

Nanostructured materials for Lithium Separation from Produced Water: A Multiscale Approach from Computational Screening to Pilot-Scale Validation

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Developing technologies based on advanced materials plays a significant role in the current energy transition scenario, driving a more efficient process with reduced environmental impact. At the same time, it is crucial to consider social, economic, and environmental aspects to achieve a sustainable balance between technological innovation and collective responsibility. In this context, the management of produced water (PW) is critical to the sustainability and viability of the oil and gas industry. Additionally, PW can be seen as a potential secondary source for extracting valuable materials such as lithium ions (Li^+). This study aims to develop nanofiltration systems based on nanostructured materials and electrochemical processes to extract these valuable ions from PW efficiently. The core innovation methodology focuses on applying materials informatics and computational screening to design and optimize materials with morphologies that enhance Li^+ selectivity, and introducing an economic risk assessments to ultimately contribute to the sustainable upscaling of the developed technologies. Initially, an extensive literature review of different PW studies was conducted to create a detailed database of ion concentration, which was essential for defining relevant concentration ranges for testing nanomaterials' selectivity. This approach ensures precise comparisons between computational predictions and experimental findings. This research contributes to advancing material design, manufacturing processes, and separation methodologies by tailoring technologies to specific ionic compositions. Recent studies highlight that membranes incorporating nanomaterials (NMs), such as graphene derivatives, metal-organic frameworks (MOFs) and lithium-ion sieves (LIS), effectively enhance Li^+ separation. These materials exhibit unique properties, including surface charge, pore size, and channel morphology, critical for improving recovery efficiency. Here, we show the challenges and latest developments in computational materials screening, applying techniques such as Density Functional Theory (DFT) and Molecular Dynamics (MD), and for the synthesis and characterization of NMs for incorporation in membranes, targeting Li^+ ions in the presence of other dissolved monovalent and divalent ions in a synthetic brine solution, such as sodium (Na^+), potassium (K^+), magnesium (Mg^{+2}), and calcium (Ca^{+2}).

