Structure and Dynamics of Molecules in Liquid Environments

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Structure and dynamics of solutions of non-aqueous liquids containing ions has received unique attention in chemistry and physics in recent years, due to their technological potential. Being 'in-between' gases and solids, the liquid state is most difficult to describe and numerical simulations must be carried out since normally no analytical theories are available.

We work together with experimental and other computational/theoretical groups in order to find and understand the properties of such systems. For example, we have investigated the importance of polarisation corrections to pair potentials that describe molecule-ion interactions.

Experimentally, X-ray and neutron diffraction are the techniques of choice to determine structures in liquid solutions. These techniques are limited, however, due to the large number of interatomic distances which are measured and must be assigned to a proper structure. The more complicated the system, the more inaccurate they are and therefore numerical simulations are indispensable to check experimental results and to guide their refinement. As a recent example, we have investigated solutions of singly charged gold cations in nitromethane. This special system is important for a variety of possible applications: (a) Au+ ions are cores for the self-assembly of rigid nanostructures (triangles, squares and so on) if organic molecules, for example fused pyridine rings, are added to their nitromethane solution. (b) such solutions can be used in processes that help to extract gold from electronic scrap – an environmental issue of dramatically increasing importance.

The picture above displays an isoenergy map that shows how gold ions 'feel' the nitromethane molecules in their neighborhood. The energy function that is displayed in this map is then used to perform computer simulations. The small inset on the upper right is one of the most important results of such simulations: The probability of finding a gold ion at a given distance from the oxygen atoms of nitromethane. From such a radial distribution function most other properties can be readily derived. All the potential energy function developments and MD simulations are carried out at the Linux-cluster of the HPC consortium in Innsbruck.
Participation:

- Schwerpunkt Ionen- und Plasmaphysik / Angewandte Physik (Universität Innsbruck)
- Schwerpunkt Hochleistungsrechnen (Universität Innsbruck)
- Plattform Computer Science & Applied Computing (Universität Innsbruck)

International cooperations:

- Chemical Research Centre of the Hungarian Academy of Sciences, Budapest II, Hungary
- Departament de Física i Enginyeria Nuclear, Universitat Politecnica de Catalunya, Barcelona, Spain
- Center of Nanotechnology, Kasetsart University, Bangkok, Thailand

Selected publications:


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