Modeling Gate-Tunable Ionic Transport Using Atomically Thin Patterned Graphene Membrane

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Abstract

Patterned two-dimensional (2D) materials have recently become promising candidates for separation processes in both gaseous and aqueous phases, due to mechanical strength and atomic thickness. Conventional separation technique using 2D materials are limited by the surface charge of 2D material, which is hard to control during fabrication process. In this report, using patterned porous graphene as an example, we show that the ionic transport can be tuned by applying a bias between the graphene membrane and water. We model the gate-tunable ionic transport through graphene nanopores using the Electrochemistry module in COMSOL Multiphysics®. The transport and electrostatic phenomena are studied near a single graphene nanopore with diameter ranging from 5 to 50 nm. The material transport and potential distribution are described by a Poisson-Nernst-Planck setup, with inlet boundary conditions for the boundaries connecting the system studied with the bulk phase. Our numerical simulations reveal a rectified ionic transport at low positive bias on graphene, in consistent with experimental results. The ionic transport exhibits strong spatial dependency, with cations transported through the center, while anions near the edge of the graphene nanopore. The rectification is further found to be closed related with the Debye length in the solution, indicating that the gate-tunable rectification is feasible for nanopores even as large as 20 nm, which is hardly achievable by conventional method with similar diameter. Out numerical simulation using COMSOL Multiphysics® reveals the mechanism behind the gate-tunable ionic transport through patterned 2D materials, and related applications.