Materials and models for wearable hemodialysis

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Abstract:

Hemodialysis (HD) is a therapy replacing kidney functionality, which has a huge impact on the patients' life and is not equally accessible to all. Ideally, a wearable dialysis device would allow for a more frequent treatment, reduce the stress on the body and the need for strict dietary regime. Such a treatment would also improves the patients' lifestyle and make HD more accessible to those living in remote areas, with mobility issues or with poor heart condition. Furthermore, it will enable significant water and energy savings.

The miniaturization of HD requires the introduction of a water regeneration device after the dialysis unit, that purifies the toxin-rich water and recirculates it to the blood cleaning section. The majority of compounds present in dialysate water can be abated with conventional sorbents or ion exchangers, while urea is too small a molecule to be completely depleted with standard materials. Previous prototypes adopted a biochemical reaction mediated by urease, a method creating by-products that can enter the patient's blood causing health issues.

Membranes, sorbents and mixed matrix membranes working via diffusion and adsorption have the potential to capture such molecules, but conventional adsorbents have low urea/water selectivity. In this work, we performed a comprehensive computational study of 560 porous crystalline adsorbents comprising mainly covalent organic frameworks (COFs), as well as some siliceous zeolites, metal organic frameworks (MOFs) and graphitic materials. An initial screening using Widom insertion method assessed the excess chemical potential at infinite dilution for water and urea at 310 K, providing information on the strength and selectivity of urea adsorption. From such analysis it was observed that urea adsorption and urea/water selectivity increased strongly with fluorine content in COFs, while other compositional or structural parameters did not correlate with material performance. The results agree with those of the Widom method and allow to identify the urea binding sites, the contribution of electrostatic and van der Waals interactions, and the position of preferential urea-urea and urea-framework interactions. This study paves the way for a well-informed experimental campaign and accelerates the development of novel sorbents for urea removal, ultimately advancing on the path to achieve wearable artificial kidneys.

Keywords: hemodialysis, sorbents, water purification, modelling, screening, bioseparation.