

Atomistic Simulations of Biofouling and Molecular Transfer of Crosslinked Aromatic Polyamide Membrane for Desalination

Md Symon Jahan Sajib¹, Ying Wei², Ankit Mishra³, Lin Zhang⁴, Ken-ichi Nomura^{3,5}

Rajiv K. Kalia^{3,5,6,7}, Priya Vashishta^{3,5,6,7}, Aiichiro Nakano^{3,5,6,7,8}, Sohail Murad^{9*}, Tao Wei^{1*}*

1. Chemical Engineering Department, Howard University, 2366 Sixth Street NW, Washington, D.C., 20059, United States

2. School of Information Science and Technology, Xiamen University, Tan Kah Kee College, 422 Siming South Road, Zhangzhou, Fujian, 363105, China

3. Mork Family Department of Chemical Engineering & Materials Science, University of Southern California, 925 Bloom Walk, HED 216, Los Angeles, CA 90007, United States

4. Engineering Research Center of Membrane and Water Treatment of MOE, College of Chemical and Biological Engineering, Zhejiang University, 38 Zhe Da Road, Hangzhou, 310027, China

5. Collaboratory for Advanced Computing and Simulations, University of Southern California, 3651 Watt Way, VHE 608, Los Angeles, CA 90089, United States

6. Department of Physics & Astronomy, University of Southern California, 825 Bloom Walk, ACB 439, Los Angeles, CA 90089, United States

7. Department of Computer Science, University of Southern California, 941 Bloom Walk, Los Angeles, CA 90089, United States

8. Department of Biological Sciences, University of Southern California, 3616 Trousdale Parkway, AHF 107, Los Angeles, California, 90089, USA

9. Department of Chemical Engineering, Illinois Institute of Technology, 10 West 35th Street, Chicago, IL 60616, United States

KEYWORDS: Atomistic Simulations, Polyamide Membrane, Desalination, Nonequilibrium, Steady-State, Biofouling

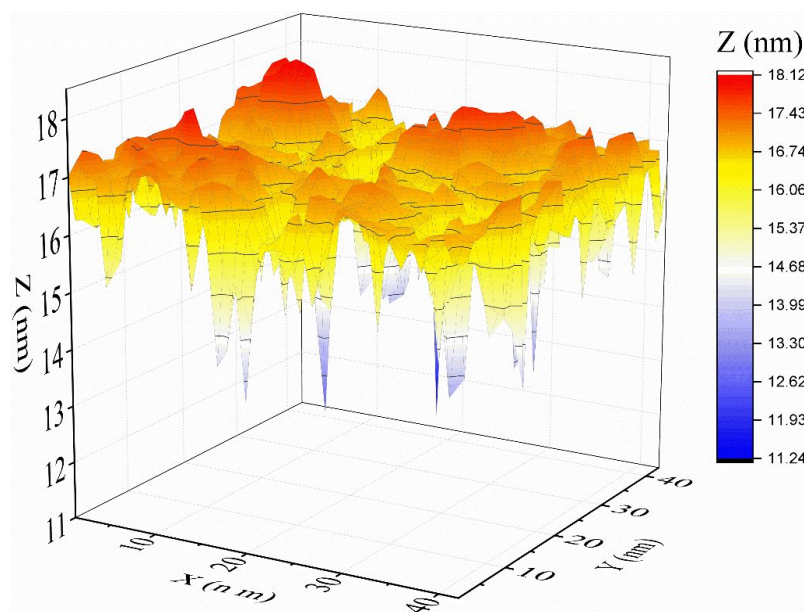


Figure S1: The interface of the PA membrane. To define a membrane top surface, the system is divided into grids with the resolution of $0.2 \times 0.2 \text{ nm}^2$ in the X-Y plane and atoms of the largest value in the Z-axis are selected as top atoms to define the membrane surface.

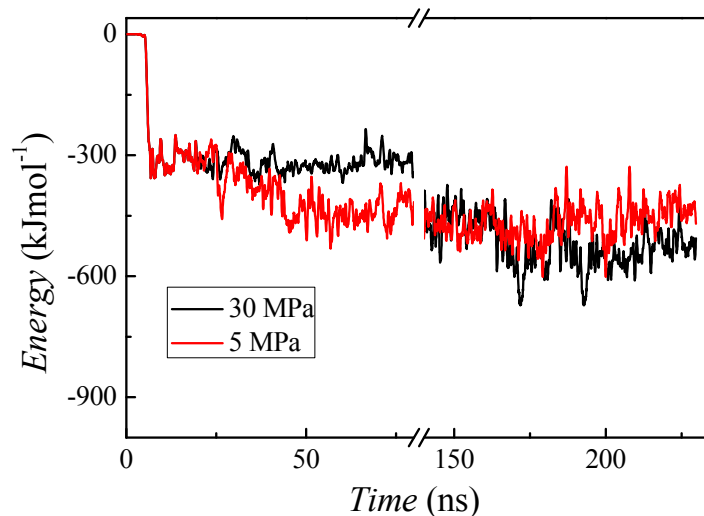


Figure S2: Interaction energy (i.e., the sum of the Lennard-Jones and electrostatic energies) of protein and membrane Surface.

From the estimated interaction energy, when the protein from the bulk got attached on the surface at around 5.5 ns, an increase amount of interaction between the polymer membrane and protein was recorded. The change in interaction energies for 30 MPa over the 230 ns of simulation was larger than the lower pressure case, which also explains the greater secondary structural changes of protein for 30 MPa case.

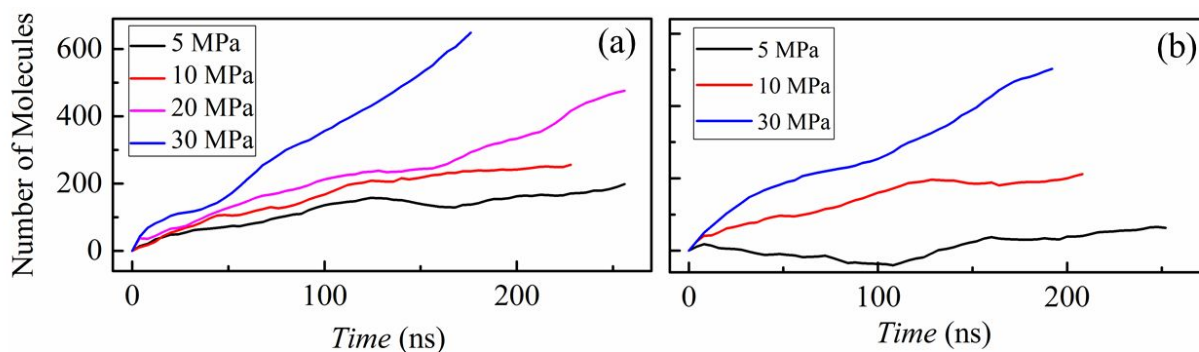


Figure S3: Net molecule number of waters passed through membrane for different pressure a) Without Protein attachment b) with protein attachment

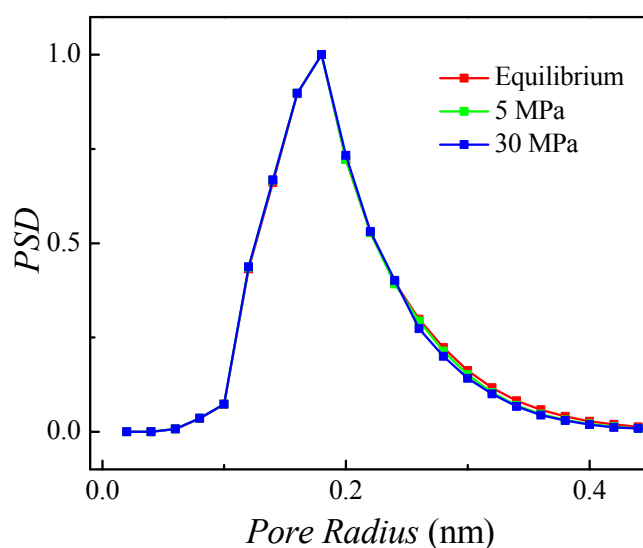


Figure S4: Pore size distribution of PA membrane at $\Delta P = 5$ MPa, 30 MPa and equilibrium. Pore size distribution was measured using the Monte Carlo approach¹.

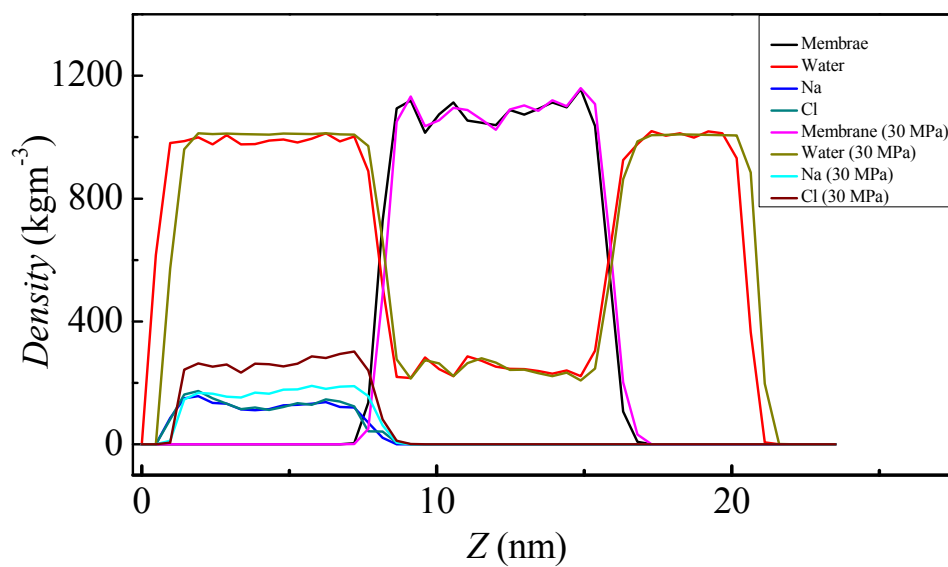


Figure S5: Density distribution at $\Delta P = 30$ MPa without the addition of protein.

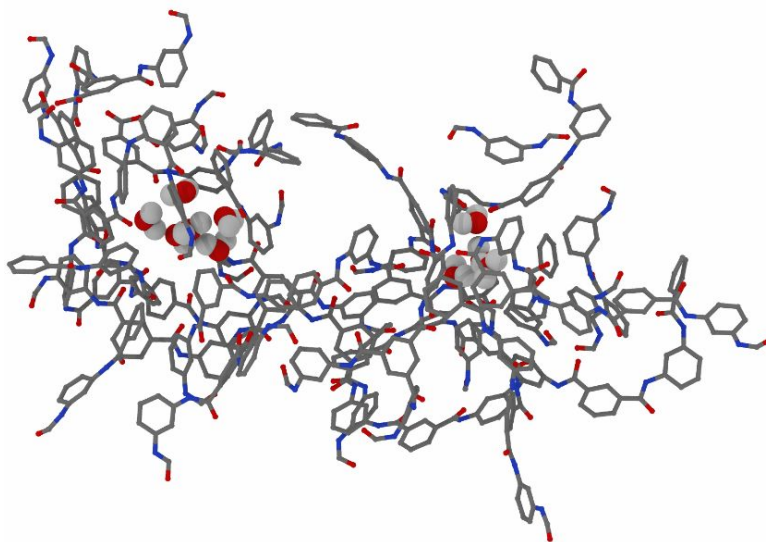


Figure S6: Water molecules shown in red & white are shown trapped around PA membrane in cage-like structure. The membrane fragments are drawn with water molecules in the center and marking all the membrane fragments within 6 Å.

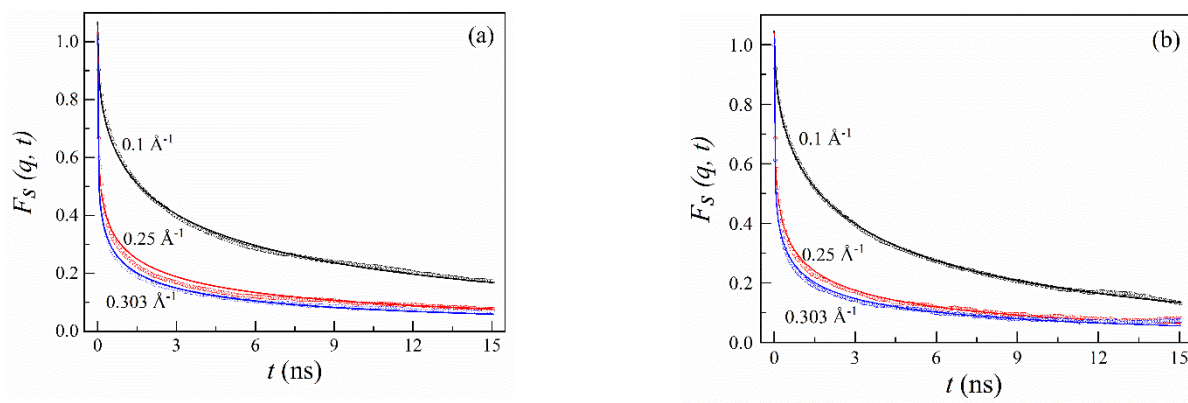


Figure S7. The comparison of the original simulation data (circle symbols) and the curve fitting data (line) of self-intermediate scattering function $F_s(k, t)$ of oxygen atoms of water molecules inside the membrane at wavenumbers $k = 0.1, 0.25$ and 0.303 Å^{-1} for the membrane at the equilibrium condition (a) and the nonequilibrium with $\Delta P = 0.5 \text{ MPa}$ (b). The fitting parameters are listed in Table 1.

REFERENCES

1. Wei, T.; Zhang, L.; Zhao, H.; Ma, H.; Sajib, M. S. J.; Jiang, H.; Murad, S. Aromatic polyamide reverse-osmosis membrane: An atomistic molecular dynamics simulation. *The Journal of Physical Chemistry B* **2016**, *120* (39), 10311-10318.