molecular simulations that have been used to study the role of interfacial water on amino-acid-specific binding to metal surfaces.

Mittwoch, den 3.12.2008
16:00 Uhr
Raum PH 3344

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