Supplementary Information

Mechanisms of efficient desalination by a two-dimensional porous nanosheet prepared *via* bottom-up assembly of cucurbit[6]urils

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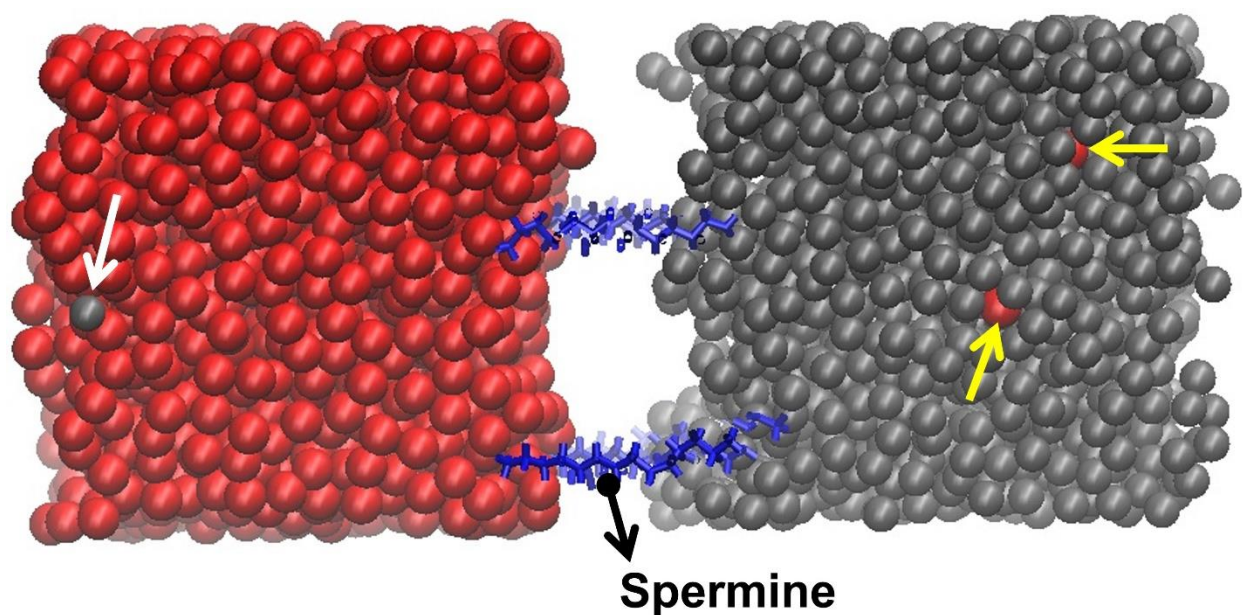[†] These authors contributed equally to this work.

Spermine

Figure S1. Simulation system consisting of the 2D nanosheet with four CB[6]-spermine complexes, 2880 water molecules, 44 sodium, and 60 chloride ions at 100 ns. The thioether bridges, dangling arms, CB[6], and NaCl ions are not represented for clarity. Red and gray spheres are indicative of water molecules on the freshwater and saltwater sides, respectively. The yellow arrows show two water molecules that moved from the fresh water to salt water, while the white arrow exhibits one water molecule that moved from the salt water to fresh water.
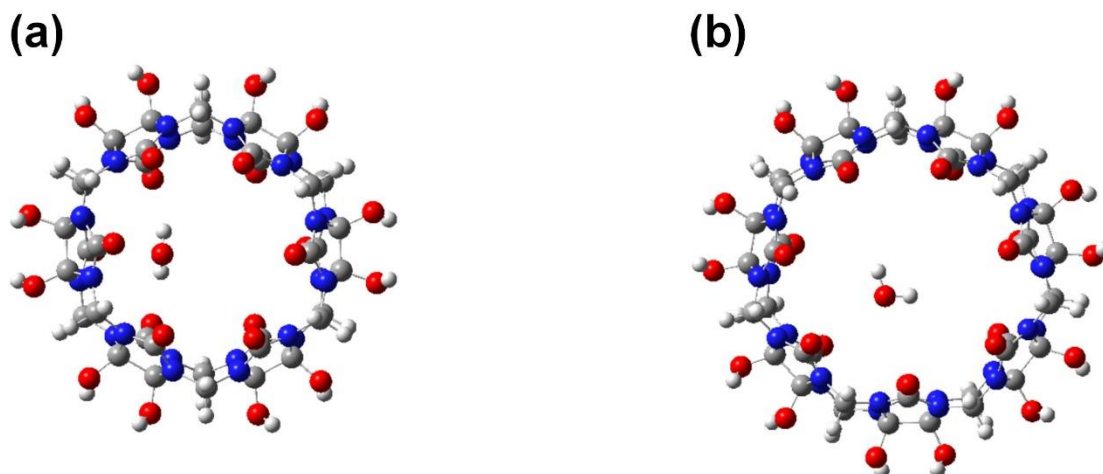
(a)

(b)

Figure S2. Optimized structures of (a) CB[6] and (b) CB[7] with one water molecule (color scheme: C, grey; N, blue; H, white; O, red). Gaussview was used to generate initial molecular structures [1], which were optimized with the Gaussian 09 package unless stated otherwise [2].

References

[1] R. Dennington, T. Keith, J. Millam, GaussView, version 5, (2009).

[2] M. Frisch, G. Trucks, H. Schlegel, G. Scuseria, M. Robb, J. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. Petersson, Gaussian 09, revision E. 01 (2009) Gaussian Inc, Wallingford, CT See Supporting Information for full citation.