

# Functionalized Nanostructured Materials for Selective Ion Recovery in Capacitive Deionization



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### Motivation

Capacitive deionization (CDI) is a promising technology in the field of desalination and water treatment, which can efficiently separate and recover salts at high purity without using chemicals [1]. It makes use of a pair of porous electrodes and an electrical potential difference to remove charged species from aqueous solutions (Figure 1).

The current focus in CDI research is to selectively separate valuable ions, such as precious metals and nutrients. For that, the traditional activated carbon electrodes can be replaced with more selective alternative materials. 3D intercalation materials like Prussian Blue Analogous (PBAs) have been shown to have high salt adsorption capacity and, by adding different transition metals in their lattice structure, also tunable selectivity [2,3].

## Technological challenge

The ion selectivity of PBAs can be controlled by using different transition metals, their combinations and composites. However, to successfully address the challenge of improving selectivity, a full understanding of PBAs structure-property relationships is needed, which is currently still lacking. This needs to focus on various chemical properties such as crystal structure, functionality, redox activity and pore/cavity size.

Furthermore, the new materials must also remain stable and effective during long-term operation. Predicting the stability of a material will require a combination of both theoretical knowledge and experimental testing such as working with certain chemicals or repeated cycles of charging and discharging.

# Research goals

The objective of this project is to understand, optimize and tune the ion-selective properties of selected intercalation materials.

The research goals of the project are to:

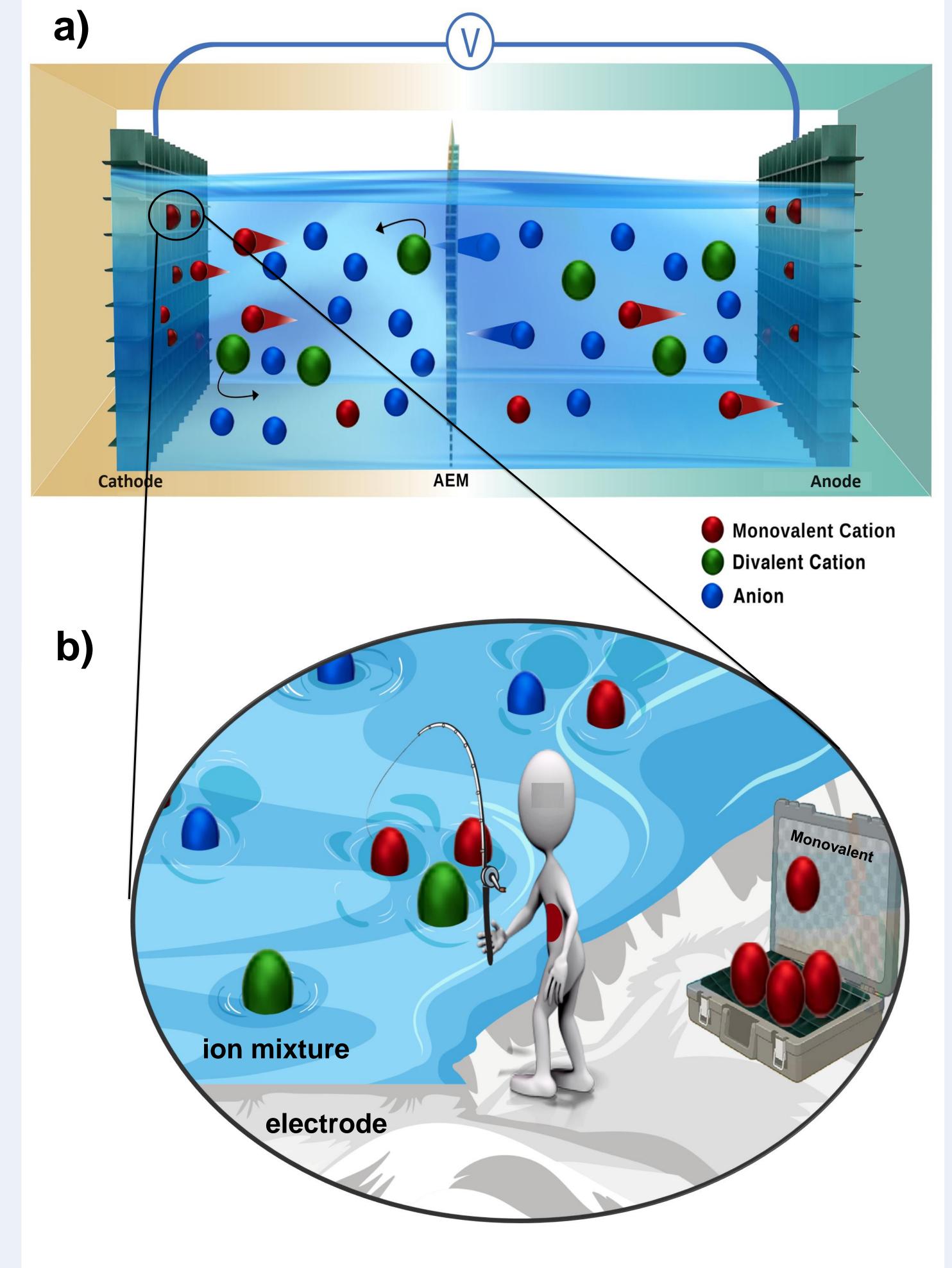
- Explore different transition metals (Ni, Cr, Mn, Co, Cu, Zn, etc.) for making PBA electrodes, to increase their selectivity and compare them with traditional activated carbon electrodes.
- Understand structure-property relations of the electrodes (PBAs) to obtain different cation selectivity.
- Improve the stability of electrodes by metal combination to get simultaneously high stability and selectivity.

### References

[1] Porada, S., Zhao, R., van der Wal, A., Presser, V., & Biesheuvel, P. M. (2013). Review on the science and technology of water desalination by capacitive deionization.

[2] Singh, K., Porada, S., De Gier, H. D., Biesheuvel, P. M., & de Smet, L. C. P. M. (2019). Timeline on the application of intercalation materials in Capacitive Deionization.

[3] Singh, K. (2022). Advanced materials for electro-driven ion separation and selectivity. PhD Thesis Wageningen University.



**Figure 1.** a) CDI setup consists of two PBA electrodes acting as an anode and a cathode, with an anion exchange membrane (AEM) placed between them, within a mixture of monovalent and divalent ions. The PBA electrodes are designed to selectively intercalate monovalent cations from the ion mixture. The membrane allows the passage of anions, enabling them to move across to the de-intercalating compartment. b) PBA electrode selectively removes monovalent cations from the solution.



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