Subin Sahu
Justin Elenewski, Christoph Rohmann, & Michael Zwolak
University of Maryland, College Park, MD, USA
National Institute of Standards and Technology, Gaithersburg, MD, USA

subinsahu@gmail.com

Optimal transport and colossal ionic mechano-conductance in graphene crown ethers

Directly interrogating the mechanism of ion transport in sub-nanoscale pores is challenging as several processes contribute to ion translocation: van der Waal repulsion, dehydration, electrostatic interactions, structural fluctuations, etc. Biological ion channels, for example, balance electrostatic and dehydration effects to yield large ion selectivity alongside high transport rates. These macromolecular systems are often interrogated through point mutations of their pore domain, limiting the scope of mechanistic studies. In contrast, using all-atom molecular dynamics simulations, we demonstrate that graphene crown ether pores afford a simple platform to directly investigate optimal ion transport conditions, i.e., maximum current densities and selectivity. We show that small pore strains (1%) give rise to a colossal (100%) change in conductance. This process is electromechanically tunable, with optimal transport in a primarily diffusive regime, tending toward barrierless transport, as opposed to a knock-on mechanism. These observations suggest a novel setup for nanofluidic devices while giving insight into the physical foundation of evolutionarily optimized ion transport in biological pores.

References

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Figures

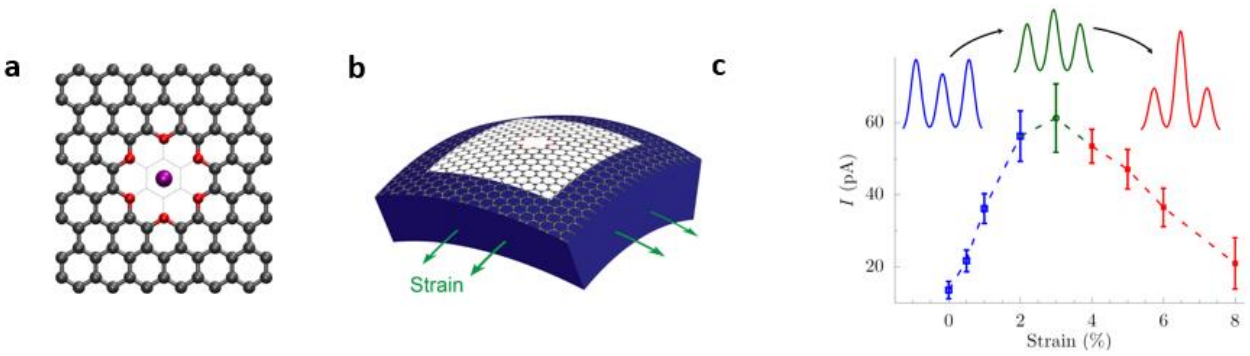

Figure 1: Optimal transport in graphene crown ether pore. a) K^+ ion (purple) in an 18-crown-6 pore embedded in graphene. b) Schematics of potential experimental setup. c) MD results of current versus strain, showing a colossal rise in the current at small strains, optimal transport around 3 % strain, and subsequent drop in the current at large strain. The insets show the schematics of the free-energy profile in each regime.