# O 16: Focus Session: Structure and Dynamics of Solvent at Electrochemical Interfaces – Poster

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: Monday 18:00–20:00 Location: P2

O 16.1 Mon 18:00 P2

**Ab initio study of water clusters and thin film adsorption on Bi(111) surfaces** — •Yingjie Xie, Adriana Bocchini, Uwe Gerstmann, and Wolf Gero Schmidt — Universität Paderborn, Paderborn, Deutschland

Bismuth, as a semimetal with strong spin-orbit coupling, plays an important role in many electrochemical applications, including electrocatalysis, electrode materials, and seawater desalination [1]. In these environments, interaction between Bi surfaces and water is unavoidable. The Bi(111) surface is both the natural cleavage plane of bulk Bi and the preferred growth surface in epitaxial processes, and is therefore suitable for studying water adsorption. While the atomic and electronic structures of Bi(111) surfaces have been well characterized, understanding of the water-Bi interface remains incomplete, and existing theoretical studies report partially conflicting results [2,3].

In this work, we employ density functional theory (DFT) to systematically investigate the adsorption behavior of isolated water molecules, molecular clusters, and thin water films on Bi(111). We examine the interplay between water-water and water-metal interactions and determine energetically favorable adsorption sites and configurations for water clusters and ultrathin films.

[1] V. Jovanovski, *et al.*, Curr. Opin. Electrochem. **3**, 114-122 (2017).
[2] V. Ivanistsev, *et al.*, E. Lust, Surf. Sci. **609**, 91 (2013).
[3] W. Oh *et al.*, J. Phys. Chem. C, **122**, 23084 (2018).

O 16.2 Mon 18:00 P2

**Structure and Dynamics of Na$^+$ and Cs$^+$ adsorbed on Cu(111) and solvated by D$_2$O molecules** — Florian Denizer[1], Jayita Patwari[1,2], John Thomas[1], Inga Langguth[2], Karina Morgenstern[2], and •Uwe Bovensiepen[1] — [1]Fakultät für Physik, Univ. Duisburg-Essen — [2]Phys. Chemie I, Ruhr-Univ. Bochum

Alkali cations in liquid water represent widely studied model systems of solvation science in which the water-water interaction competes with the local water-cation coupling. On electrode surfaces additional interactions become relevant. In our investigation using time-resolved two-photon photoemission and low-temperature scanning tunneling microscopy we compare Na$^+$ and Cs$^+$ on Cu(111) coadsorbed with individual D$_2$O molecules. D$_2$O/Na$^+$/Cu(111) forms 10 nm wide, flat-lying aggregates. We observe a linear increase of the electronic lifetime of the 3$s$ electron transfer resonance at the Cu(111)-Na$^+$ interface as a function of the number $n$ of adsorbed D$_2$O molecules per ion combined with a maximal energy transfer to solvent modes $\Delta E$ of 0.6 eV at $n = 6 - 7$ [1]. On D$_2$O/Cs$^+$/Cu(111) we find exclusively one or three D$_2$O attached to Cs$^+$. This leads to a stepwise increase in the corresponding 6$s$ electron lifetime with $n$. $\Delta E$ is half that of Na$^+$/Cu(111) which we associate with difference in ion core diameter and modified interactions with Cu(111) [2]. Comparing both systems we identify pronounced differences rooted in the microscopic connection between structure and dynamics.

[1] Kühne et al., JPC C **129**, 2054 (2025). [2] Thomas et al., JPC C **127**, 23467 (2023).