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Molecular dynamics simulations in membrane material design for desalination

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Motivation

- Next-generation membranes require molecular-level design to achieve high selectivity and permeability.
- The composition-structure-property-performance relations of membrane materials can be built using molecular dynamics (MD) simulations, which can contribute to not only the fundamental understanding but also the tailored design of advanced membrane materials.
- Computation acceleration schemes and coarse-graining techniques has enabled the simulations of complex systems and processes involving vaporization.

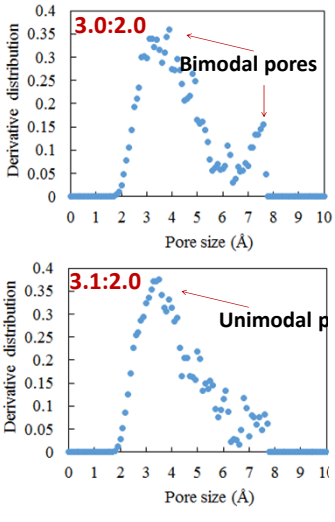
Polyamide thin films in RO membranes

- Despite the experimental effort in improving the performance of polyamide (PA) thin-film composite (TFC) membranes, the fundamental understanding of membrane structure and transport has been largely empirical.
- Atomic compositions under various MPD/TMC ratios

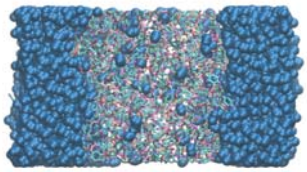
	2.8:2.0	2.9:2.0	3.0:2.0	3.1:2.0	[b] RMS data
COOH%	1.05	0.58	0.29	0.14	0.41-0.71
O/N	1.16	1.08	1.02	0.98	1.00-1.12
[a] DC%	91.95	94.29	95.40	94.78	94.1-96.2

[a] Degree of cross-linking
[b] data from Karan *et al.*, *Science* 2015

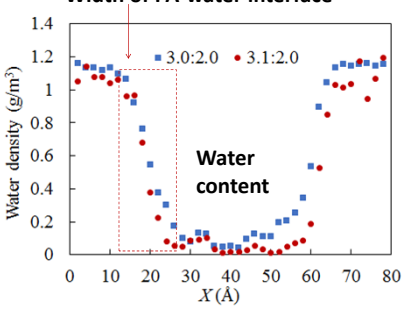
- Dry PA structures



- Hydrated PA structures

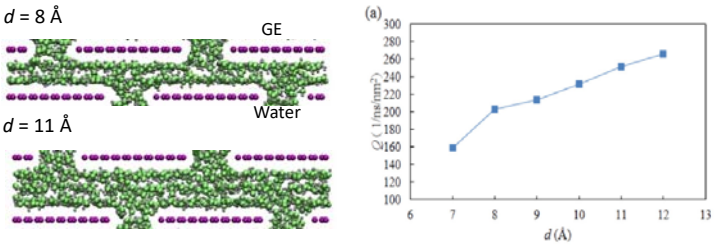


Width of PA-water interface

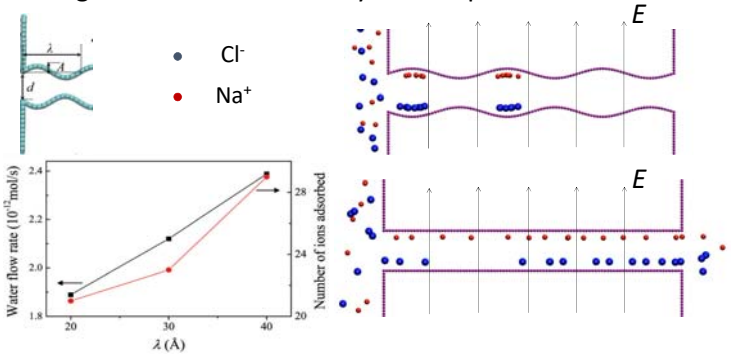


Graphene structure design for desalination

- Effect of graphene (GE) interlayer spacing on water flux in pressure-driven desalination.

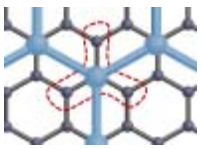


- Corrugated structure of GE layer for capacitive deionization

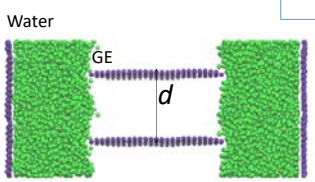


Coarse-grained MD for membrane distillation

- Simulating evaporation process and obtaining statistical results in all-atom (AA) MD is time consuming.
- Coarse-grained (CG) approach to save computational cost



	CPU time (hour)
AA-MD	3820.6±32.5
CG-MD	336.5±5.7



- A transition from surface diffusion-dominated transport to activated Knudsen transport occurs at d = 30 Å.