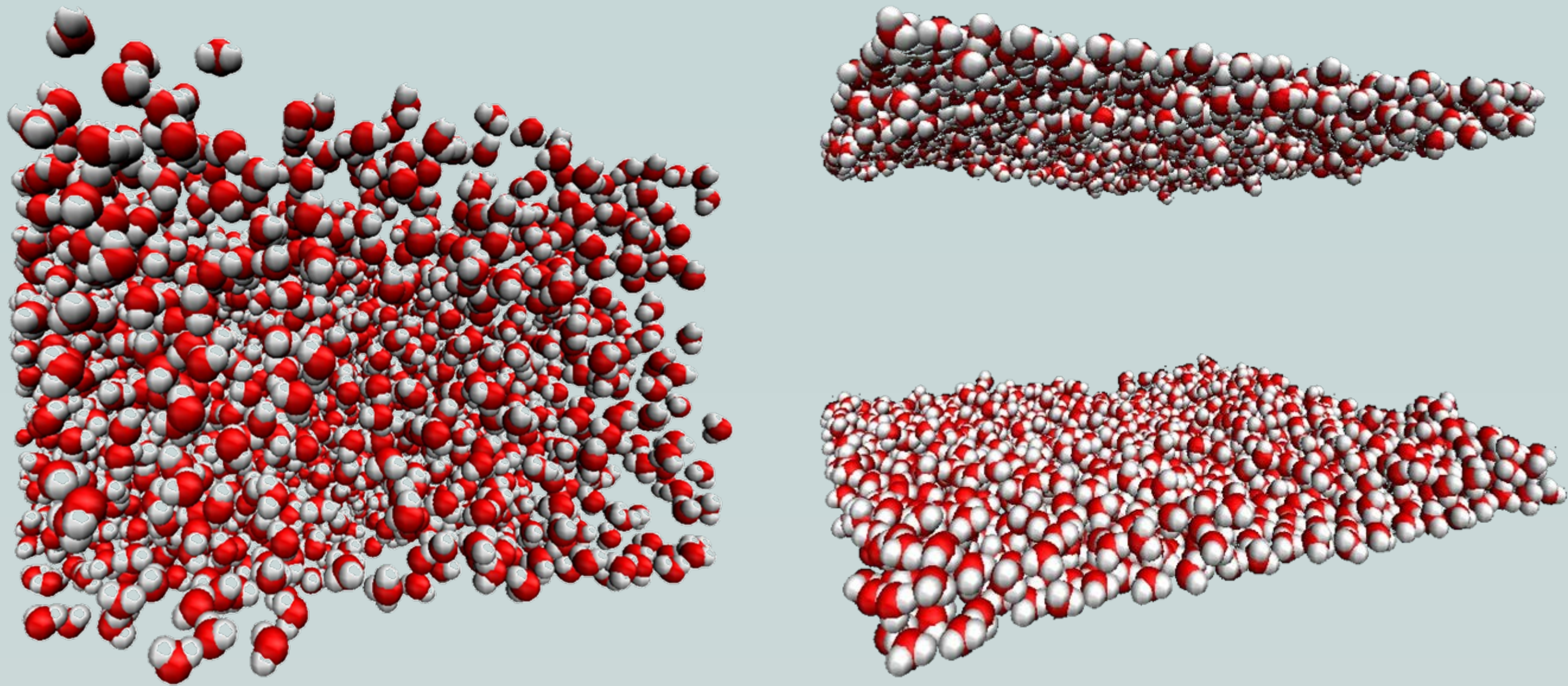


Simulations of confined water under electric field & Water purification with tip-charged carbon nanotubes

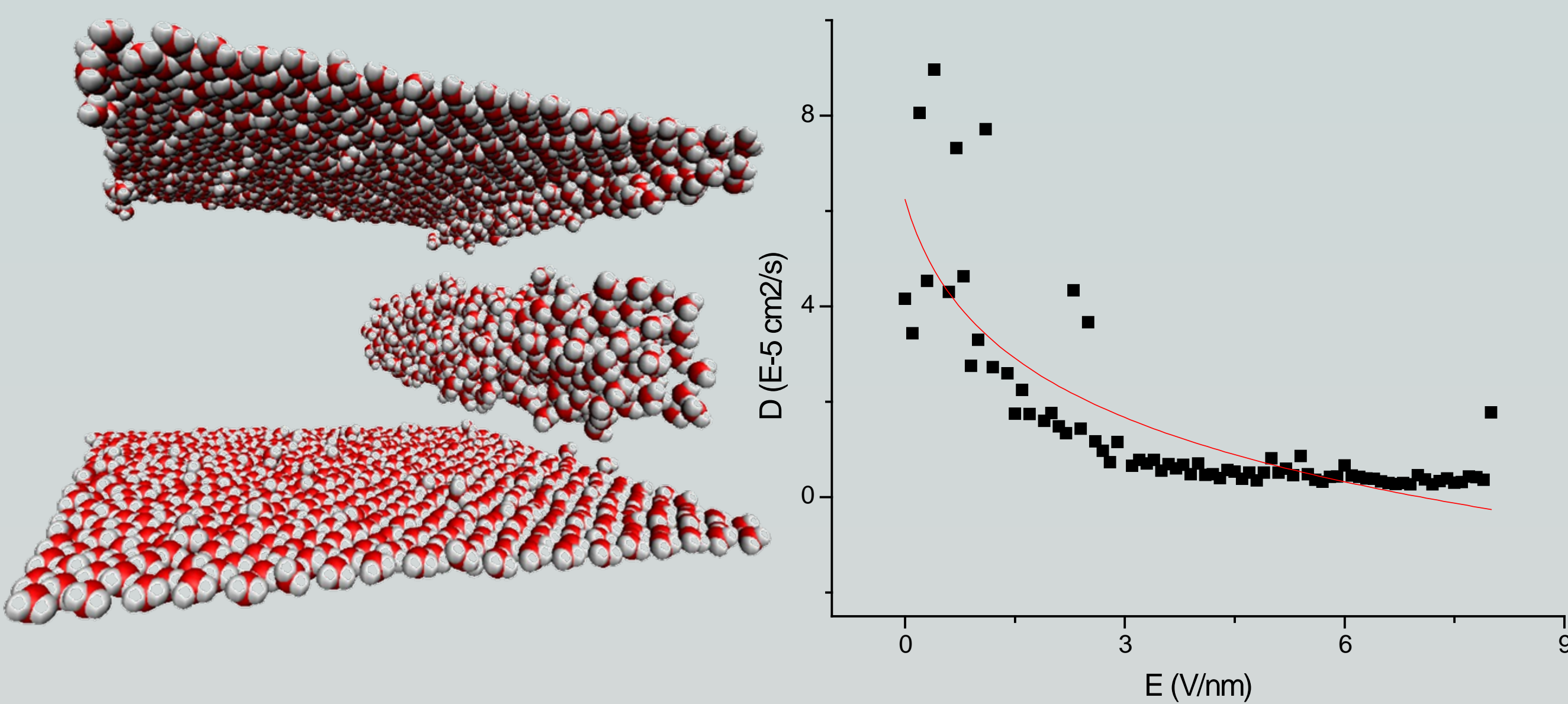
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The behavior of confined water is very different from that of the bulk one[1]. And the investigation into it has a big meaning for the understanding of anomalous behavior of water. In our job, we apply electric field on the randomly distributed water molecules between two graphene sheets, and find a phase transition from water to ice, and a water column under high electric field.



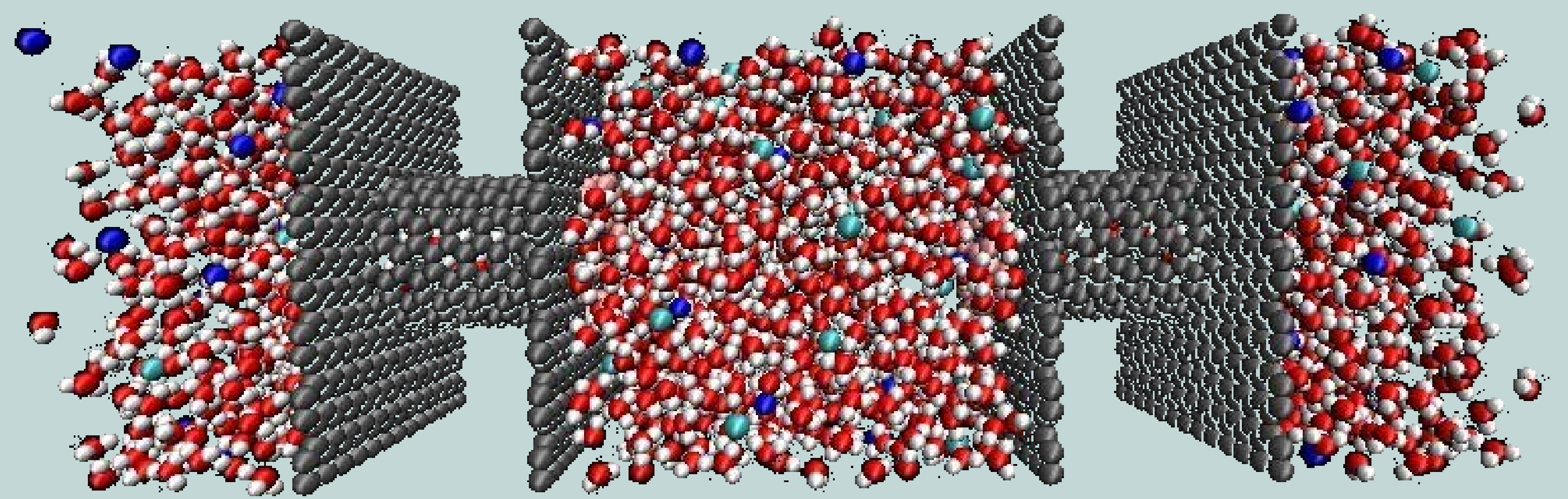
Initial state: randomly distributed. $E=1\text{V/nm}$, and water molecules distribute mainly along the two sheets in lower order.



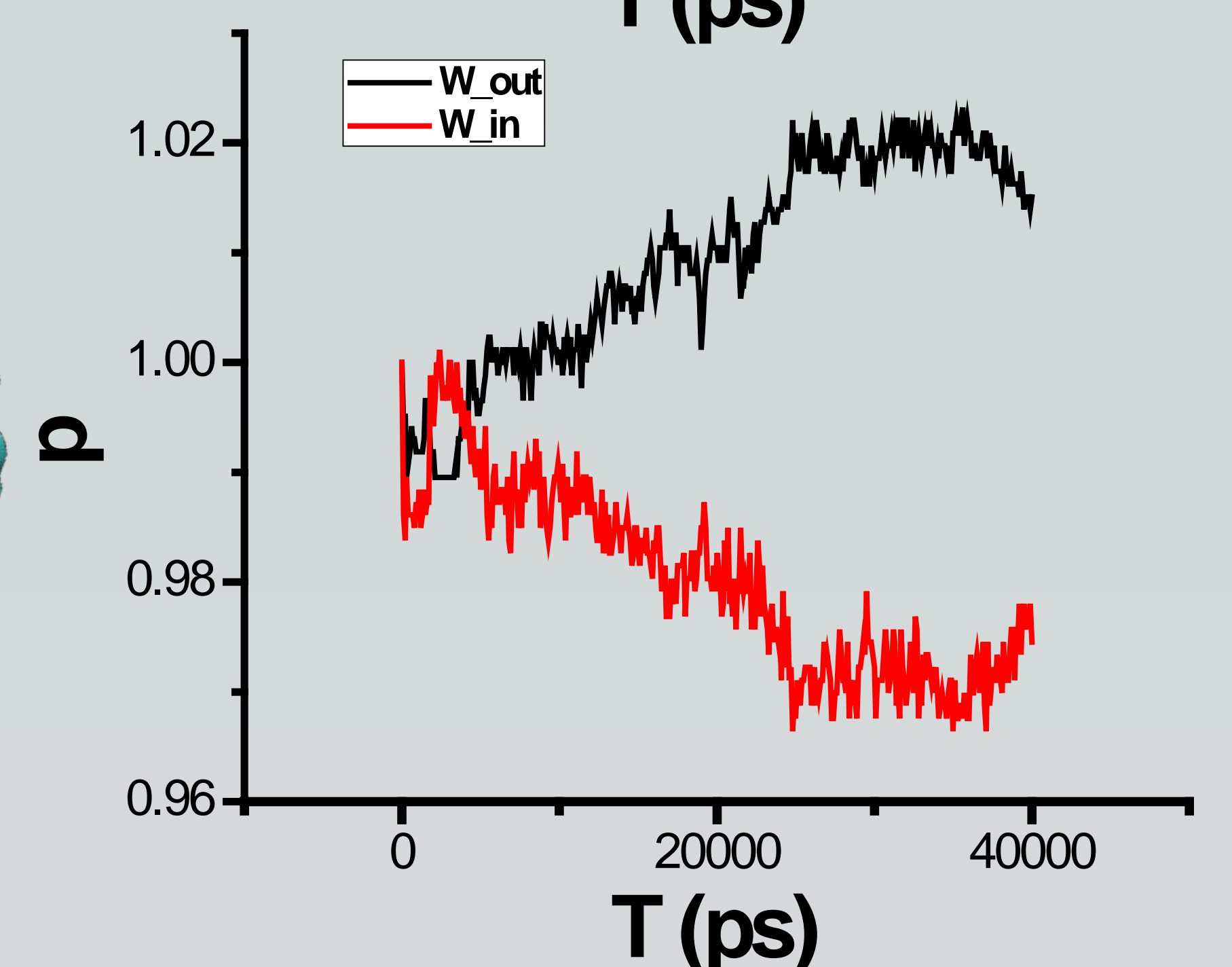
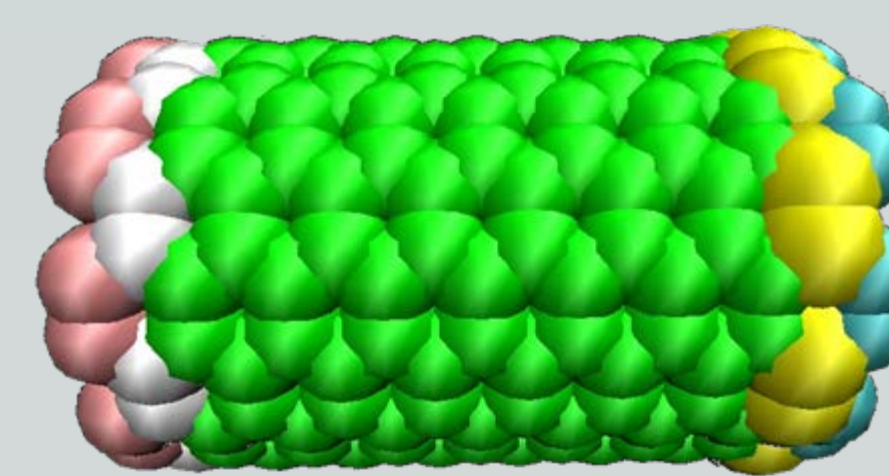
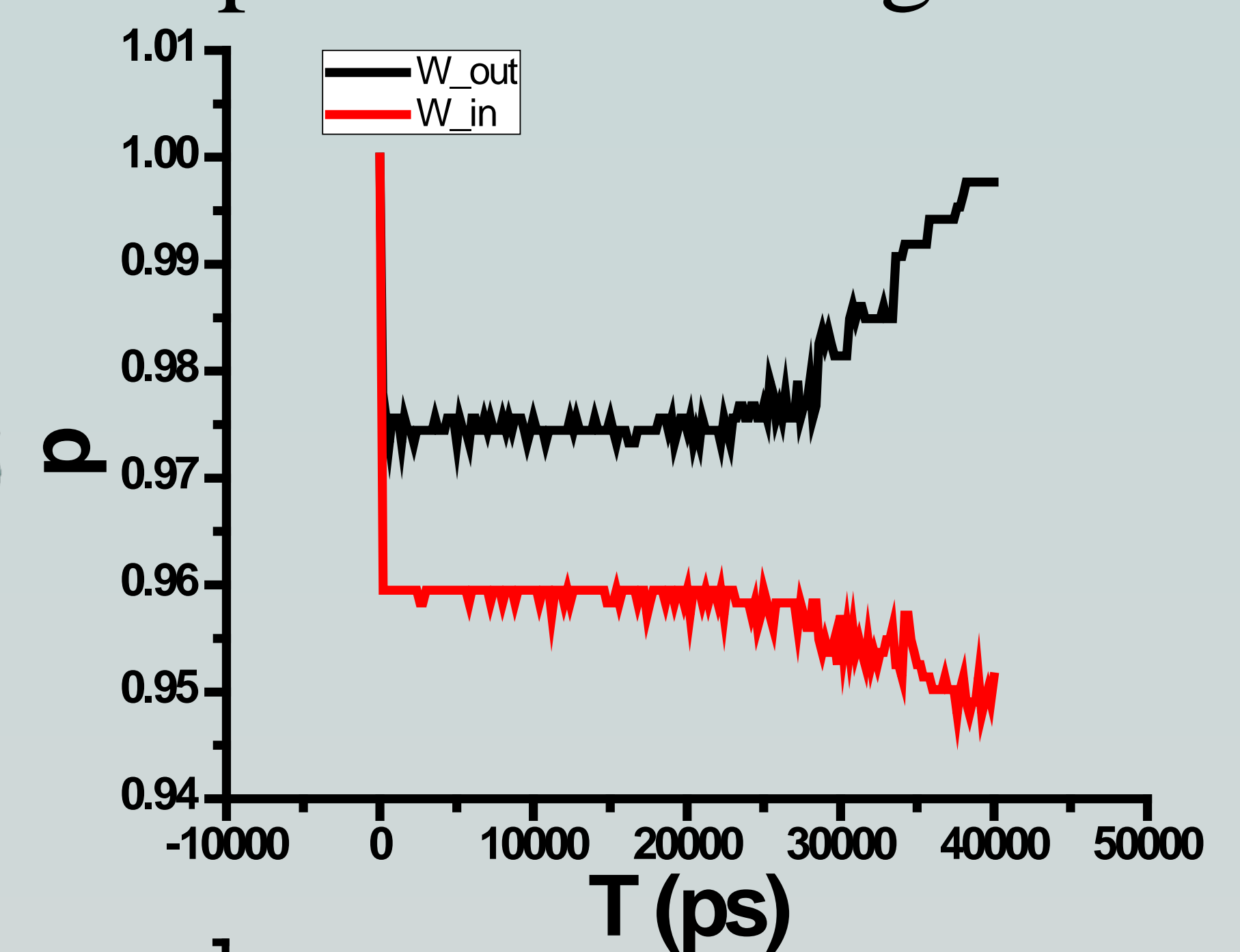
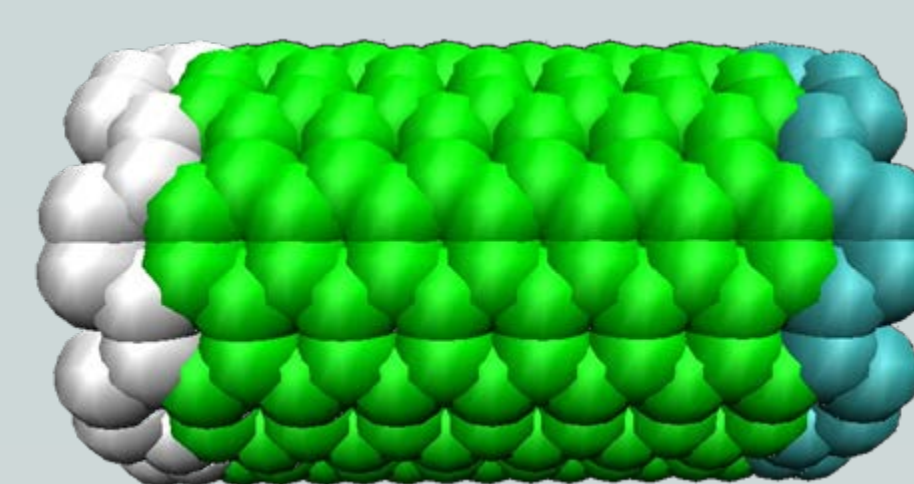
$E=8\text{V/nm}$, monolayer ice and a water column formed.

Diffusion coefficients of water molecules decrease with increasing electric field.

Extract water from sea water is an important project due to the lack of pure water on the earth[2]. The study of desalination with MD simulations has a wide applications for engineering and agriculture field.



In our job, based on the job before[3], we imposed charges on the tips of nanotubes instead of hydrophobic or hydrophilic molecules, with $1e/\text{atom}$ and $0.001e/\text{atom}$ on the outside and inside respectively. And another design with positive and negative on both sides.



Two types of carbon nanotubes

The difference of water density in two boxes. With less charge, water molecules can pass more easily. And because of the neutral property of the 2nd type, ions will not prevent the effective passages of water.

Reference:

- 1, R. Zangi et al, Physical review letters 2003, 91, 025502
- 2, R. F. Service, Science 2006, 313, 1088
- 3, Q. W. Chen et al, Small 2011, 7, 2225