Supporting Information

Insights into the water permeability and Hg^{2+} removal using two-dimensional nanoporous boron nitride

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1. Computational method of the diffusion coefficient for Hg^{2+}

Diffusion coefficient of Hg^{2+} in solution from a MD simulation using Eq. (1),

$$D = \lim_{t\to\infty} \frac{\left\langle \left| r_{(t)} - r_{(0)} \right|^2 \right\rangle}{6t} \quad (1)$$

where D is the diffusion coefficient, t is time, $r_{(t)}$ is the position of the ion at the time t and $r_{(0)}$ is the initial position. The diffusion coefficient can be obtained by calculating the mean square displacement (MSD). We performed independent MD sampling runs at pressure of 10^5 Pa and temperature of 298 K. Firstly, the steepest descent method was used to minimize the energy of the system during 500,000 steps. Then, it was equilibrated in the canonical ensemble (NVT) for 1 ns. Finally, the simulations were performed in NPT ensemble for 2 ns. The diffusion coefficient of Hg^{2+} was obtained as $0.9235\times10^{-5}cm^2\cdot s^{-1}$ in this work.

2. Computational method of the surface tension

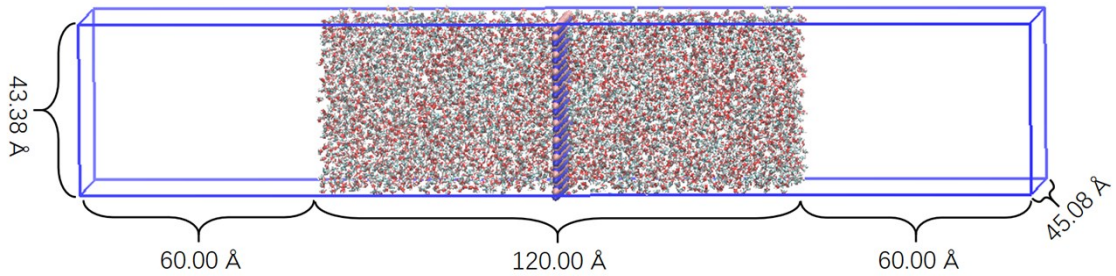

Fig. S1. Snapshot of molecular dynamic trajectory in simulation.

In order to calculate the surface tension of water on h-BN, we constructed the simulation box shown in Fig. S1.[1] Firstly, the h-BN membrane was placed in the center of 120 Å simulation box, and 7441 water molecules were randomly filled into the box. Then, the energy of the system was minimized during 500,000 steps. In order to equilibrate, MD simulation was performed in NPT ensemble for 1 ns. Next, the simulation box was lengthened from 120 Å to 240 Å, and 60 Å vacuum parts appeared at both ends of the box. Finally, the h-BN membrane was frozen and the simulations were performed in NVT ensemble for 5 ns. For all simulations, the pressure was always 10^5 Pa, and other parameters were set the same as the non-equilibrium MD simulation. The surface tension of water on a single h-BN layer was

obtained as 68.66mN·m^{-1} in this work.

3. PEs for Hg^{2+} across N4, N6, B4 and B6 pores.

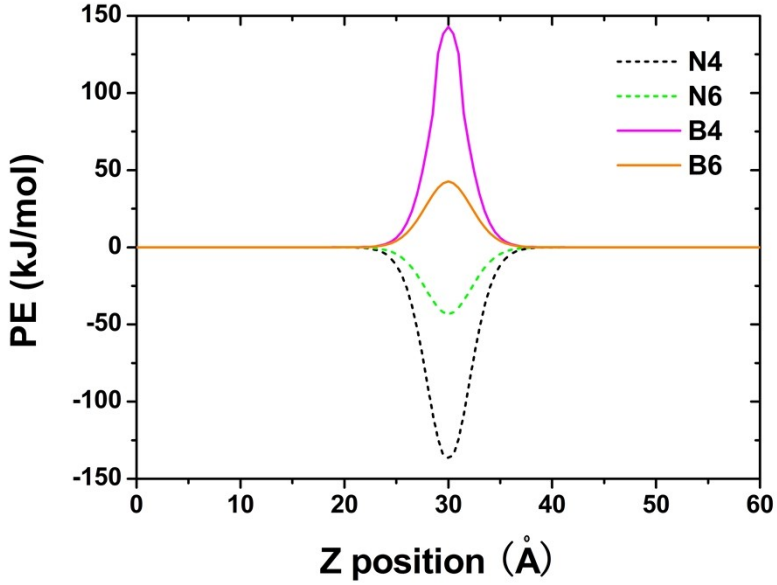

Fig. S2. PEs for Hg^{2+} across N4, N6, B4 and B6 pores. The distance is the position of Hg^{2+} along the z axis, 30 Å is the middle point of the membrane.

1. L. T. CHEN Fei Wu, WU Zhao, *Acta Physico-Chimica Sinica*, 2015, **31**, 5.