SEMINAR
Department of Mechanical Engineering

From Fundamentals to Applications of Solid–Liquid Interfaces: An Atomistic Simulation Perspective

SPEAKER

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ABSTRACT

The key mechanisms governing the processes at solid-liquid interfaces remain largely elusive, and requires atomic-level understanding of the interfacial structure, dynamics, chemical composition, thermodynamics and charge distribution. While continuum theories are often used to model solid–liquid interfaces, they tend to break down at molecular scales. At the same time, the resolution of many experimental techniques usually lacks the spatial resolution needed to fully capture and interpret nanoscale interfacial changes. To bridge this gap, we employ molecular simulations that provide detailed insights and complement experimental measurements and theoretical approaches. In this seminar, we present a series of case studies on solid–liquid interfacial phenomena, including ion adsorption, hydration, electric double layer (EDL) formation, and ion/liquid transport; all explored through density functional theory and molecular dynamics simulations. Our simulations demonstrate a certain ion-specificity towards the adsorption and hydration, primarily attributed to the ionic properties (e.g., hydration shell, size, valency, etc.) and surface features (e.g., surface chemistry, charge density), resulting in an overscreening and underscreening phenomena. This is complemented by high-resolution atomic force microscopy imaging at mica interfaces, which resolves the crystal structure of the mica surface immersed in aqueous solution and adsorbed ions from the salt-rich solutions at different concentrations. Furthermore, we demonstrate that the solution chemistry is a critical factor tuning the surface properties. With an increased pH of electrolyte solution, an enhanced deprotonation of the silanol groups of silica surface is observed which increase the net negative surface charge. This effectively restructures the EDL, and subsequently affecting both ion adsorption and electrokinetic transport. Using surface force apparatus measurements backed by molecular simulations, we capture real-time transport processes of ionic species in electrochemically modulated and molecularly confined gold surfaces. Overall, such atomistic understanding of solid–liquid interfaces is essential to unravelling many natural phenomena and a wide range of technological applications. For instance, surface charge regulated membranes can enable high ion selectivity, and effective flow control for desalination and electrochemical energy storage systems.

ABOUT THE SPEAKER

Alper T. Celebi is a Unv.Ass.Dr. at the Institute of Applied Physics, TU Wien, where he serves as the computational group leader in the Applied Interface Physics. His research focuses on the computational modelling and simulation of surfaces and interfaces at the molecular scale, with a vision of developing energy-saving, cost-effective, durable, and sustainable materials and processes for applications in energy storage and conversion, corrosion, adhesion, and surface cleaning. Prior to joining TU Wien, Alper worked as a postdoctoral researcher at the Chair of Engineering Thermodynamics at TU Delft, The Netherlands, where he focused on the atomic-level characterization of ionic liquids (ILs) and deep eutectic solvents (DESs) for the design of novel green solvents. A native of Turkey, he earned his B.Sc. in Mechanical Engineering from Istanbul Technical University and received his Ph.D. from Southern Methodist University in 2019. His doctoral thesis, titled "Molecular Dynamics Studies on Nanoscale Confined Liquids," was supervised by Prof. Dr. Ali Beskok. Dr. Celebi has actively involved in various academic and industrial projects in different roles addressing multiscale challenges in interfacial phenomena, mass and momentum transport, and materials characterization. He was lately awarded a research grant by the Austrian Research Promotion Agency (FFG) with an industrial partner for his project on the "Computational Modeling of Wet Cleaning Processes for Semiconductor Nanostructures", and an industrial grant on "Atomistic modelling of the interfacial adhesion mechanism of epoxy-based coatings". His expertise is reflected in peer-reviewed journal publications, book chapters, review articles, and academic and industrial collaborations.

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