# Selective transport of water molecules through cation-controlled interlayer spaces in graphite and vermiculite systems

### Gopinadhan Kalon

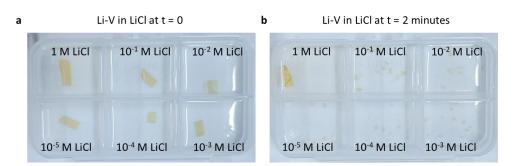
Lalita Saini, and Aparna Rathi Discipline of Physics and Materials Engineering, Indian Institute of Technology Gandhinagar, Gujarat 382355, India gopinadhan.kalon@iitgn.ac.in

Ion channels of living cells play a crucial role in life's day to day functioning. Understanding and mimicking their functionalities will provide a breakthrough in the membrane-based desalination, chemical separation, and dialysis technologies. Moreover, when the fluidic channel dimensions approach the sizes of ions and molecules, interesting effects such as deformation of hydration shells, steric effects, van der Waals and even quantum related effects are expected to emerge. These studies require channels of sizes in the sub-nm range which is extremely difficult to fabricate. We chose single crystals of graphite and vermiculite and modified the interlayer spaces with the help of salt intercalation. In the case of graphite, the use of aqueous KCI ions and an electric field is found to expand the interlayer spaces sufficiently large to allow the passage of water molecules. When low voltage or a concentration gradient is applied across the expanded graphite samples, it rejects > 99 % of the sea salt ions, making them ideal for desalination applications. Majority of the ions are rejected based on the steric exclusion, however a small proportion (< 1%) is transported exhibiting hydration energy dependant conductance. On the other hand, vermiculite interlayer spaces are tuned by the intercalation of cations such as K<sup>+</sup>, Na<sup>+</sup>, Ca<sup>2+</sup> and Al<sup>3+</sup>, which made them water stable. 600 nm thick Na-intercalated vermiculite membrane exhibits dye rejection efficiencies >99% with high water permeation rates. We also achieved a high salt rejection efficiency of 95% with a 1.2 µm thick membranes. The water flux and salt rejection are found to be a function of external pressure and membrane thickness. These cation-intercalated vermiculite membranes exhibit several properties related to highly confined systems such as conductance saturation at low concentrations of 10 mM, and K<sup>+</sup> mobility enhancement.

#### References

- [1] L. Saini, S.S. Nemala, A. Rathi, S. Kaushik, G. Kalon, Nature Communications 13, 498 (2022).
- [2] A. Rathi, K. Singh, L. Saini, S. Kaushik, B. Dhal, S. Parmar, G. Kalon, Materials Today Nano. 22, 100328 (2023).

#### Figures



**Figure 1:** The stability of Li-Vermiculite membrane in aqueous LiCl solution. Li-V membrane in various concentrations of LiCl ranging from 1 M to  $10^{-5}$  M at time (a) t = 0, and (b) t = 2 minutes.

## Graphene2023