Transport via Ion-Trapping Artificial Crown Ether Nanopores in Atomically Thin Membranes

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Crown ethers have been long known to bind non-covalently to metal cations, with binding selectivity depending on the crown type. Recently, ion-trapping crown-ether-like nanopores in monolayer graphene have been described [1], owing to the hexagonal symmetry of the graphene lattice. Given the importance of reliable ion trapping in nanoporous membranes for applications ranging from battery technology to healthcare and water desalination, we describe simulated aqueous binding and transport behavior of cation-trapping crown nanopores created in monolayers of graphene and molybdenum disulfide (MoS_2). For the graphene-based 18-crown-6 nanopores, we use detailed atomistic molecular dynamics simulations to estimate Na^+ and K^+ binding free energies of -4.79 kJ/mol and -11.72 kJ/mol, respectively – in good agreement with the experimental data on stand-alone crown ethers. In addition, we demonstrate ion species-dependent semiconductor-like transport properties of the resulting nanoporous membranes, as well as their zero permeability for anions. Finally, using density functional theory calculations, we utilize hexagonal symmetry of MoS_2 monolayers to create novel crown-like nanopores with tailored binding free energies and selectivities.

References

[1]. Guo, J., et al., *Crown ethers in graphene.* Nature Communications, 2014. **5**: p. 5389.