O 25: Solid-liquid interfaces: Structure, spectroscopy – Poster

Time: Monday 18:00–20:00 Location: P2

O 25.1 Mon 18:00 P2

Role of Interfacial Water for CO_2 Reduction Reactions in Ionic Liquid/Acetonitrile Electrolytes — •Björn Ratschmeier[1], Arik Geringswald[1], Alisa Kamaric[1], Angel Cuesta[2], and Björn Braunschweig[1] — [1]University of Münster, Institute of Physical Chemistry, Münster, Germany — [2]Advanced Centre for Energy and Sustainability (ACES), School of Natural and Computing Sciences, University of Aberdeen, UK

Room-temperature ionic liquids (RTILs) such as 1-butyl-3-methylimidazolium bis(trifluoromethanesulfonyl)imide ([BMIM][NTf_2]) are promising electrolytes for CO_2 reduction reaction (CO_2RR), where the availability of water at the electrode/electrolyte interface is known to play a decisive role in the reaction mechanism. We find that the addition of acetonitrile (ACN) to [BMIM][NTf_2] with 1.5 M H_2O markedly increases the CO yield, while the onset potential for CO formation remains essentially unchanged. *In situ* IRAS of bulk intermediates formed during CO_2RR are indicative for a reaction pathway [1] via a [BMIM]-COOH intermediate that requires the presence of interfacial H_2O as shown in previous work. In contrast, *in situ* ATR-SEIRAS reveals ACN-induced modifications of the electrode/electrolyte interface. OH vibrational bands increase significantly at cathodic potentials, indicating enhanced water accumulation at the interface, thus, causing larger availability of water for CO_2RR. Ref.: [1] Ratschmeier et al. ACS Catalysis 14, 1773 (2024).

O 25.2 Mon 18:00 P2

Capacitance of Nanoconfined Salt Solutions: Interplay between Concentration and Temperature — •Caterina Sartori, Haoyuan Quan, Louis Lehmann, and Roland Netz — FU Berlin, Fachbereich Physik, Arnimallee 14 14195 Berlin, Germany

The capacitance of confined aqueous salt solutions is important for a variety of applications, including thermal energy conversion, but remains poorly understood. Performing Molecular Dynamics simulations and treating bulk electrolytes as a reservoir, we determine the temperature and bulk-concentration dependent density, slit concentration and capacitance of confined salt solutions. On a microscopic level, the capacitance is determined by the inverse dielectric profile, which we also present. Our results constitute a crucial step towards understanding the electrostatic behavior of confined electrolytes.