

Supplementary Materials

Investigation into the Simulation and Mechanisms of Metal-Organic Framework Membrane for Natural Gas Dehydration

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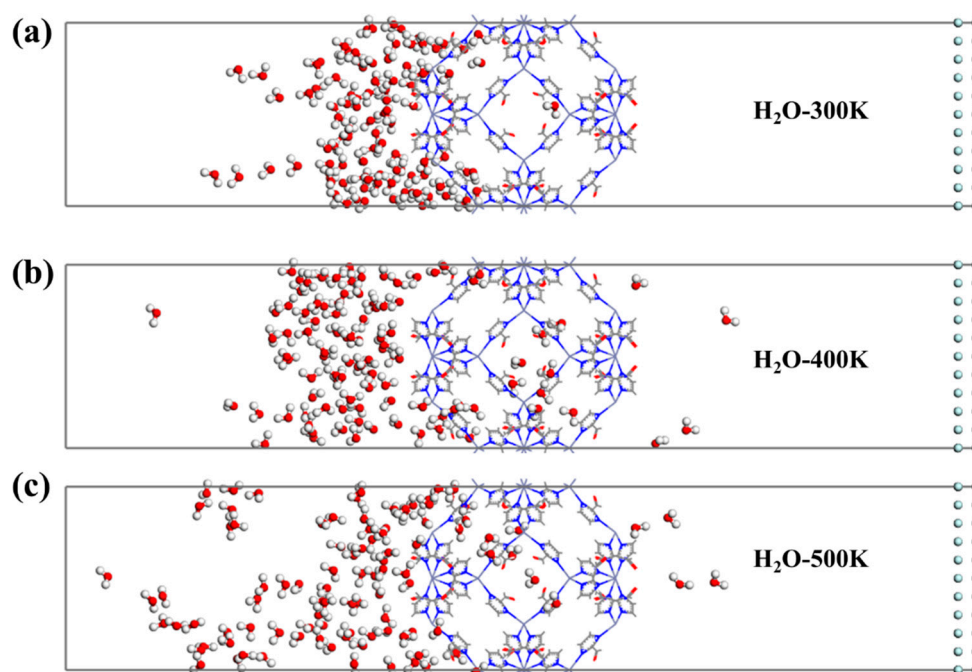
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(1) 100 H₂O molecules



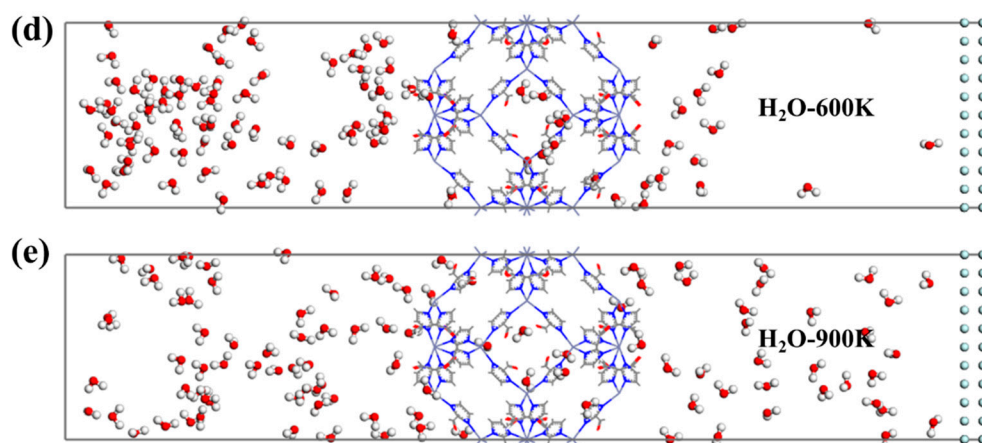


Figure S1. The final state simulation snapshots of H₂O molecules permeating through the ZIF-90 membrane at (a) 300K, (b) 400K, (c) 500K, (d) 600K and (e) 900K for 5 ns.

(2) 200 H₂O molecules

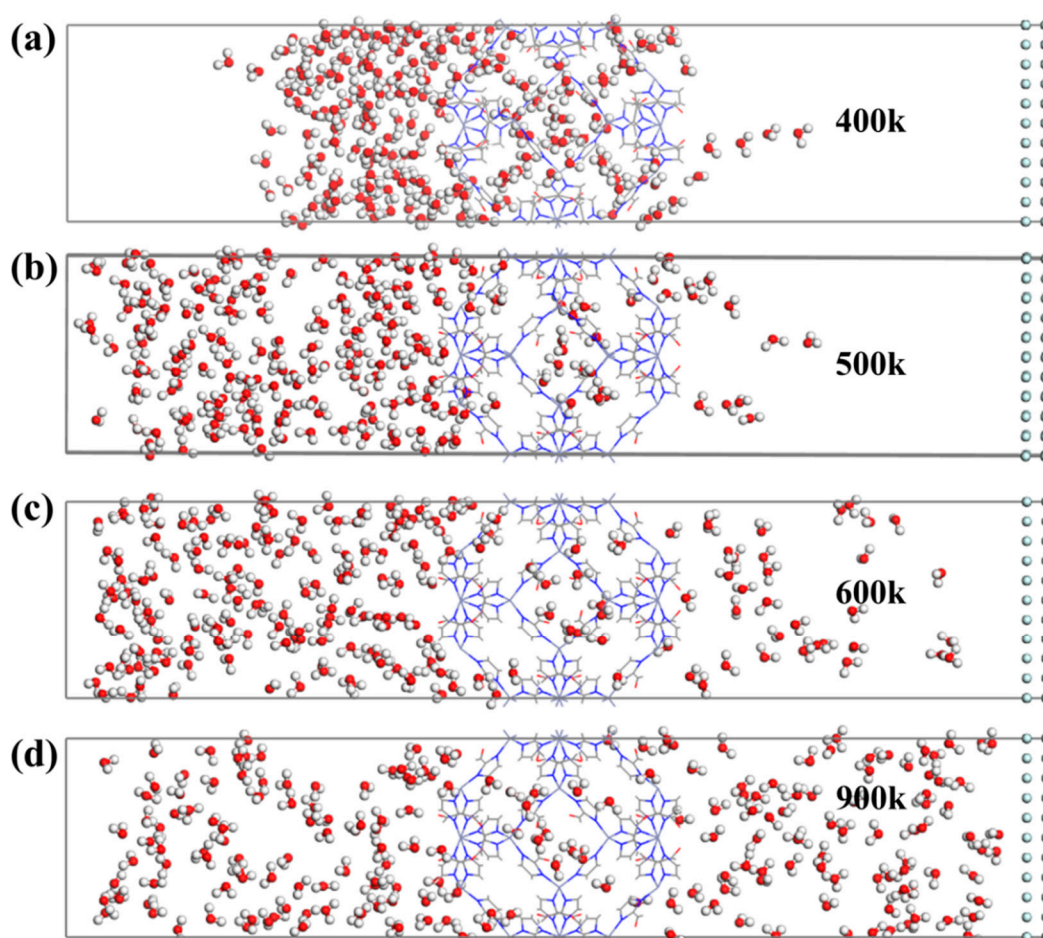


Figure S2. Final state simulation snapshots of H₂O molecules permeating through the ZIF-90 membrane at (a)

400K, (b) 500K, (c) 600K and (d) 900K for 5 ns.

(3) 100 CH₄ molecules

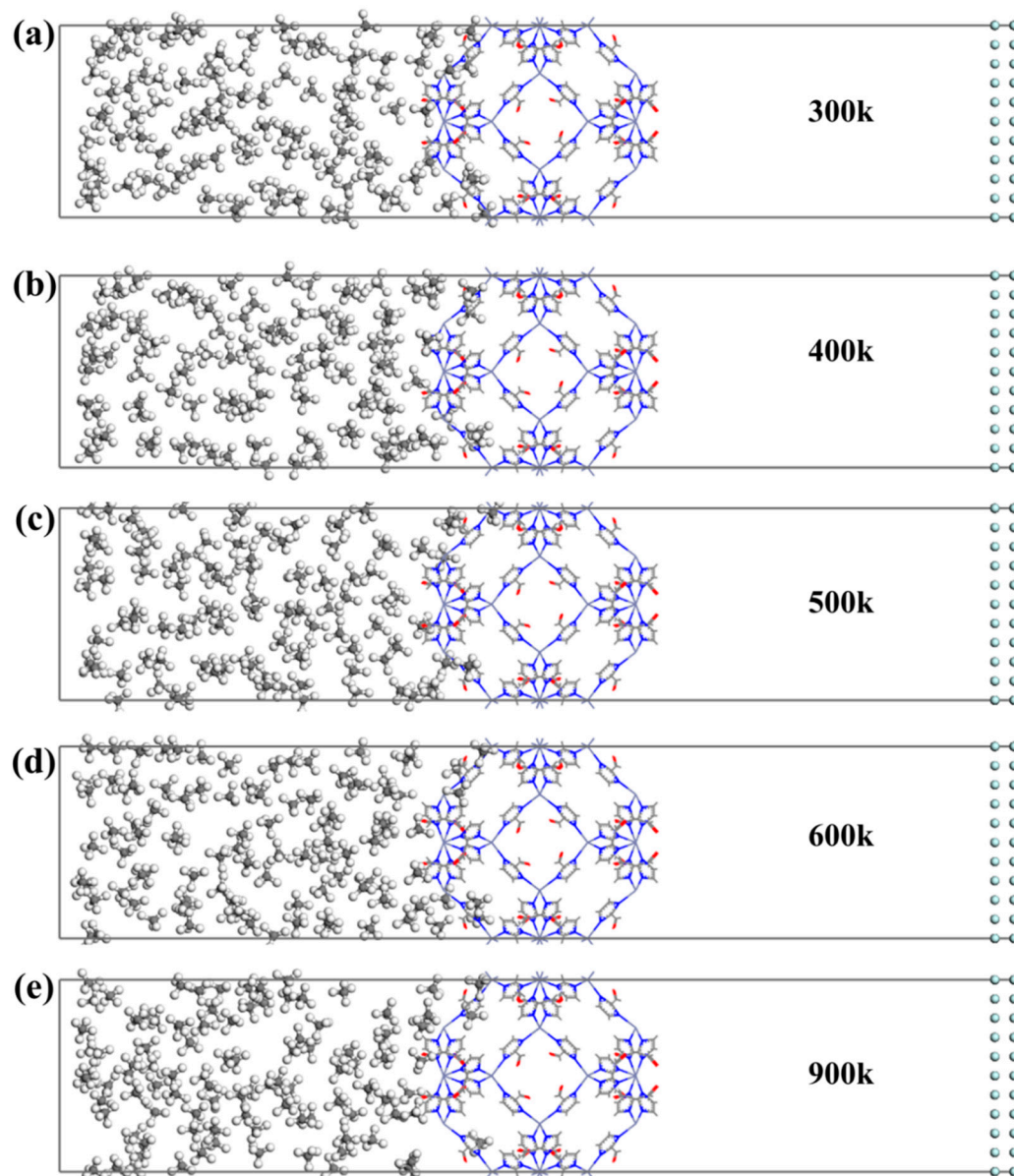


Figure S3. Final state simulation snapshots of CH₄ molecules permeating through the ZIF-90 membrane at (a) 300K, (b) 400K, (c) 500K, (d) 600K, (e) 900K temperatures for 5 ns.

(4) 200 H₂O molecules

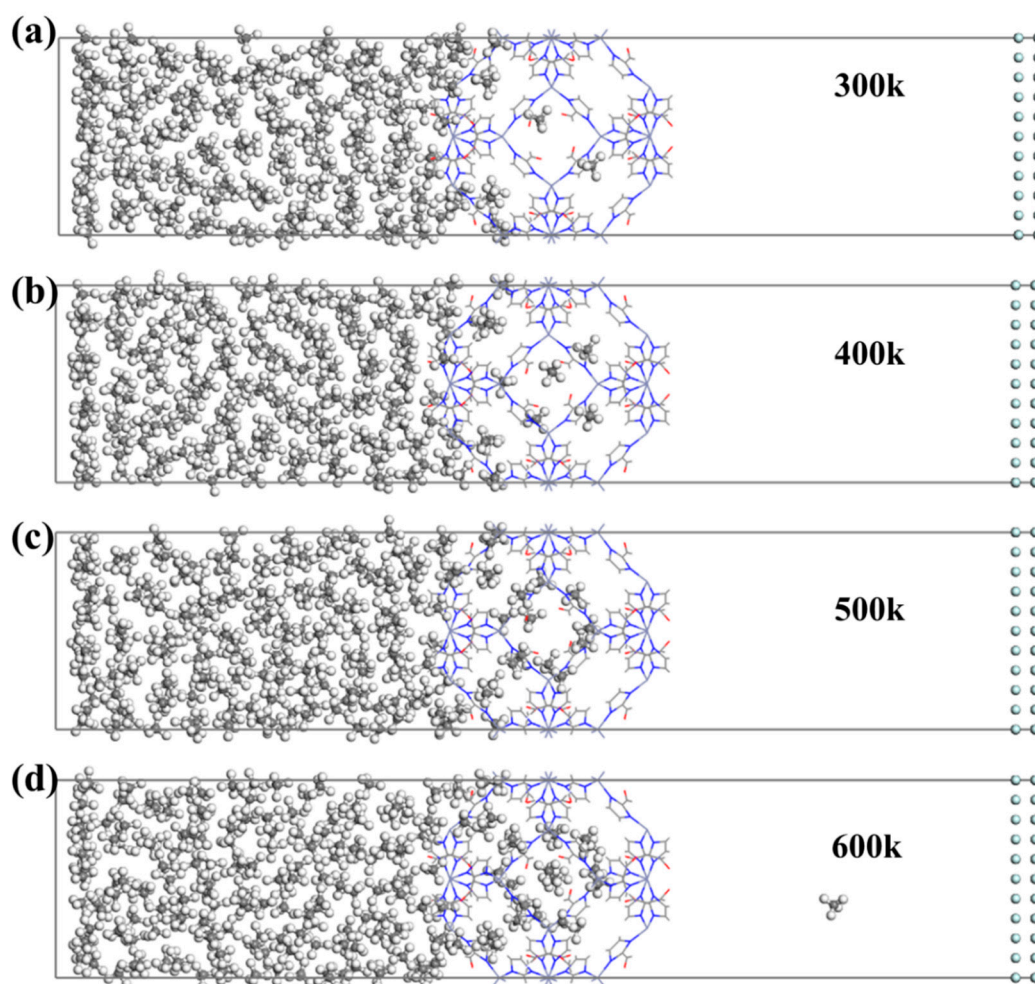


Figure S4. Final state simulation snapshots of CH₄ molecules permeating through the ZIF-90 membrane at (a) 300K, (b) 400K, (c) 500K, (d) 600K for 5 ns.