

INM-KOLLOQUIUM

“THE ROLE OF CHARGE-TRANSFER INTERACTIONS IN ELECTROCHEMICAL SEPARATIONS: TUNABILITY AND SELECTIVITY”

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INM, Leibniz-Saal, Campus D2 5

Host: Prof. Dr. Volker Presser

Molecular level design is crucial for the development of new, more efficient electrochemical interfaces for a wide range of industrial and environmental applications. Selective separations remain one of the most important processes in the chemical and biochemical industries, and are crucial for water purification and environmental remediation. Electrochemical modulation presents an avenue for minimizing both energy consumption and secondary pollution. In our work, we leverage redox-active materials as an attractive platform for performing selective electrochemical separations. We focus on the principal role of charge-transfer interactions in achieving molecular level selectivity. Organometallics, metallopolymers and associated metal-organic complexes offer a wealth in flexibility in terms of metal/ligand design, and control of electronic properties. First, the development of a range of redox-active metallopolymer electrodes is presented, with specific interactions towards micropollutant anions of concern [1-2]. The underlying intermolecular mechanisms are then unraveled by a combination of electronic structure calculations and spectroscopy, and leveraged for fine chemical separations. Second, the capabilities of redox-electrodes are leveraged towards not only selective capture, but also the environmental transformation of emerging contaminants and heavy metal pollutants. Chromium and arsenic oxyanions are separated selectively in the presence of excess competing ions, and down to 10-100 ppb concentrations, based on differential charge-transfer between the redox-sites and the molecular targets [3]. Finally, we present some new directions in the fine tuning of redox-processes for wider classes of chemical transformations.

From a fundamental perspective, these concepts point towards an emerging direction in electrochemical interface design – by superimposing properly tuned chemical interactions, we can reach beyond double-layer effects and achieve unprecedented molecular selectivity.

References:

- [1] X. Su, et al, “Anion-selective redox electrodes: electrochemically-mediated separation with organometallic interfaces,” *Advanced Functional Materials*. 2016, 26(20), 3394-3404.
- [2] X. Su, et al, “Asymmetric Faradaic systems for selective electrochemical separations,” *Energy & Environmental Science*, 2017, 10, 1272-1283.
- [3] X. Su, et al. “Electrochemically-mediated selective capture of heavy metal oxyanions chromium and arsenic from water,” *Nature Communications*, 2018, 9, 4701.

You are invited to have coffee with the speaker 15 minutes before the talk starts.

KONTAKT

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