Advanced materials for electro-driven separation for selective resource recovery

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Motivation

Capacitive deionization is an upcoming water desalination technology [1]. It has the potential to rival existing technologies for treatment of water with moderate to low salt concentration because of its cheap and energy-efficient nature. This technique can be made to function in a continuous mode resulting in a constant production of desalinated water. The material used for the fabrication of porous electrodes is of prime importance as it underlines the performance of the cell (salt removal capacity, stability over time, energy consumption). The most-studied and used electrode materials for the CDI technique are made of carbon [2]. This research explores the field of advanced materials for CDI, other than carbon. The first potential candidate chosen for electrode is a class of material called Prussian blue analogues (PBAs). These compounds are of interest for the purpose of water desalination (apart from cost-effective and easy fabrication) because of their open framework structure, lower energy consumption than conventional CDI materials, fast charge transfer kinetics and long cycle life [3]. The ions are stored in the lattice spaces of the PBA by a process referred to as intercalation. It is a redox reaction and is given in Figure 1. A schematic of the desalination cell is given in Figure 2.

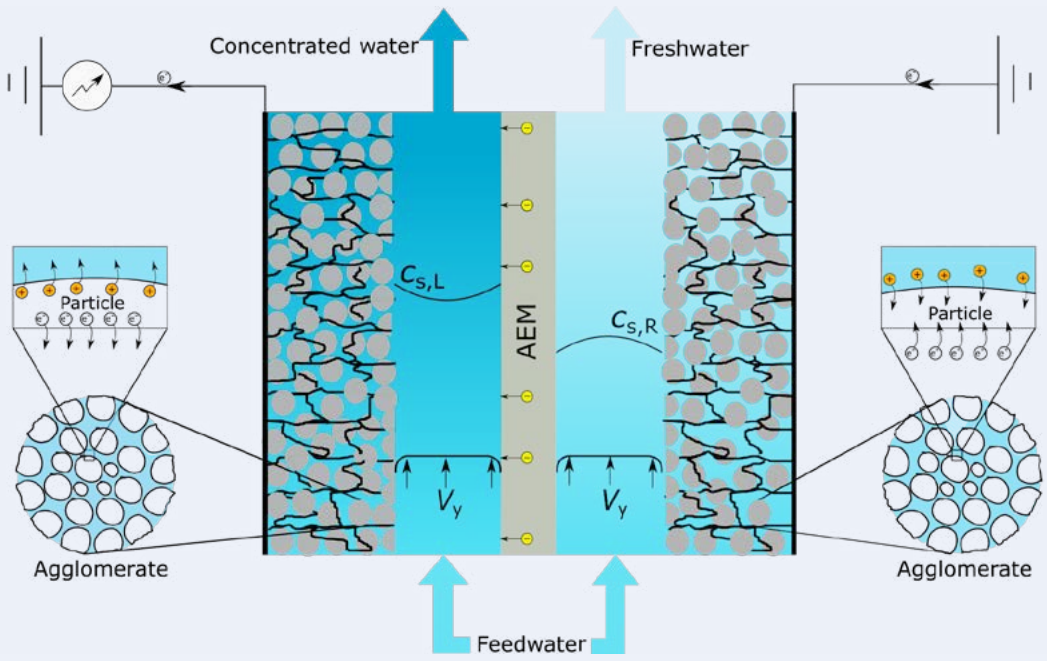

Figure 2: Schematic of the desalination experiment demonstrating the functioning of the desalination cell with PBA electrodes. Intercalation in one electrode (right) is complimented by de-intercalation in the other electrode(left).

Technological challenge

The Prussian blue analogue to be used for electrode material has the chemical formula of $Na_xNi[Fe(CN)_6]_yZ_{1-y}.mH_2O$ ($0 < x < 2$; $0 < y < 1$; Z: $Fe(CN_6)$ vacancy). These compounds have a face cantered cubic (FCC) structure. The main challenges to integrate PBAs with the CDI technology are :

- Synthesis of PBA. Imperfect reaction conditions may lead to a defective crystal structure.
- Deficiency of lattice sites in the crystal structure.
- Porosity of the electrodes and their characterization.

Research goals

In this research, we aim to:

- Investigate the synthesis of PBAs to reduce the defects in the crystal structure.
- Understand the impact of electrode porosity on the kinetics of ion and charge transfer.
- Study the influence of synthesis of the electrodes on their salt intake capacity.
- Introduce selectivity in the electrodes towards different kinds of ions.
- Develop a theoretical model to explain charge storage in PBAs.

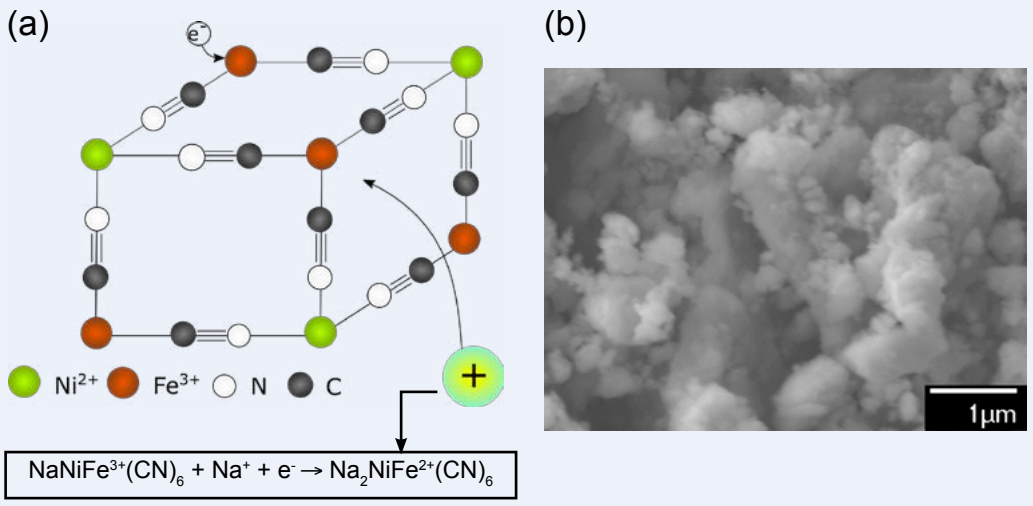

Figure 1: The PBA molecule (a) Unit cell of PBA depicted with the mechanism of charge storage observed in PBA electrodes (b) SEM image of as-synthesized PBA. Agglomerates of size < 1 µm are formed during the co-precipitation reaction.

[1] S. Porada, R. Zhao, A. Van Der Wal, V. Presser, and P. M. Biesheuvel, “Review on the science and technology of water desalination by capacitive deionization,” Prog. Mater. Sci., vol. 58, no. 8, pp. 1388–1442, 2013.

[2] C. Kim, P. Srimuk, J. Lee, S. Fleischmann, M. Aslan, and V. Presser, “Influence of pore structure and cell voltage of activated carbon cloth as a versatile electrode material for capacitive deionization,” Carbon N. Y., vol. 122, pp. 329–335, 2017.

[3] Porada, S., Shrivastava, A., Bukowska, P., Biesheuvel, P.M. and Smith, K.C., 2017. Nickel hexacyanoferrate electrodes for continuous cation intercalation desalination of brackish water. Electrochimica Acta, 255, pp.369-378.

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