chemisch
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Gegründet im Jahre 1869 von H. Hlasiwetz, J. Loschmidt, J. Petzval und J. Stefan

EINLADUNG

zum Vortrag
von

Univ.Prof. Dr. Andras Baranyai

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Development of classical molecular models for water and other species

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Dienstag, 13. Mai 2014, um 17:30 Uhr

Ort: Lise-Meitner-Hörsaal, Fakultät für Physik, Universität Wien,
1090 Wien, Strudlhofgasse 4 / Boltzmanngasse 5, 1. Stock

Barrierefreier Zugang: Boltzmanngasse 5, Lift, 1. Stock rechts über den Gang zum Hintereingang des Hörsaals

Abstract:

Computer simulations mimicking the matter in atomic, molecular details are invaluable tools for research. During the past decades numerous technological advancements emerged to make these time-consuming calculations more efficient. However, the most important thing is to devise a force-field which accurately describes the inter- or possibly the intramolecular forces acting in the system. Unsurprisingly, water, the most ubiquitous material in nature attracted special attention. In this talk, after a short overview of the history in this field, I present our model for water which is rigid and polarizable. Our model is a synthesis of several separate attempts in the area. It uses Gaussian charge distributions, classical harmonic springs to express polarization and exponential repulsion with a new combining rule for them. Despite its simplicity our model gives excellent estimates for ambient liquid properties and reasonably good results from high-pressure solids to gas-phase clusters using the same parameter set. Using this model of water as solvent we created interaction potentials for the complete set of alkali and halide ions. Each ion has a transferable pair-potential which using the same combination rules are applied to calculate water-ion clusters, hydration enthalpy, and ion crystal densities and internal energies. The results agree well with experiments.