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Curriculum Vitae

Publications and Reprints

Research Interests

During my PhD. studies my work was focused on the coherent electronic transport in the Landauer-Buttiker formulation through simple two-atomic model molecules and quantum dots. Using a non-equilibrium Green functions technique and the Hartree–Fock approximation, we were able to perform calculations for such nanodevices connected to para- and ferromagnetic leads, including the voltage drop effect on the molecule. Interesting results were: finding a negative differential resistance in the current–voltage characteristics, and significant magnetoresistance in the system with ferromagnetic leads. Recently, I am involved in the project on classical MD simulation of hydrated biochemical structures, in different water models (TIP3P & TIP4P), performing the geometrical analysis of the orientation of dipoles and hydrogen-bonds of the solvent. Using the proximal criterion, which enables to determine the distribution functions for non-spherically symmetrical solutes together with presenting the results as conditional probability graphs makes the hydration structures analysis more clear and meaningful.

Current Research Projects

- **Hydration structures of the quaternary ammonium cations**

We are investigating the hydration structures of the quaternary ammonium cations (QACs) in water (TIP3P/TIP4P) using MD simulations. The geometrical analysis of the orientation of dipoles and hydrogen-bonds of the surrounding water were performed. The results are presented as three dimensional histograms of conditional probability of the angles distribution given a distance from the solute. In order to determine the distance from the solute we have used the proximal criterion, which enables to properly construct the angular distribution functions also for non-spherically shaped molecules. We show, that starting with purely hydrophilic hydration structure of ammonium cation, the behaviour of water surrounding subsequent molecules in the QACs series shows a tendency towards hydrophobicity, which is partially reached for the TBA cation. We observe the clathrate-like ordering of water in this case, but traces of these features can be found also for more hydrophilic compounds, due to the exertion of such ordering by the bulk water. As a reference hydrophobic molecule we have taken the cyclohexane. In order to compare our results with other theoretical works, we have performed for this solute a simulation in TIP4P water and presented the results also as joint probability graphs.