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

EINLADUNG

zum Vortrag
von

Dr. Philipp Honegger

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für seine an der Universität Wien durchgeführte Dissertation

Computational Spectroscopy of Reverse Micelles

Betreuer: emer.Univ.Prof. Dr. Othmar Steinhauser, Institut für Computergestützte Biologische Chemie

am Dienstag, 3. Dezember 2024, 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:
We want to understand the inner workings of biological cells and why biochemical reactions therein differ from those in test tubes. The biomacromolecules constituting the machinery of life evolved and function encapsulated in a cell and surrounded by up to 400 g/L of organic matter, impacting reaction rates and equilibrium constants compared to the diluted bulk-liquid buffers used in experiments. While existing literature focuses on the excluded volume available to biomolecules and frequent intermolecular contacts, our approach is centered on the altered properties of the confined solvent.
Molecular dynamics simulations are a mathematical microscope allowing the observation of the molecular scale and computational spectroscopy forms the link joining simulation and experiment. Due to computational limitations we use reverse micelles, nanoscopic pools of water surrounded by a surfactant and immersed in a hydrophobic oil, as cellular mimetics.
Our simulations show that while single-particle properties near surfaces are slowed down, collective observables such as dielectric relaxation spectra indicate acceleration. This paradoxical finding can be explained by a Faraday effect exerted by confinement boundary conditions. This prediction has been confirmed experimentally. The drastically lowered dielectric constant of water in confinement implies an impact on electrostatic interaction energies of the solutes and thus on their thermodynamic and kinetic properties.

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