Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Seawater desalination using pillared graphene as a novel nano-membrane in reverse osmosis process: nonequilibrium MD simulation study

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Electronic Supporting Information (SI)

To validate the potential model and parameters used in the present study, MD simulation was conducted to evaluate the seawater properties. The dimension of the simulation box was 5×5×5 nm^3 in X, Y, and Z directions respectively. MD simulation was run for 1 ns in NPT ensemble at 1 atm and 300 K to reach the equilibrium and then continued for further 3 ns for data extraction. The hydration enthalpies (ΔH_{Hyd}) of salt ions were calculated from the enthalpy of pure water and enthalpy of ions in seawater. The calculated values of ΔH_{Hyd} are -4.05 and -3.61 eV, for Na^+ and Cl^-, respectively which are in good agreement with those reported previously.[1]

The hydration coordination number (N_{Hyd}) of Na^+ and Cl^- ions were also calculated from integration of radial distribution function (RDF) of (Na^+-O_w) and (Cl^--O_w) pairs from $r = 0$ to $r = r_{min}$, where r_{min} is the location of the first minimum (Figure S1). The simulated N_{Hyd}s are 5.75 and 7.95 for Na^+ and Cl^- ions, respectively which are in good agreement with those reported using Monte Carlo simulation of 6.0 and 8.3.[2]

Figure S2 presents the snapshots of the simulation box at t = 19 ns and t = 8 ns for (6,6)@G (7,7)@G membranes, respectively.

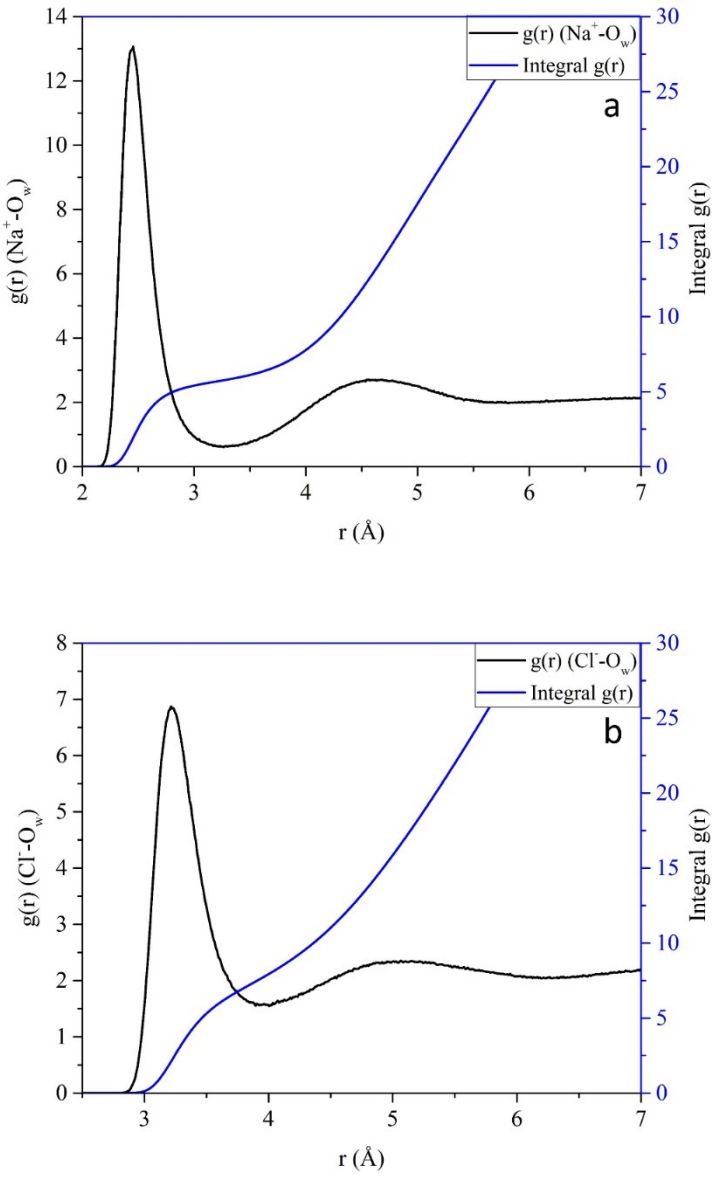

Figure S1. The RDF and its integration for (Na^+/O_w) and (Cl^-/O_w) pairs.

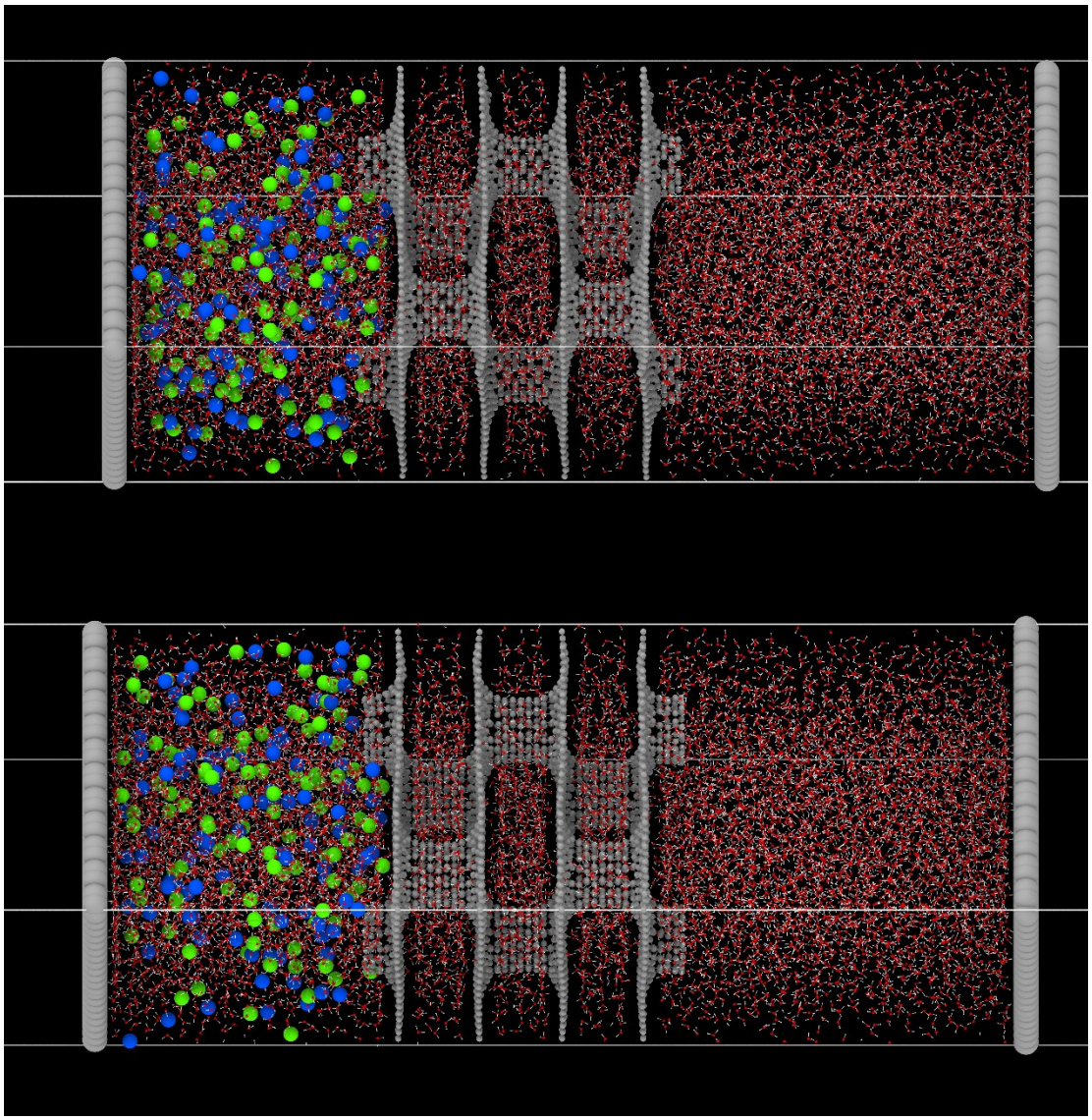

Figure S2. Snapshot of simulation box at t = 19 ns for (6,6)@G (top) and t = 8 ns for (7,7)@G (bottom). The red, white, grey, blue, and green spheres represent the oxygen, hydrogen, carbon, Na^+, and Cl^-, respectively.

1. Y. Marcus, *Journal of the Chemical Society, Faraday Transactions 1: Physical Chemistry in Condensed Phases*, 1987, **83**, 339-349.
2. M. Mezei and D. L. Beveridge, *The Journal of Chemical Physics*, 1981, **74**, 6902-6910.