O 51: Focus Session: Structure and Dynamics of Solvent at Electrochemical Interfaces II

Understanding how solvent molecules organize and move at electrochemical interfaces is central to catalysis, energy conversion, and electrochemical materials science. This Focus Session will bring together experimental and theoretical leaders using complementary surface specific spectroscopies as vibrational sum frequency generation, advanced X ray/electron techniques, and multiscale simulations to reveal intermolecular structure, hydrogen bond networks, ion-solvent coupling, and field driven dynamics from single crystal electrodes to complex battery interfaces. By highlighting recent breakthroughs in time-resolved measurements and operando platforms, the session aims to connect fundamental interfacial physics with macroscopic performance in electrocatalysis, corrosion, and electrochemical energy storage.

Organized by Yujin Tong (U Duisburg-Essen) and Angelika Kühnle (U Bielefeld).

Time: Tuesday 14:30–15:45 Location: TRE/MATH

Invited Talk O 51.1 Tue 14:30 TRE/MATH

Ultrafast aqueous electric double-layer dynamics — •Mischa Bonn — Max Planck Institute for Polymer Research

The formation of electric double layers (EDLs) at solid-liquid interfaces is universal, yet their molecular structure and dynamics remain incompletely understood. Building on recent advances in interface-specific spectroscopy and nanofluidic model systems, this talk will address how interfacial polarization, geometric confinement, and charge density collectively shape the structure and dynamics of water at electrochemical interfaces. We will highlight new femtosecond-resolved optical spectroscopy measurements that access the genuine ultrafast response of the aqueous EDL, revealing that field-driven ionic rearrangements and solvent reorganization occur on time scales of only a few tens to hundreds of picoseconds - significantly faster than expected from classical diffusion-limited models. These results demonstrate that collective many-body interactions and short-range correlations dominate the EDL response long before macroscopic diffusion sets in. Taken together, the studies provide a molecularly consistent picture in which interfacial polarization and charge act in concert to control water structure and dynamics across electrochemical interfaces, with direct implications for energy conversion, ion transport, and operando spectroscopies of electrified surfaces.

O 51.2 Tue 15:00 TRE/MATH

Second-order nonlinear vibrational spectroscopy: from depth-resolved studies at charged aqueous interfaces towards determining excitonic-vibrational coupling in hybrid heterostructures — •Debojyoti Roy, Sarabjeet Kaur, Álvaro Díaz Duque, Martin Wolf, Alexander P. Fellows, and Martin Thämer — Fritz-Haber-Institut of the Max Planck Society, 14195 Berlin, Germany

The properties of charged aqueous interfaces are governed by interfacial electric fields that influence ion distributions in the liquid phase, forming an electric double layer. While the evolution of the electric potential is relatively well described by theoretical models, much less is known about the influence of the DC fields on the interfacial molecular structure of water and its evolution with depth. Using our recently developed combined sum- and difference-frequency generation spectroscopy (SFG/DFG), we investigate the depth-dependent water structure at charged interfaces as a function of ionic strength, obtaining deep insight into the anisotropic orientational distribution of water and detailed information on the properties of the hydrogen bond network at different distances from the phase boundary.

Besides depth-resolution, the complementary information from SFG and DFG responses can also be used to isolate coupling terms in doubly-resonant studies. Here we also explore this possibility conceptually and propose such studies on exciton-vibrational coupling in 2D material/organic interfaces, which have various applications in solar cells but still lack understanding of their physicochemical properties.

Invited Talk O 51.3 Tue 15:15 TRE/MATH

Interface-specific nonlinear THz spectroscopy — •Chuanshan Tian — Department of Physics, Fudan Univ. China

Quantum confinement and proximity effects at material interfaces give rise to a range of novel physical and chemical phenomena, substantially advancing our ability to understand and control material properties. The development of in situ and interface-sensitive characterization techniques is therefore critical for uncovering the microscopic mechanisms governing interfacial systems and for improving device performance. This presentation will outline recent advances in interface nonlinear optical spectroscopic techniques, with a particular focus on their extension into the (multi-)terahertz spectral regime. Applications of these methods in probing interfacial microstructures and dynamic processes will be discussed, highlighting their potential for resolving complex interfacial phenomena with high specificity.