Supplementary Information

High-performance Desalination through Tortuous Pathways in Multilayer ABC-stacked Large-pore Covalent Organic Frameworks: A Theoretical Study

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Supplementary Figures

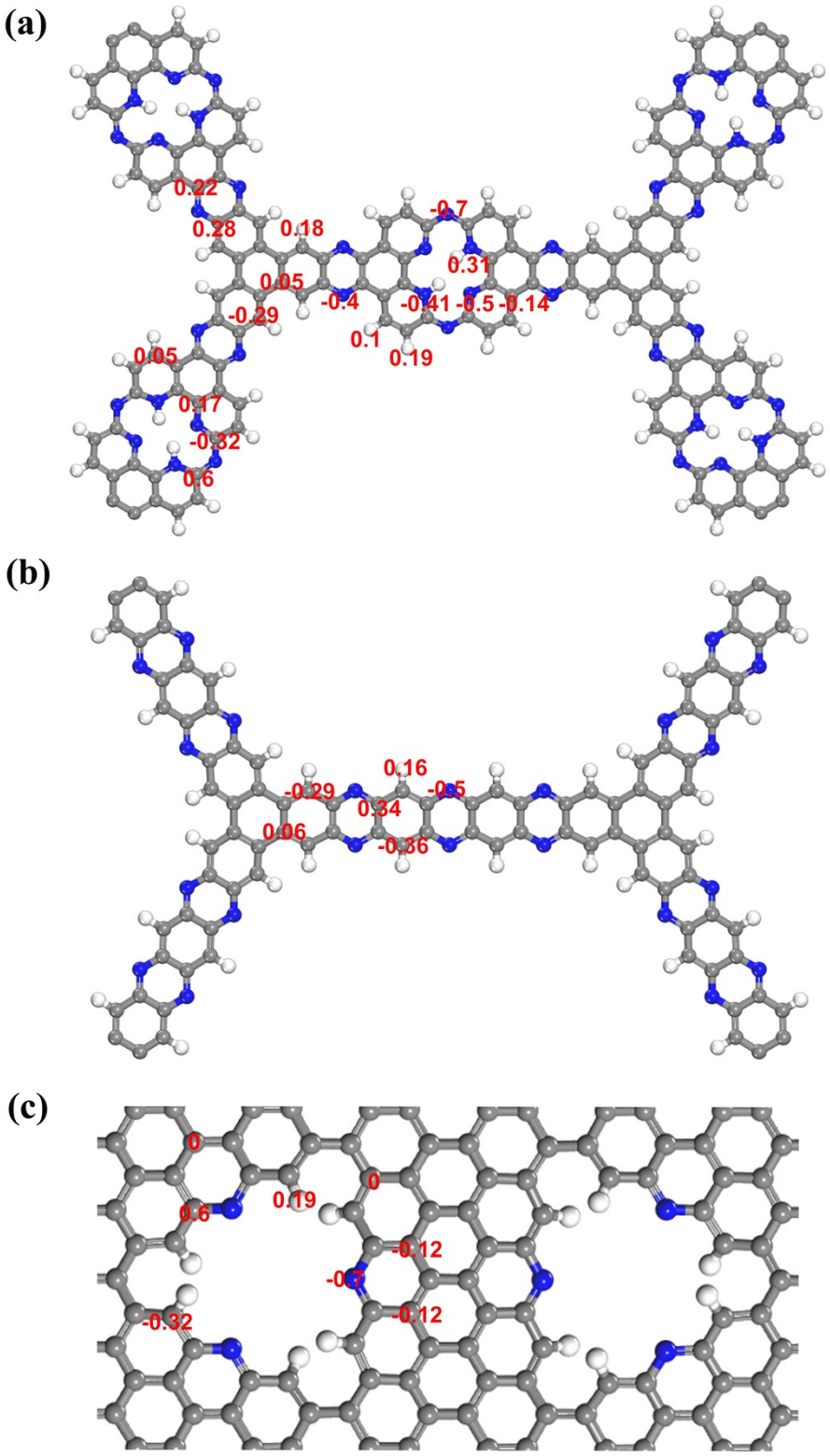

Fig. S1 The information of atomic charges of the ABBPM COF membrane (a), the 3L-pseudo COF membrane (b), and the monolayer pseudo-graphene membrane (c).

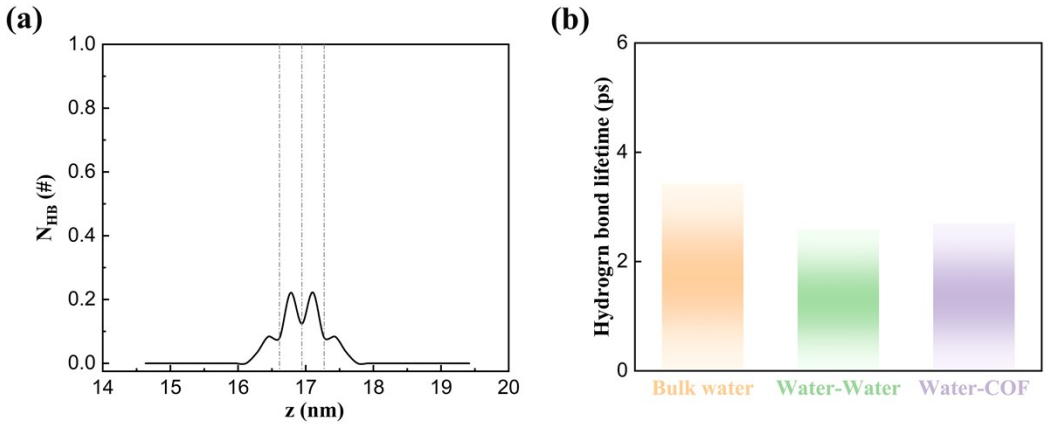

Fig. S2 (a) The average number of hydrogen bonds between the nanochannel and the water molecules along the z-direction with 3L ABBPM COF membranes. The grey dashed lines represent the position of the monolayers. (b) The lifetime of hydrogen bonds in the bulk water, between water molecules and between water and membranes within the 3L ABBPM filter.

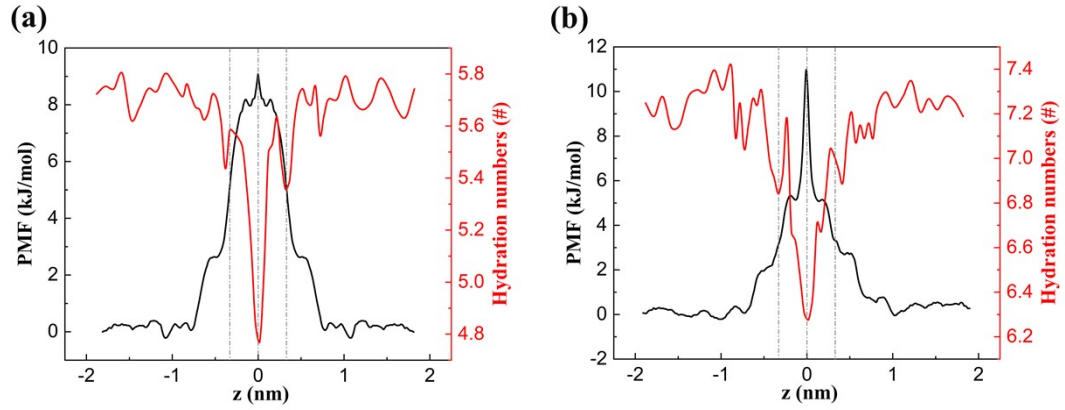

Fig. S3 The hydration numbers for the first hydration shells compared with the PMF profile as Na^+ (a) and Cl^- (b) translocating the 3L ABBPM COF nanopores.

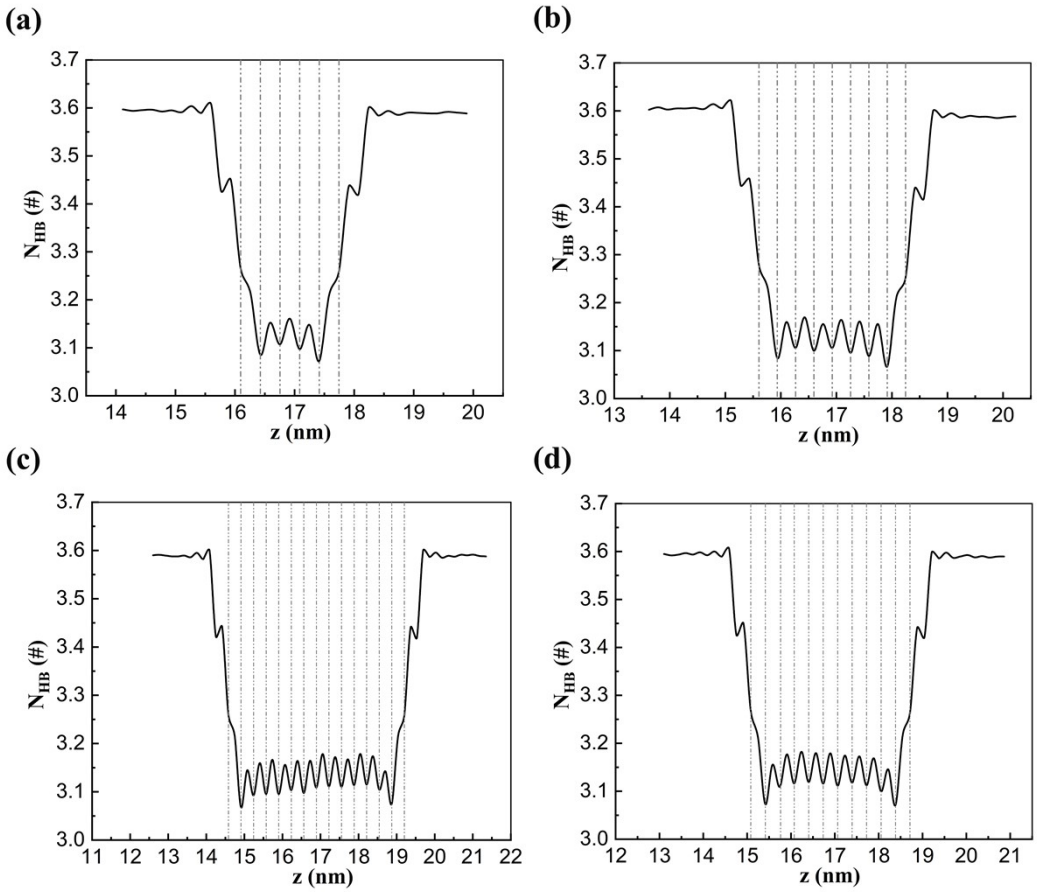

Fig. S4 The average number of hydrogen bonds between water molecules along the z-direction cross the pores of ABBPM-COF nanosheets with 6 (a), 9 (b), 12 (c), and 15 (d) COF monolayers, respectively.

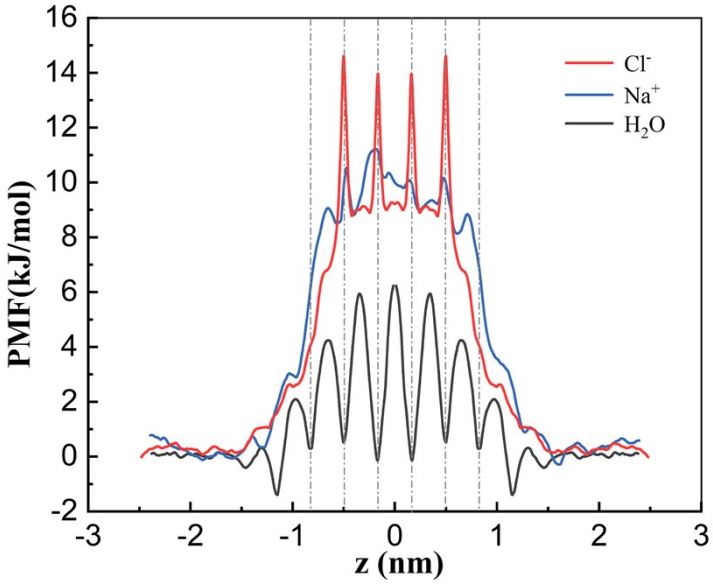

Fig. S5 Free energy of Cl^-, Na^+, and water translocating through the 6L ABBPM COF membranes.

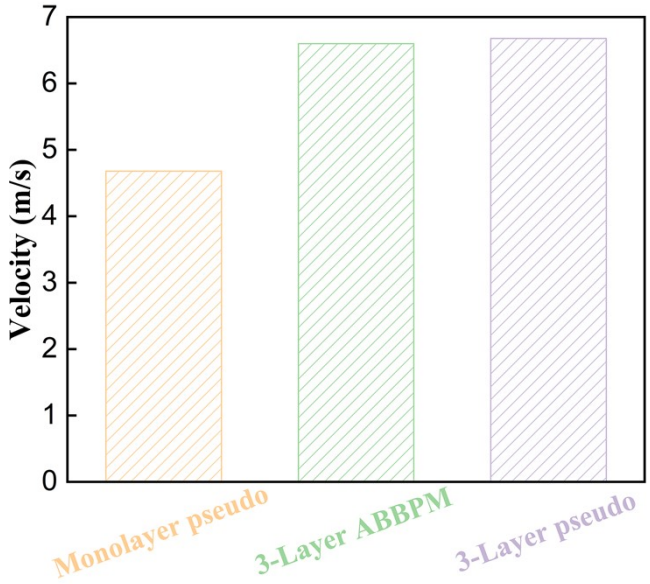

Fig. S6 The traversal velocity of the monolayer pseudo-graphene membrane, the 3L ABC-stacked ABBPM membrane, and the 3L ABC-stacked pseudo-COF membrane.

Supplementary Methods

Formulae for calculating salt rejection, water flux, water permeance

The salt rejection rate (R) is calculated by the following formula:

$$R = \left(1 - \frac{N_p}{N_o}\right) \times 100\% \quad \text{Eq. 1}$$

where N_o is the total number of ions in the initial seawater region and N_p is the number of ions in the freshwater region when the concentration of the seawater region reaches 0.8 M (twice the initial concentration).

The water flux (Q, L/m^2/h) is evaluated by the formula:

$$Q = \frac{qm}{N_A \rho S} = \left(\frac{N_{t_2} - N_{t_1}}{t_2 - t_1}\right) \times \frac{m}{N_A \rho S} \quad \text{Eq. 2}$$

where N_{t_2} and N_{t_1} are the number of water molecules in the freshwater region at moments t_2 and t_1, respectively, m is the quality of one mole of the water molecule (18 g/mol), q is the water flux (#/ns), ρ is the water density (1 g/cm^3 =10^{-3} g/L), N_A represents the Avogadro constant and S is the area of the ABBPM COF membranes (~51.25 nm^2).

The water permeance (p) is calculated by the formula:

$$p = \frac{Q}{P} \quad \text{Eq. 3}$$

where Q is water flux (L/m^2/h) and P is the pressure difference applied across the system (MPa).