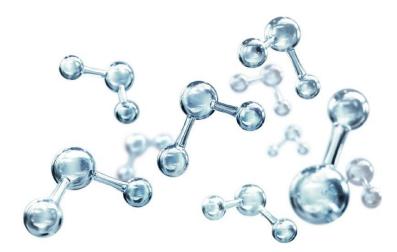
Seminar

COVS Centre for Molecular Water Science

22nd of June 2023 12:00 h

Zoom Virtual Meeting:

https://tuhh.zoom.us/j/82631283465 Meeting-ID: 826 3128 3465 Password: 978444



Oskar Paris

Chair of Physics, Department Physics, Mechanics and Electrical Engineering Montanuniversität Leoben

On the role of water for ion electro-sorption in charged carbon nanopores

Electric double-layer capacitors (EDLCs) store charge by physical adsorption of ions at the electrode-electrolyte interface within highly porous, charged electrodes. Aqueous electrolytes – despite of their low operation voltage – have a series of advantages, including high ion mobility and unbeaten environmental friendliness. Together with the currently most common electrode materials made of nanoporous carbons, functional devices from potentially cheap and readily available, thus overall sustainable materials become feasible. Prominent applications include electrical energy storage in supercapacitors for high-power applications, and water purification / water desalination in capacitive de-ionisation technologies. Yet, many details of the charge storage mechanisms remain unanswered. In particular, the specific role of the solvent water remains a topic of intense current research.

We have demonstrated that in-situ small-angle X-ray scattering (SAXS) in combination with in-situ X-ray transmission (XRT) and electrochemical measurements are promising methods to study global ion flux and local ion re-arrangement within the pores of a carbon working electrode during charging and discharging of EDLCs. Such in-situ experiments together with advanced data analysis help to understand local ion storage mechanisms such as the role of the pore geometry for charge screening (degree of confinement), or the partial loss of the water solvation shell to access pores smaller than the size of the solvated ions (degree of de-solvation) (1). The approach also allows studying ion dynamics, notably the discrimination between different mechanisms such as ion exchange, counter-ion adsorption, or co-ion expulsion (2). However, there are several assumptions and approximations involved, which need to be verified independently by individual ion-sensitive and ideally also water-sensitive techniques. Synchrotron radiation based anomalous small-angle X-ray scattering (ASAXS) extends the advantage of the structural sensitivity of SAXS to chemical sensitivity for one (or even both) ion species (3). Moreover, small-angle neutron scattering (SANS) can be employed to specifically enhance (or reduce) the scattering contribution from the solvent water. Recent SANS experiments using electrolytes with H₂O and D₂O indeed suggest that the active role of water during charging and discharging EDLC's cannot be neglected.

(1) C. Prehal, C. Koczwara, N. Jäckel, A. Schreiber, M. Burian, H. Amenitsch, M.A. Hartmann, V. Presser, O. Paris, *Nature Energy* 2 16215 (2017). (2) C. Prehal, C. Koczwara, H. Amenitsch, V. Presser, O. Paris, *Nature Communications* 9 4145 (2018). (3) C. Koczwara, C. Prehal, S. Haas, P. Bösecke N. Hüsing, O. Paris, *ACS Applied Materials & Interfaces* 11, 42214 (2019).