Advanced materials for electro-driven separation for selective resource recovery

Abstract

The electrochemical technology of Capacitive Deionization (CDI) has witnessed an exponential increase in research and development efforts over the past several years. It employs porous electrodes to remove ions of interest from water. These ions are driven to the interior of the electrodes, where they are stored, by the applied electrical current. Quite often, an ion selective membrane is used in conjunction with the electrodes for enhanced desalination. The addition of a membrane gives rise to the membrane capacitive deionization (MCDI). This PhD falls under the purview of this technology. The mechanism of ion storage depends on the selection of the electrode materials. Carbon based electrodes, widely studied and used in MCDI, store the removed ions in electrical double layers (EDLs) formed on the surface inside the pores. One of the primary objectives of this project is to look for alternative electrode materials for MCDI. Prussian blue analogues (PBAs), described by the general formula $A[Fe(CN)_6]$(A: Ni^{2+}, Co^{2+}, Fe^{2+}), will be considered as a replacement to carbon for electrode materials. These compounds can be fabricated cheaply and their open lattice framework presents a unique opportunity for ion storage using redox mechanism. This mechanism involves intercalation of ions into the PBA lattice with a simultaneous reduction of a lattice ion. A survey of the state-of-the-art provides several different performance results. A focus of this project would be to optimize the performance of electrodes to harness their full potential in terms of charge storage, over time stability and reduced energy consumption. A consequence to this change of material will be that the well understood EDL model, from porous carbon electrodes, will no longer be applicable to the PBA electrodes that utilize the redox mechanism of ion storage. Therefore, a separate theory will also be developed parallel to the experimental expertise. This will be another objective of this project. A model of ion storage and charge transfer would help in optimizing the cell design and understanding the experimental results as well. The establishment of a fundamental understanding of the experiments and the theory of deionization using PBAs will be followed by a shift in focus towards the nature of ions being removed. It will be highly desirable to tune the electrodes towards selective removal of one kind of ion from feed water. The selectivity can be based on the valency of ion (mono/di-valent) or the type of ions (Na^+, K^+ etc.) with the same valency. As a final output of this project, we aim at developing a good understanding of the intercalation phenomena in the PBA electrodes and use this knowledge to efficiently and effectively solve real world problems.