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Understanding Ion Transport and Selectivity in 2D Nanochannels

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Understanding ion transport in confined environments is crucial for designing synthetic membranes with high selectivity and efficiency. Inspired by biological systems, two-dimensional (2D) nanomembranes have emerged as promising platforms for controlling ion transport, with interlayer spacings tunable from angstroms to nanometers. However, achieving precise control over ion mobility requires deeper insights into the interplay between the aqueous fluid and the solid interface. Here, we employ large-scale molecular dynamics (MD) simulations to unravel the key physicochemical mechanisms that govern ion selectivity in functionalized MoS_2 and MXene nanochannels.

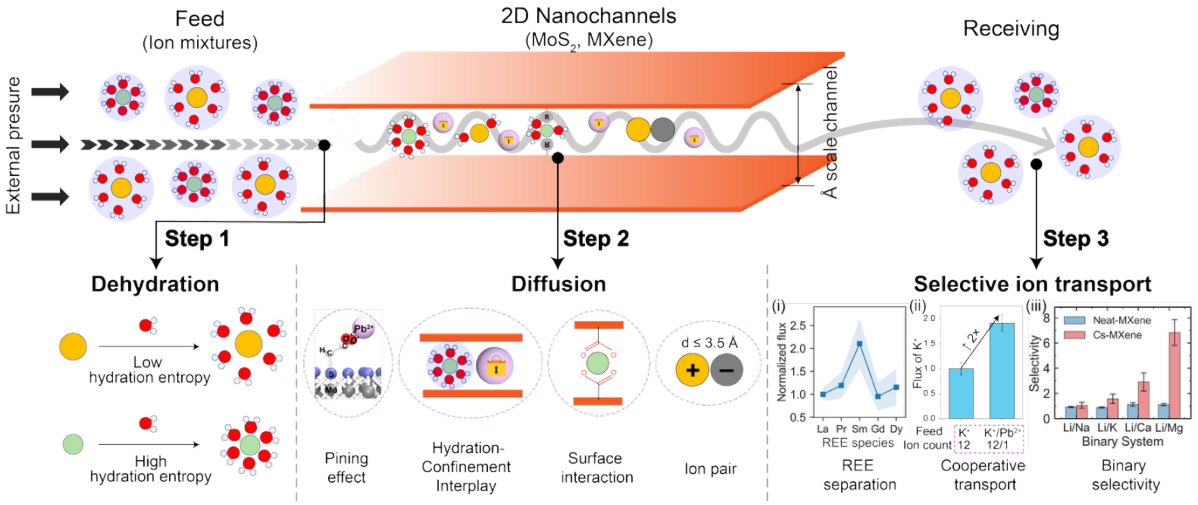

Fig. 1. Schematic of the pressure-driven ion transport process through 2D nanomembranes (e.g., MoS_2 or MXene). The process begins with Step 1, Dehydration, where hydrated ions from the feed solution shed water molecules to enter the channel, a step governed by the ion's hydration entropy. The partially dehydrated ions then undergo Step 2, Diffusion, traversing the Å-scale channel via a complex interplay between hydration-confinement effects (including pinning and hydration shell rigidity), surface chemistry, and ion-ion interactions (such as ion pairing or competition). This leads to Step 3, Selective transport, where specific ions exit into the receiving solution. Representative computational results of this process are shown, including (i) volcano-shaped permeability for rare earth element (REE) separation, (ii) cooperative transport that enhances K^+ flux in the presence of Pb^{2+}, and (iii) improved binary selectivity (e.g., for Li^+/Mg^{2+}) in Cs^+–intercalated MXene.

Our simulations reveal that ion selectivity is governed by a complex interplay of dehydration, confinement, and surface chemistry, leading to novel transport phenomena (Fig. 1). For acetate-functionalized MoS_2 membranes, we utilized the GPU-accelerated OpenMM package with 12-6-4 empirical potentials to model the complex ion-water-surface interactions under applied pressure. These simulations revealed a volcano-shaped permeability trend for rare earth elements (REEs), arising from competing dehydration and surface interaction effects.[1, 2] We also identified a "pinning effect", where transient interactions between ions and the acetate functional groups hinder diffusion. Furthermore, a cooperative transport mechanism was discovered, in which Pb^{2+} promotes the formation of neutral K^+–Cl^- ion pairs, thereby boosting K^+ permeability.[3] In the MXene system, we found that Cs^+ intercalation selectively enhances Li^+/Mg^{2+} separation. This selectivity stems from ion-specific effects: the rigid hydration shell of Mg^{2+} favors a central pathway through the channel, leading to direct steric competition with the intercalated Cs^+ ions. This effect significantly reduces Mg^{2+} permeability while having a lesser impact on the smaller, more flexible Li^+.[4]

These insights provide a deeper understanding of confined ion transport and offer guiding principles for the rational design of next generation nanomembranes for selective ion separation.

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