Supporting Information

Strain tunable nanoporous r-N-GDY membrane for efficient seawater desalination

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Supplementary Figures

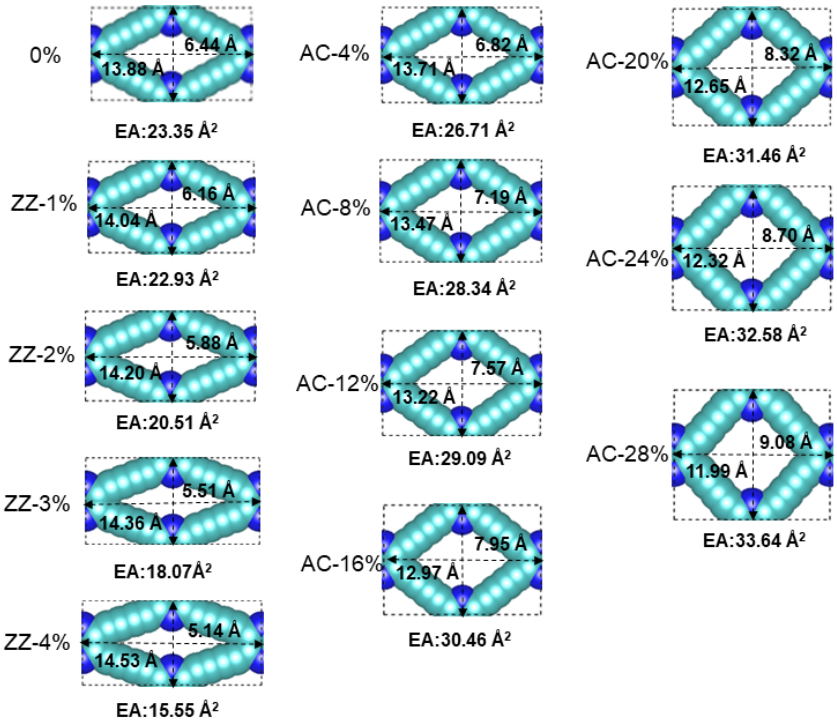


Figure S1. The pore sizes and EA under different tensile strains.

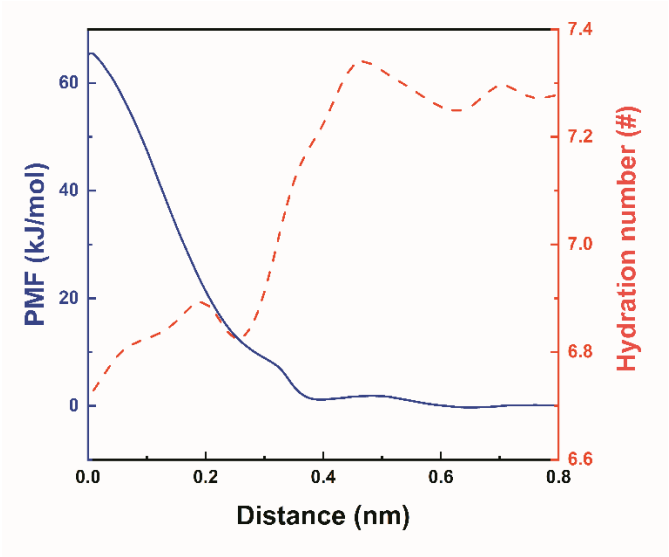


Figure S2. The hydration numbers for the first hydration shells (dashed red line) compared with the PMF profile (solid blue line) for Cl^- translocating the nanopores.

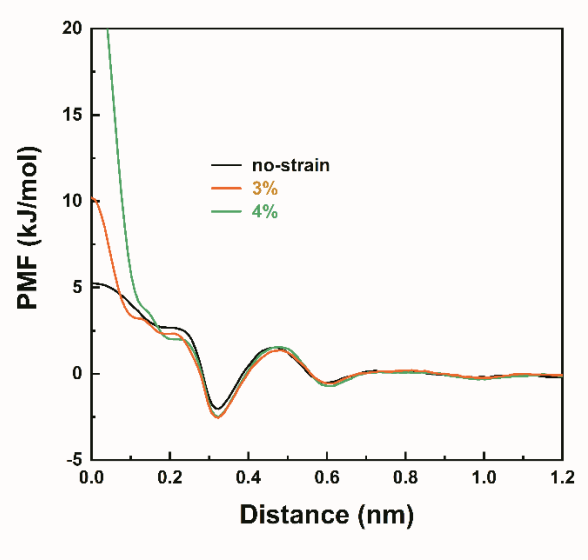
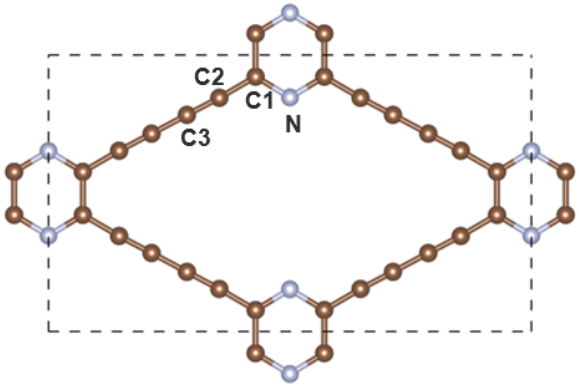


Figure S3. Potential of mean force (PMF) for H_2O translocating the nanopore of the r-N-GDY membrane under the no-strain system, and under 3%, 4% strain along the ZZ direction. The r-N-GDY membrane is placed at 0 nm.

Supplementary Tables

Table S1. Atomic charges for the r-N-GDY membrane.

Atom	Q (e)	σ (nm)	ε (kJ/mol)
C1	0.35	0.339967	0.359824
C2	-0.16	0.339967	0.878640
C3	0.04	0.339967	0.877640
N	-0.46	0.325000	0.711280



Supplementary Methods

Formulae for calculating salt rejection, water flux and water permeability

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

$$R = \left(1 - \frac{N_p}{N_0}\right) \times 100\% \qquad \text{Eq. (1)}$$

where N_p is the number of ions in the pure water region when the seawater concentration doubles (0.8 M), and the N_0 is the total number of ions in the system.

The water flux (Q) is calculated by the formula:

$$Q = \frac{N_{t_2} - N_{t_1}}{(t_2 - t_1)S} \qquad \text{Eq. (2)}$$

where N_{t2} and N_{t1} represent the number of water molecules on the pure water side at moments t_2 and t_1 respectively, and S is the area of the r-N-GDY membrane (20.41 nm^2 ~ 25.27 nm^2).

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

$$p = \frac{mQ}{\rho N_A P} \qquad \text{Eq. (3)}$$

where Q is the water flux, m is the quality of one mole of water (18 g/mol), N_A is Avogadro's number, ρ is the density of water (1 g/cm^3 = 10^{-3} g/L), P is the pressure drop across the membrane.

Method for Fitting parameters of the acetylenic bond

There is an acetylene bond C≡C in the r-N-GDY membrane, which is absent in the amber99sb force field. In order to fit the C≡C force field parameters, we constructed H - C≡C - H molecule containing C≡C. The method we adopted is to use the *GAFF* force field that comes with *antechamber* to generate the correct *LEAP* recognizable *fcomd* parameter file and *mol2* files. Then generate *promtop* and *inpcrd* files that can be recognized by amber. The force field parameters obtained for the C atoms in the C≡C are σ = 0.339967, ε = 0.878640, respectively.