# Supporting Information

## Seawater Pervaporation through Zeolitic Imidazolate Framework Membranes: Atomistic Simulation Study

Krishna M. Gupta, Zhiwei Qiao, Kang Zhang, and Jianwen Jiang*

Department of Chemical and Biomolecular Engineering, National University of Singapore, 117576, Singapore

*E-mail: chejj@nus.edu.sg

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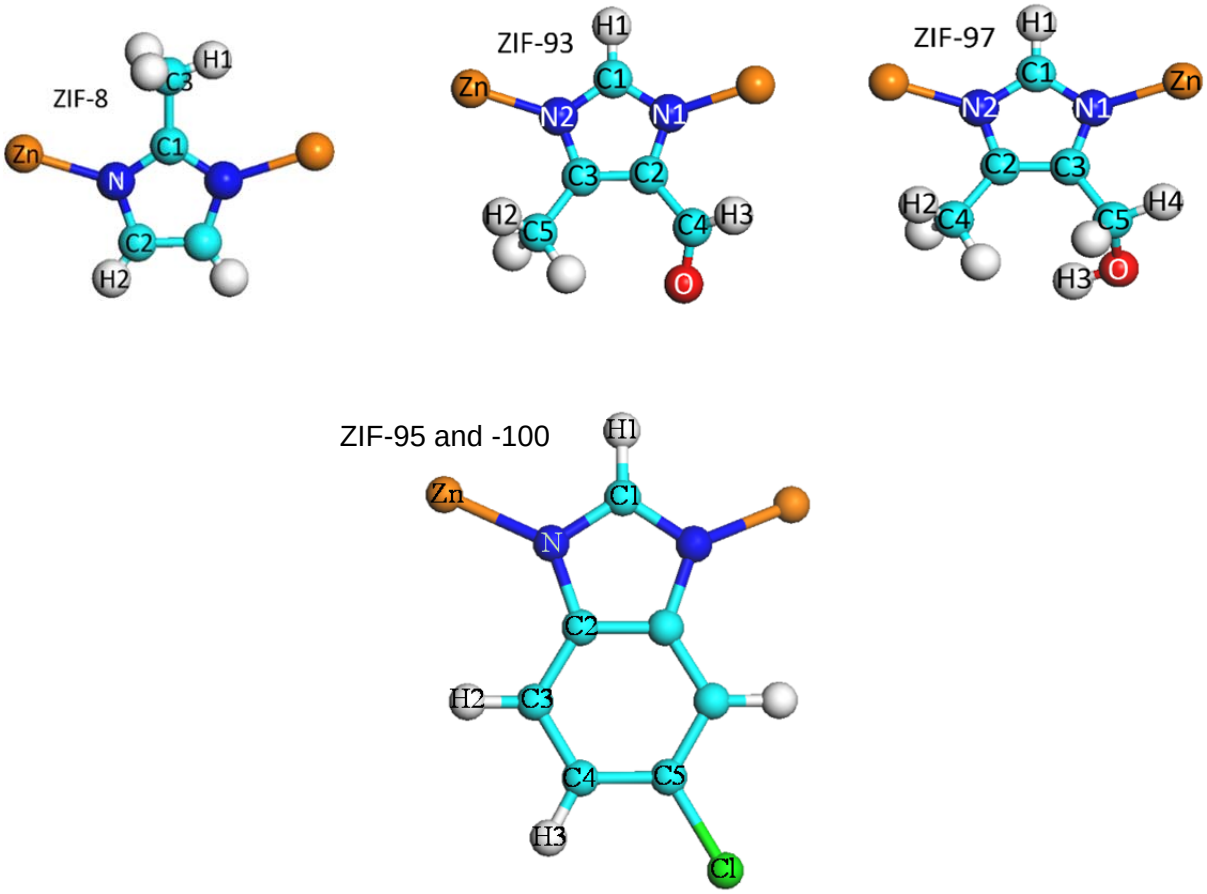


**Figure S1.** Fragmental clusters of ZIF-8, -93, -95, -97 and -100.

**Table S1**. Force field parameters of ZIF-8, -93, -95, -97 and -100.

| Atom | $\sigma$ (Å) | $\varepsilon/k_B$ (K) |
|---|---|---|
| Zn | 2.462 | 62.343 |
| N | 3.260 | 34.690 |
| C | 3.431 | 52.790 |
| Cl | 3.516 | 114.237 |
| O | 3.118 | 30.166 |
| H | 2.571 | 22.122 |

**Table S2.** Atomic charges of ZIF-8, -93, -95, -97 and -100.

| ZIF-8 | |
|---|---|
| Atom | Charge (*e*) |
| Zn | 1.0219 |
| N | –0. 4973 |
| C1 | 0. 4958 |
| C2 | 0. 0672 |
| C3 | –0. 2720 |
| H1 | 0.0632 |
| H2 | 0.1023 |

| ZIF-93 | |
|---|---|
| Atom | Charge (*e*) |
| Zn | 0.8187 |
| N1 | –0.2730 |
| N2 | –0.4166 |
| O | –0.6438 |
| C1 | 0.0608 |
| C2 | –0.2380 |
| C3 | 0.3703 |
| C4 | 0.5930 |
| C5 | –0.3476 |
| H1 | 0.2270 |
| H2 | 0.0824 |
| H3 | 0.0112 |

| ZIF-97 | |
|---|---|
| Atom | Charge (*e*) |
| Zn | 0.7797 |
| N1 | –0.3800 |
| N2 | –0.2654 |
| O | –0.6790 |
| C1 | –0.0008 |
| C2 | 0.0700 |
| C3 | –0.0024 |
| C4 | –0.1805 |
| C5 | 0.2866 |
| H1 | 0.1882 |
| H2 | 0.0592 |
| H3 | 0.3927 |
| H4 | 0.0011 |

| ZIF-95 | |
|---|---|
| Atom | Charge (*e*) |
| Zn | 0.9390 |
| N | –0.4560 |
| C1 | 0.3180 |
| C2 | 0.1524 |
| C3 | –0.2333 |
| C4 | –0.0520 |
| C5 | 0.2503 |
| H1 | 0.0080 |
| H2 | 0.1283 |
| H3 | 0.0902 |
| Cl | –0.2667 |

| ZIF-100 | |
|---|---|
| Atom | Charge (*e*) |
| Zn | 1.0082 |
| N | –0. 5230 |
| C1 | 0. 3102 |
| C2 | 0. 2779 |
| C3 | –0. 3377 |
| C4 | –0. 0643 |
| C5 | 0. 2482 |
| H1 | 0.0509 |
| H2 | 0.1311 |
| H3 | 0.1067 |
| Cl | –0. 2653 |

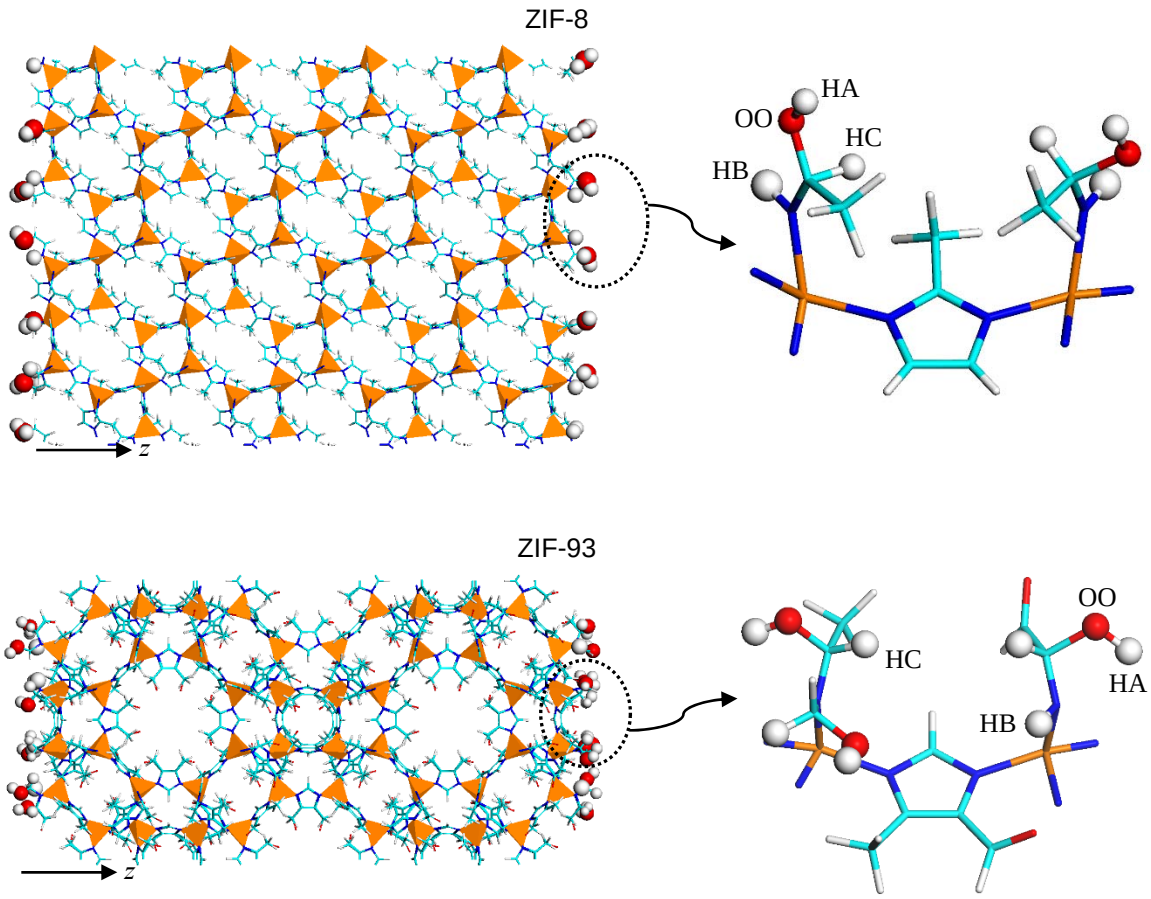


**Figure S2.** Saturated surface dangling bonds of ZIF-8 and ZIF-93.

**Table S3.** Charges of surface dangling atoms in Figure S2.

| ZIF-8 | |
|---|---|
| Atom | Charge (*e*) |
| OO | –0.7590 |
| HA | 0.3127 |
| HB | 0.2082 |
| HC | 0.0672 |

| ZIF-93 | |
|---|---|
| Atom | Charge (*e*) |
| OO | –0.6877 |
| HA | 0.3840 |
| HB | 0.2795 |
| HC | 0.0936 |

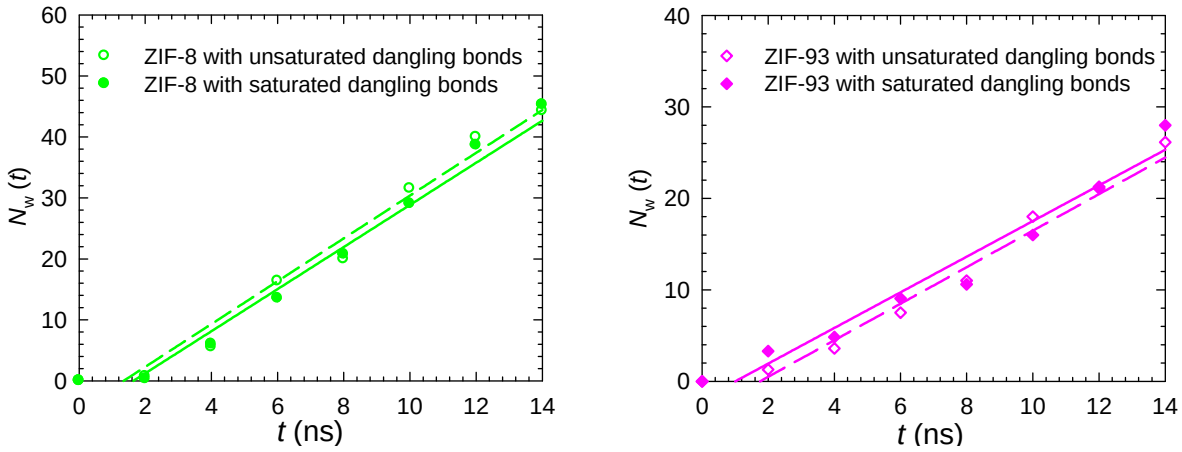


**Figure S3.** Numbers of water molecules passing through ZIF-8 and ZIF-93 membranes with saturated and unsaturated surface dangling bonds. The lines are fitted to the data points.

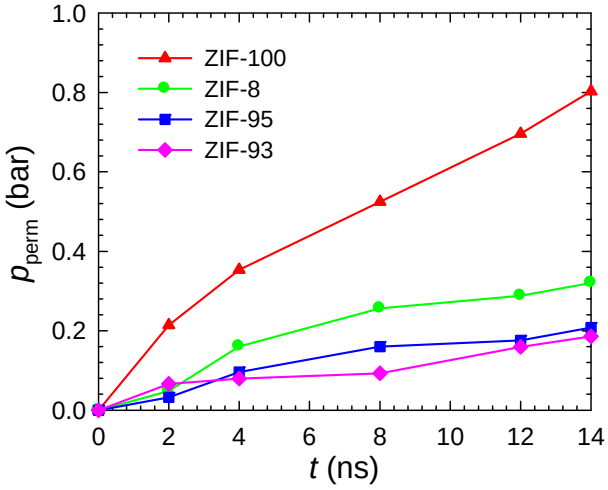


**Figure S4.** Permeate pressure versus simulation time.