Selectivity mechanisms in capacitive deionization
The seminar will be given in English

Capacitive deionization (CDI) is a fast-developing technology with primary applications in wastewater remediation, brackish water desalination, and water softening. A typical CDI cell contains two carbon-based porous electrodes electrically isolated by a separator. A constant voltage or current applied between the electrodes in the presence of a salty feedwater causes the salt ions to electromigrate into the electrode nanopores, forming electric double layers and desalting the feedwater. An emerging field of interest in water research is ion selectivity, the preferential removal of particular (harmful) ionic species relative to other (benign and beneficial) species. A thorough understanding of selectivity would be highly useful for efficiently treating complex source waters and wastewaters for use or reuse in various applications by removing undesirable species (e.g., excess sodium or heavy metals) while retaining desirable minerals (e.g. calcium and magnesium). Our aim is to deepen the understanding of ionic selectivity processes in CDI via an integrated approach, using theoretical advancements to predict observable phenomena and testing these predictions with an experimental program. We show, both theoretically and experimentally, that electrodes functionalized with an appropriate chemical charge enhance selectivity of a smaller hydrated ion (K⁺) relative to a larger hydrated ion (Li⁺). We also examine the time dependence of selectivity with functionalized electrodes, showing that monovalent ions are preferred at short charging times, while divalent ions are strongly preferred at long charging times. Lastly, we examine the removal of weak acid species (e.g. boric acid/borate), showing that CDI can perform this separation by utilizing pH gradients that form in situ across the electrodes and separator.