WORK REPORT

DYNAMIC BEHAVIORS OF WATER CONFINED IN GRAPHENE FLAKES

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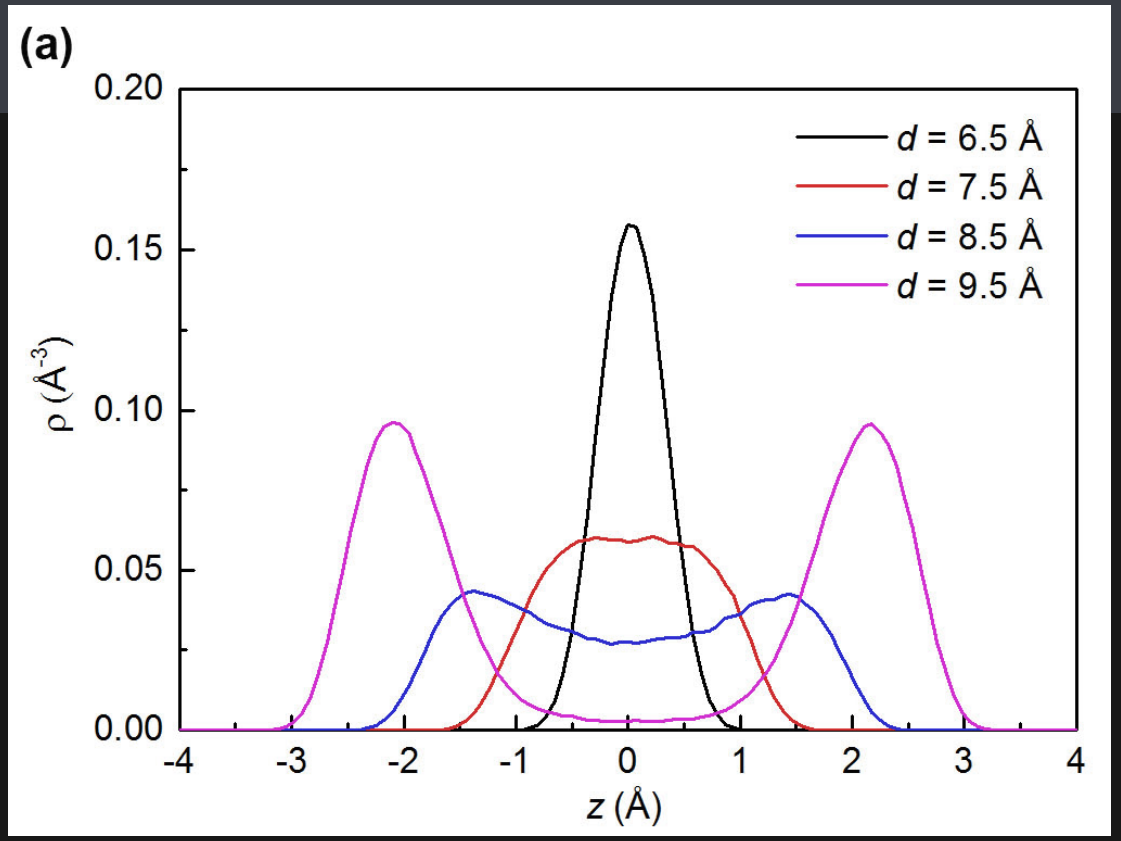
CATALOG

- Overview
- ΔZ=9.5 Å: Mechanism of Interlayer Water Transition
- ΔZ=6.5- 7.5 Å: Dynamics of Water Clusters& Nucleation
- Challenges and Prospects

OVERVIEW

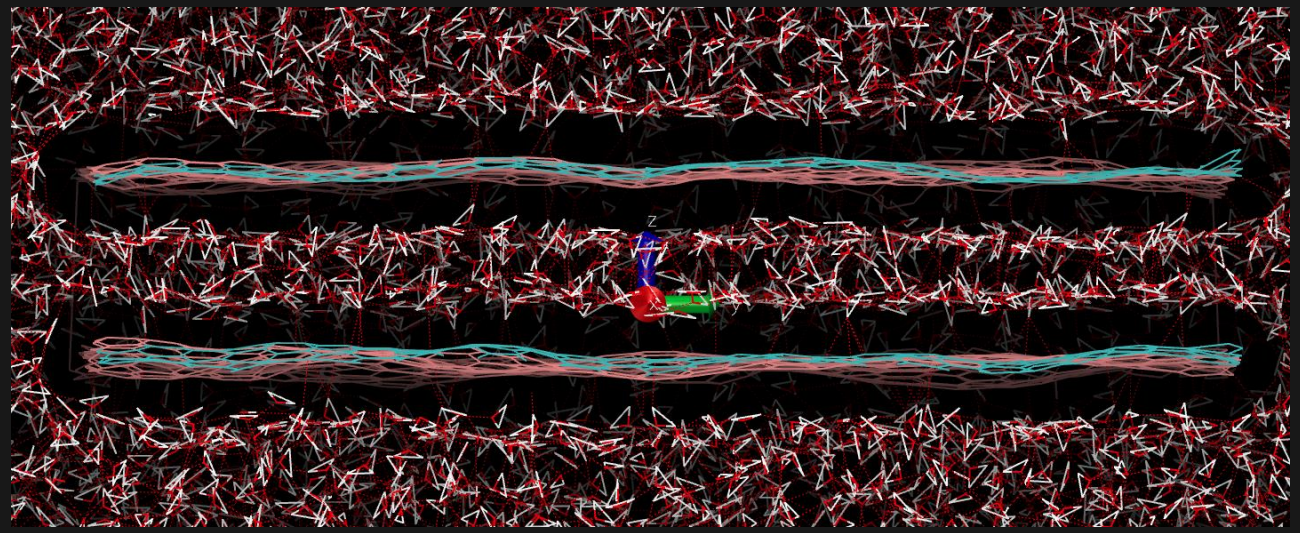
- When tuning the interlayer spacing, we observed that confined water formed different layer structures after saturation.



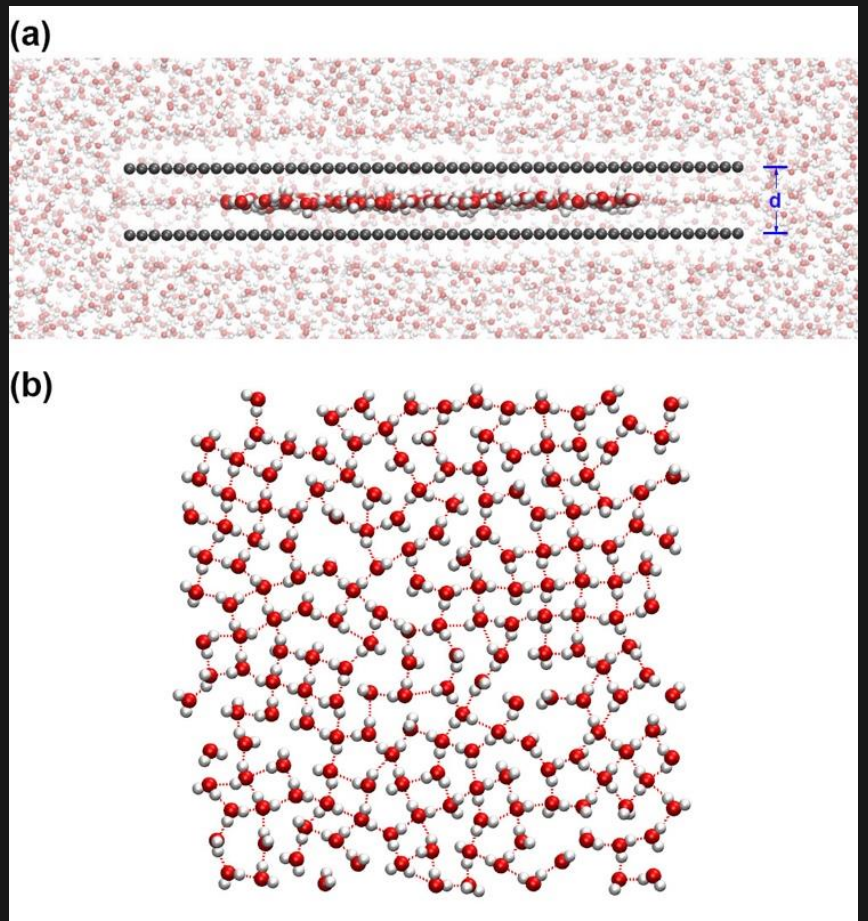
Density Distribution along Z axis.

OVERVIEW

- ΔZ=9.5 Å

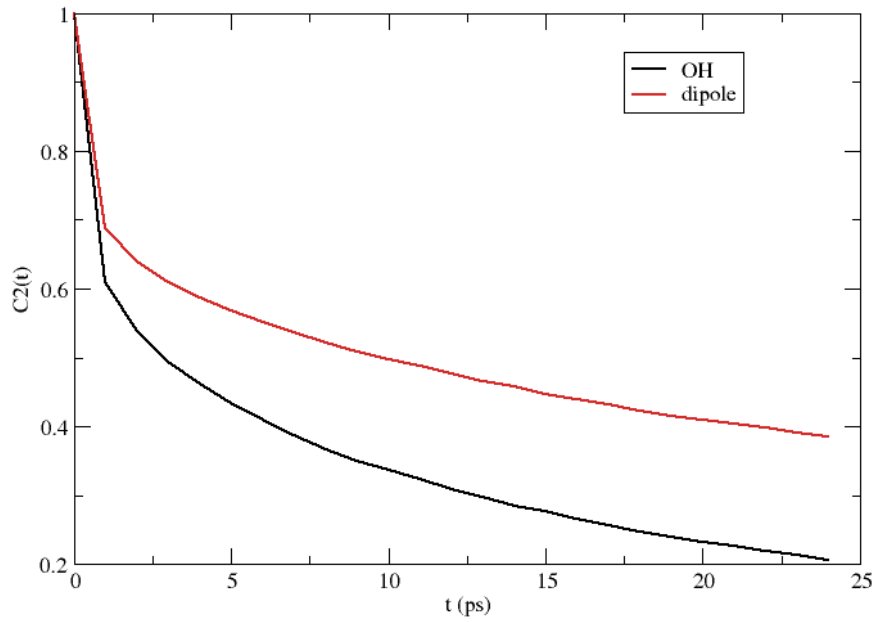


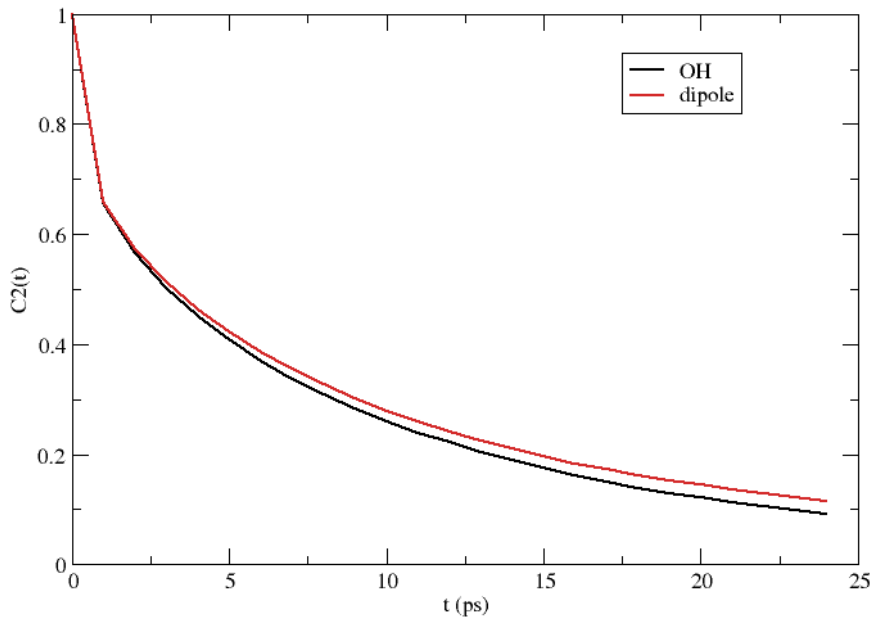
- ΔZ=6.5 Å



ANISOTROPIC ROTATIONAL RELAXATION: OH& DIPOLE

$$C_2(t) = < P_2[\mu_{OH}(0) \cdot \mu_{OH}(t)] >$$

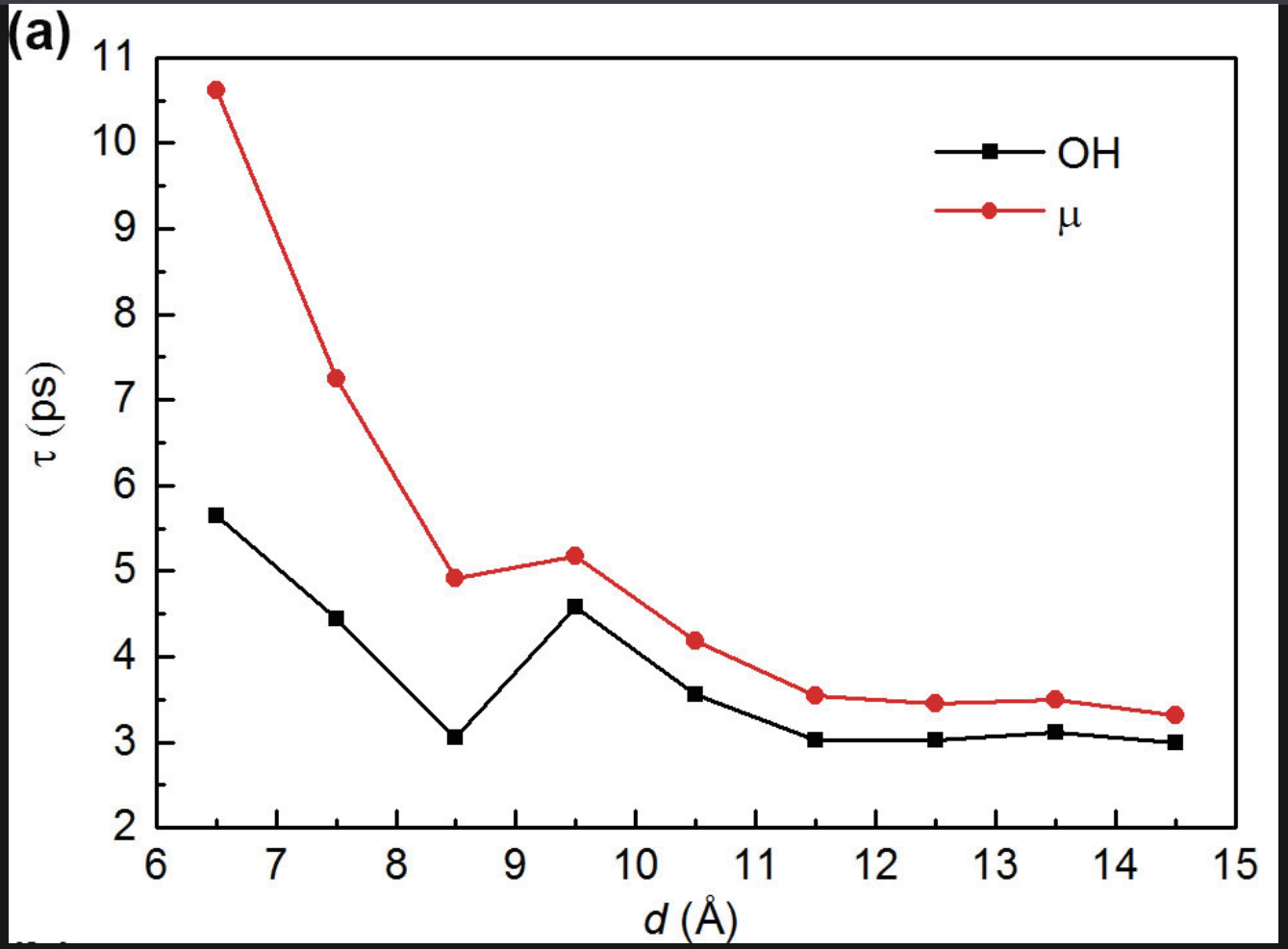




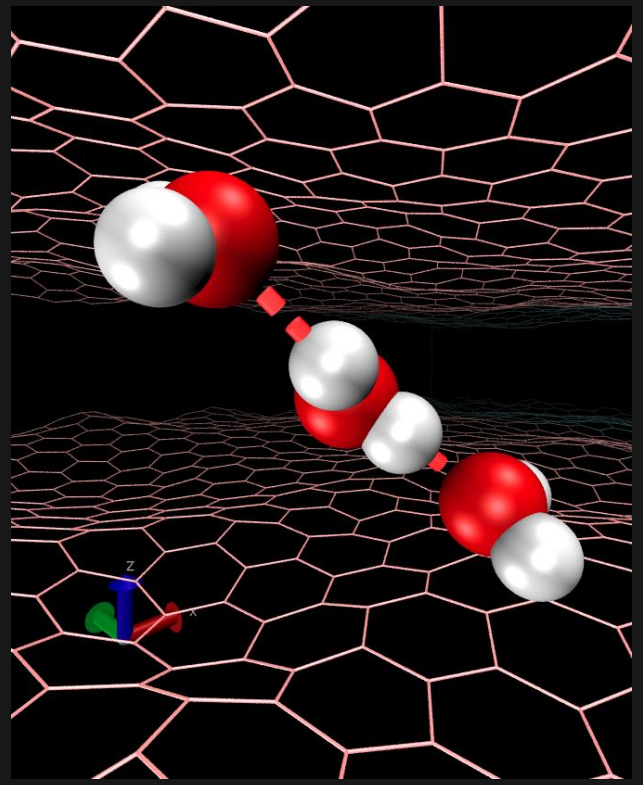
ΔZ = 6.5 angstrom

ΔZ = 14.5 angstrom

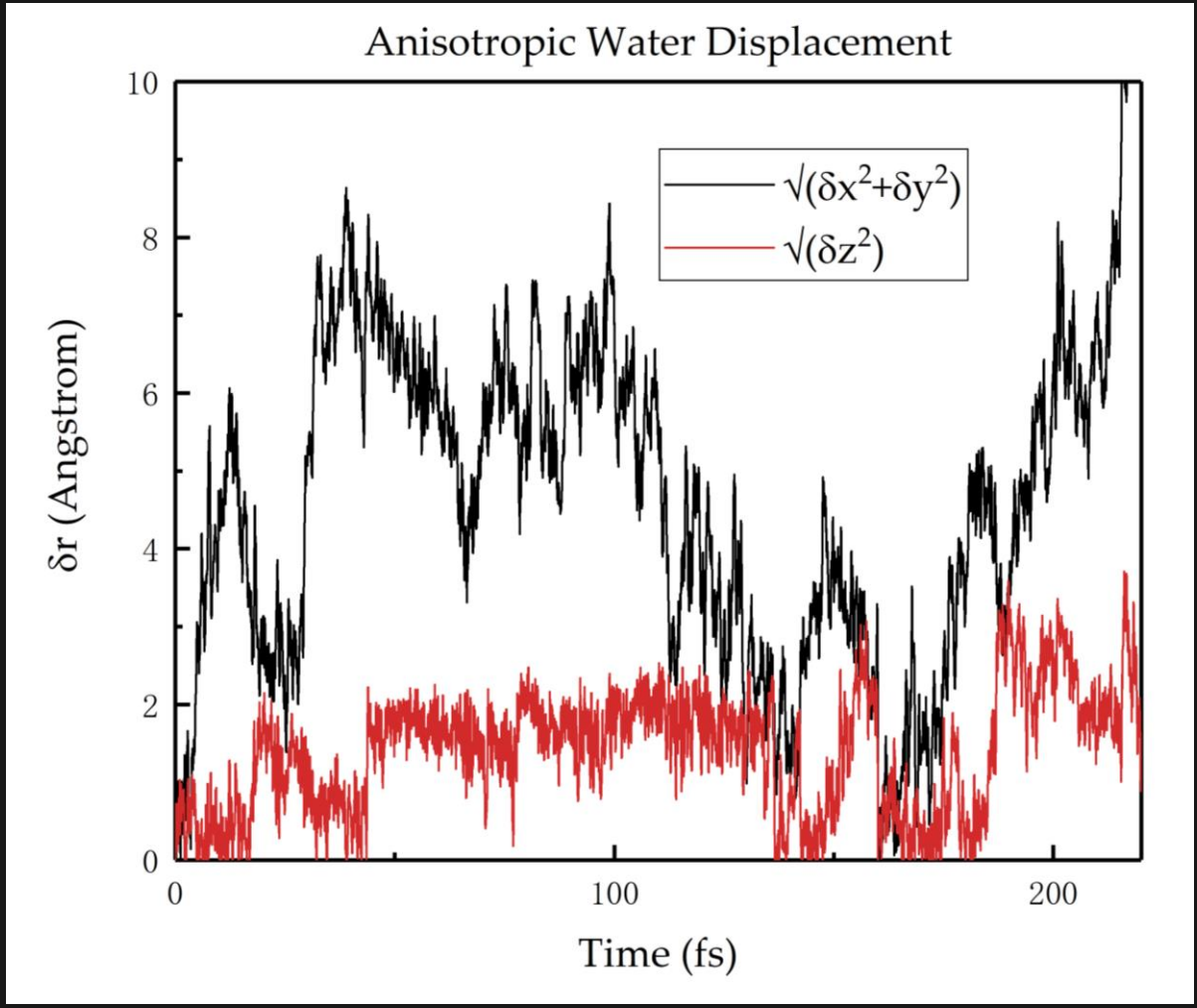
ANISOTROPIC ROTATIONAL RELAXATION: OH& DIPOLE



MECHANISM OF INTERLAYER WATER TRANSITION

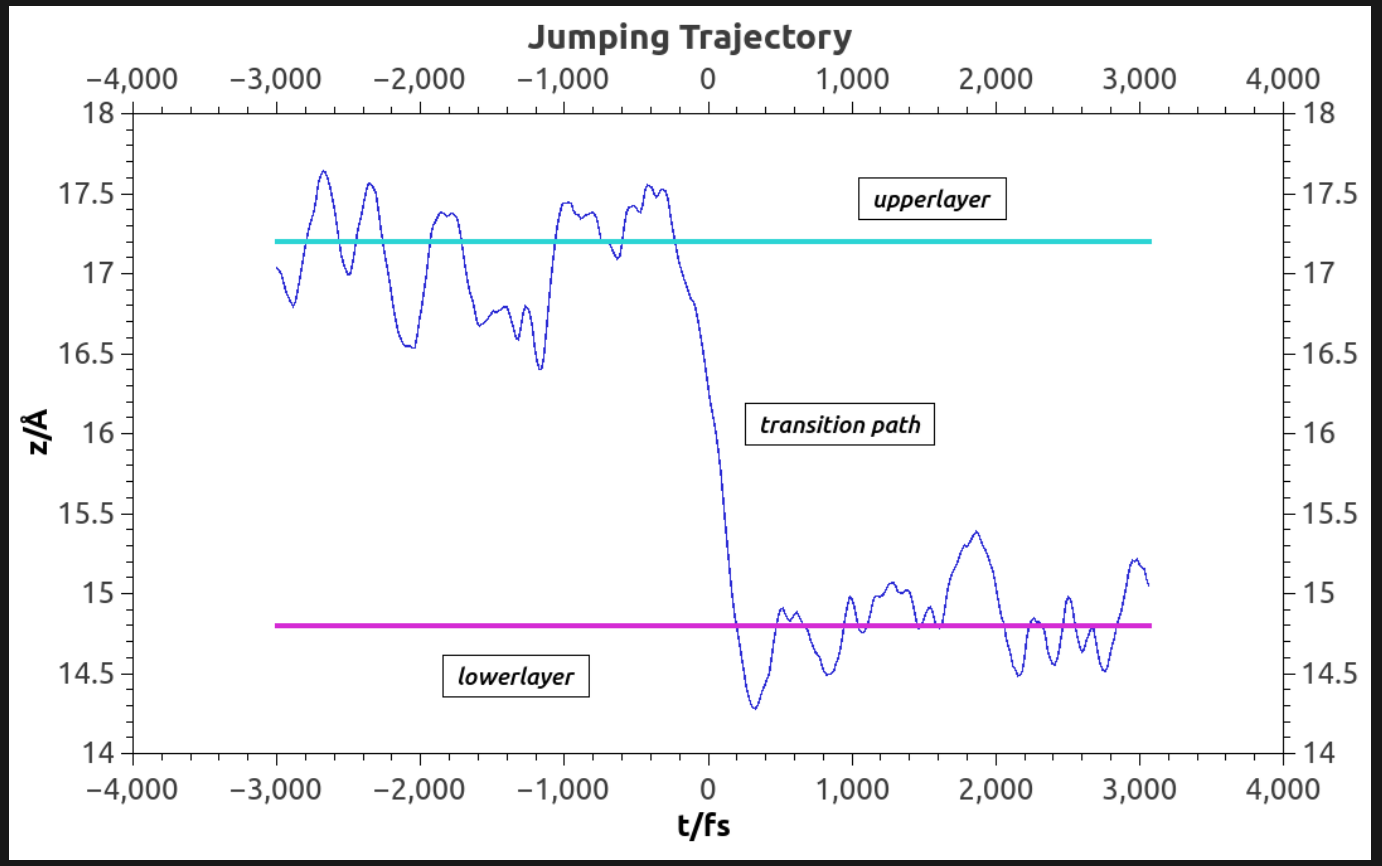


HORIZONTAL DIFFUSION VS. VERTICAL "JUMP"



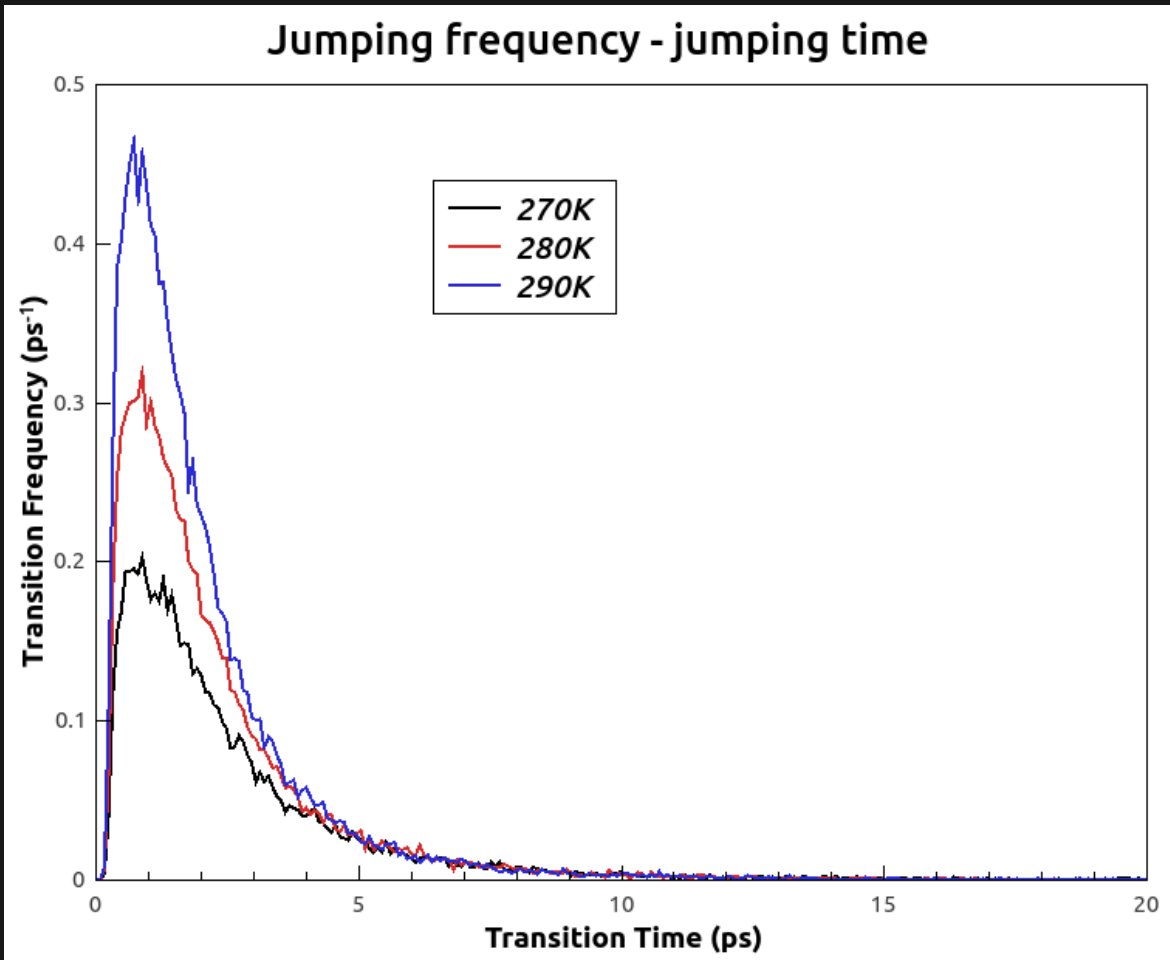
- In the ΔZ=9.5 Å system we observed discrete interlayer water transitions along z-axis, in contrast with the relatively continuous diffusion on x-y plane.

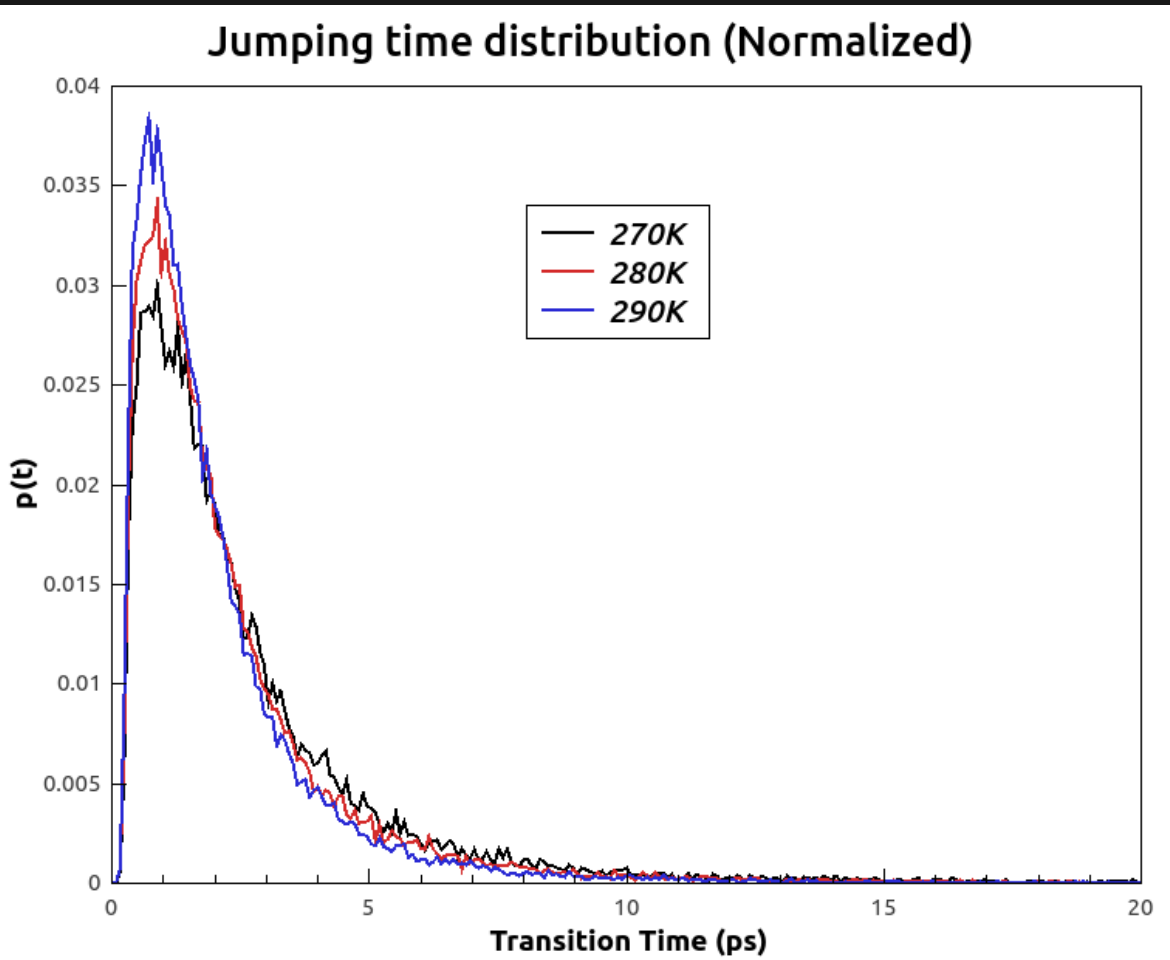
IDENTIFICATION OF A SUCCESSFUL JUMPING TRAJECTORY



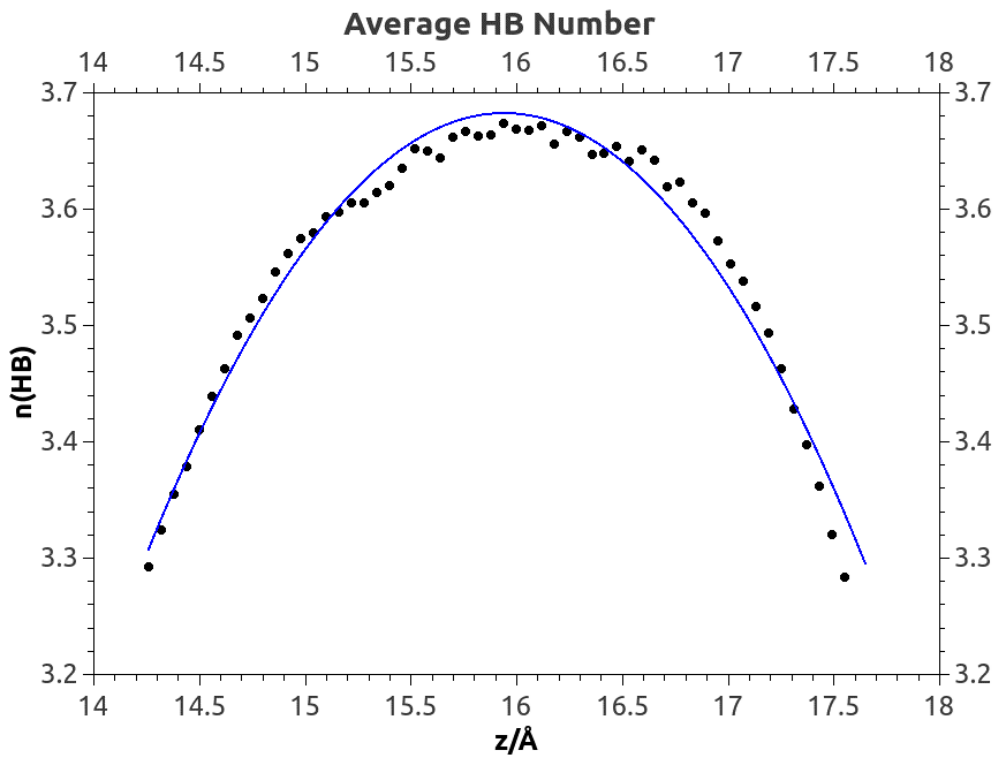
- Recrossing was precluded by setting narrower cutoff value of transition path length.

TRANSITION TIME DISTRIBUTION



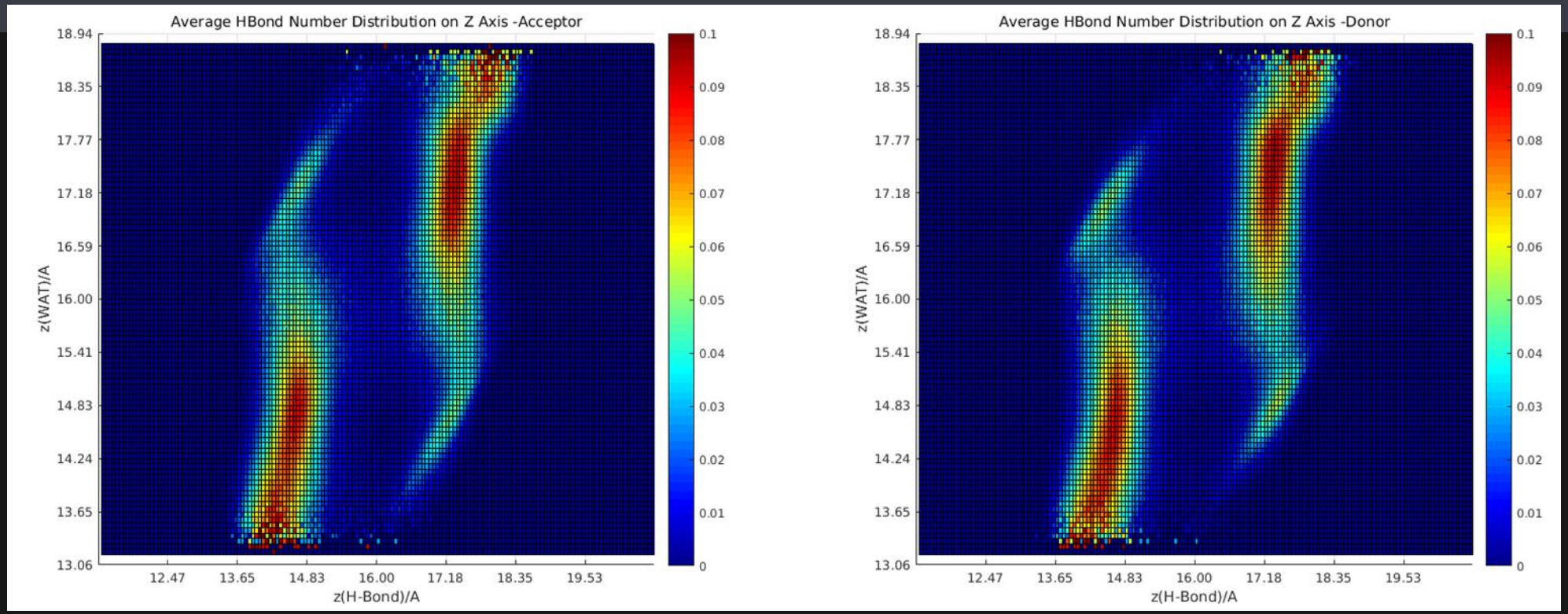


H-BOND DISTRIBUTION



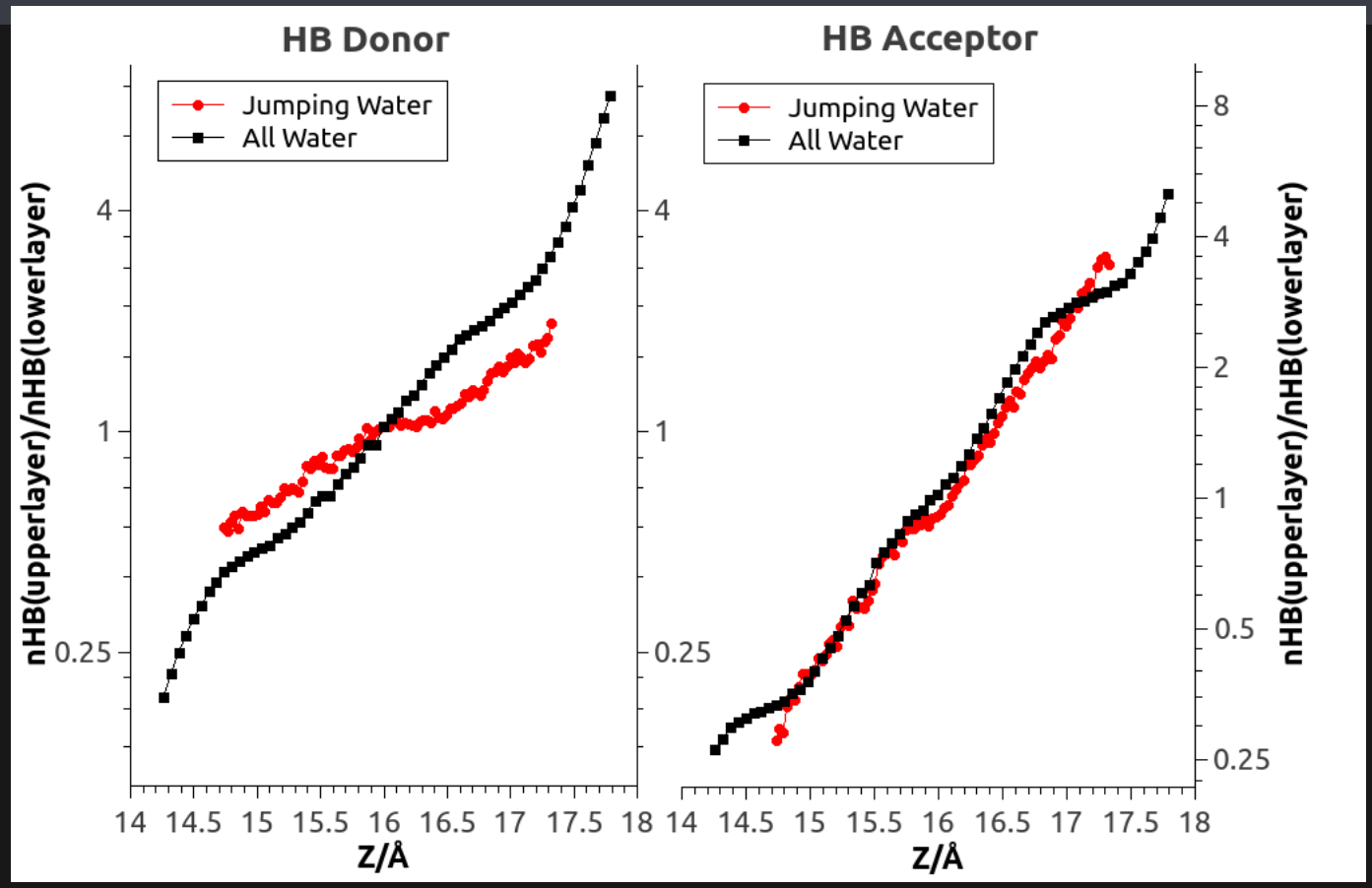
- Indicates correlation with H- Bond structure

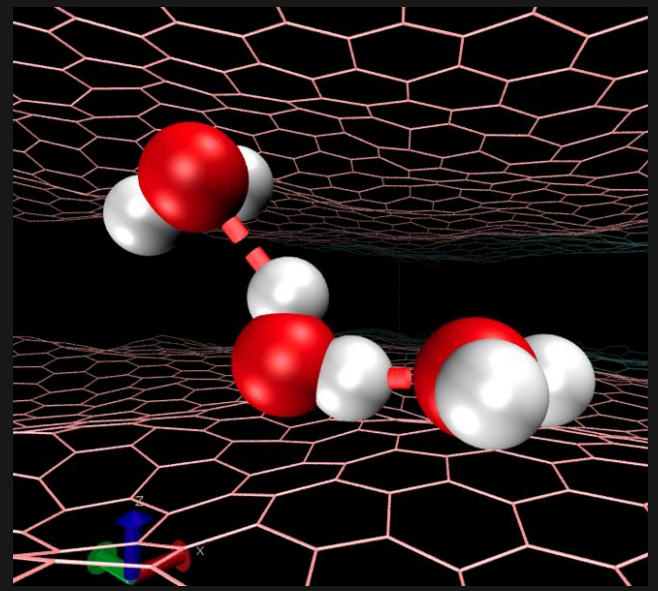
H–BOND POSITION DISTRIBUTION



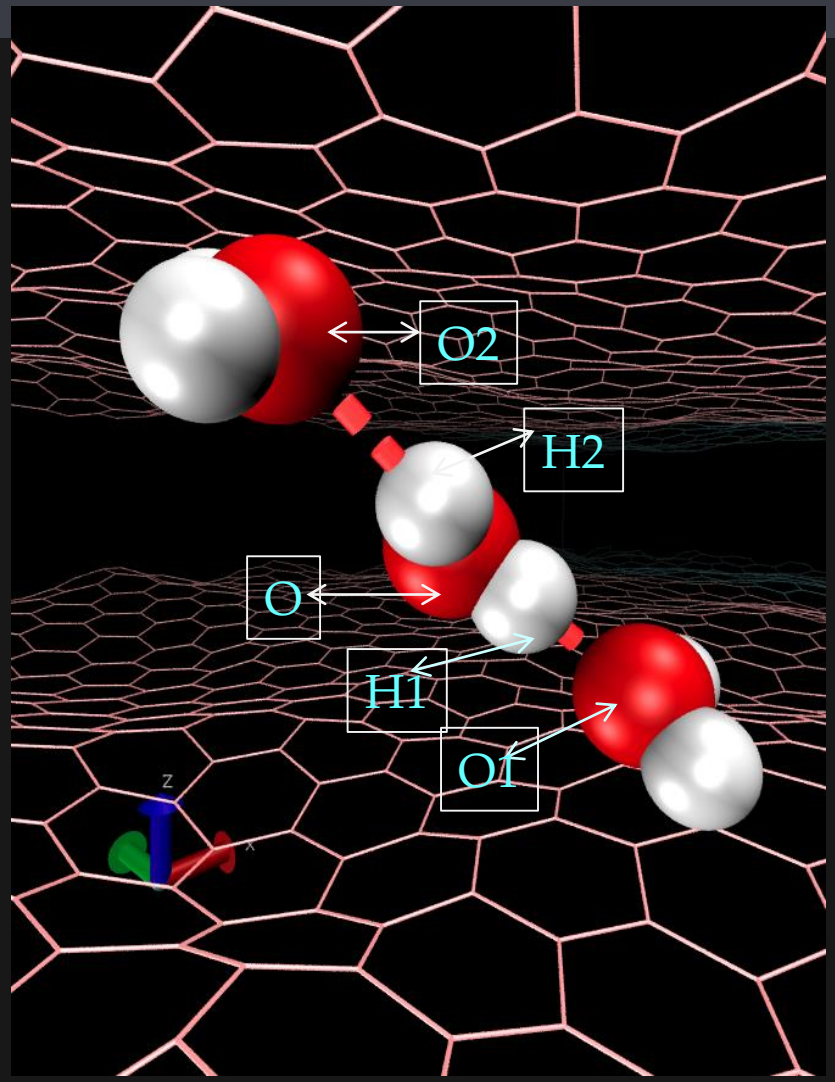
$$\rho[z(HB), z'(WAT)] = \frac{\iint \sum_i \delta\left(z' - z_{i,O(WAT)}\right) \sum_j^{n(HB,i)} \delta\left(z - z_{j,O(HB)}\right) ds}{\iint \sum_i \delta\left(z - z_{i,O(WAT)}\right)\ ds}$$

CORRELATION WITH INTERLAYER TRANSITION



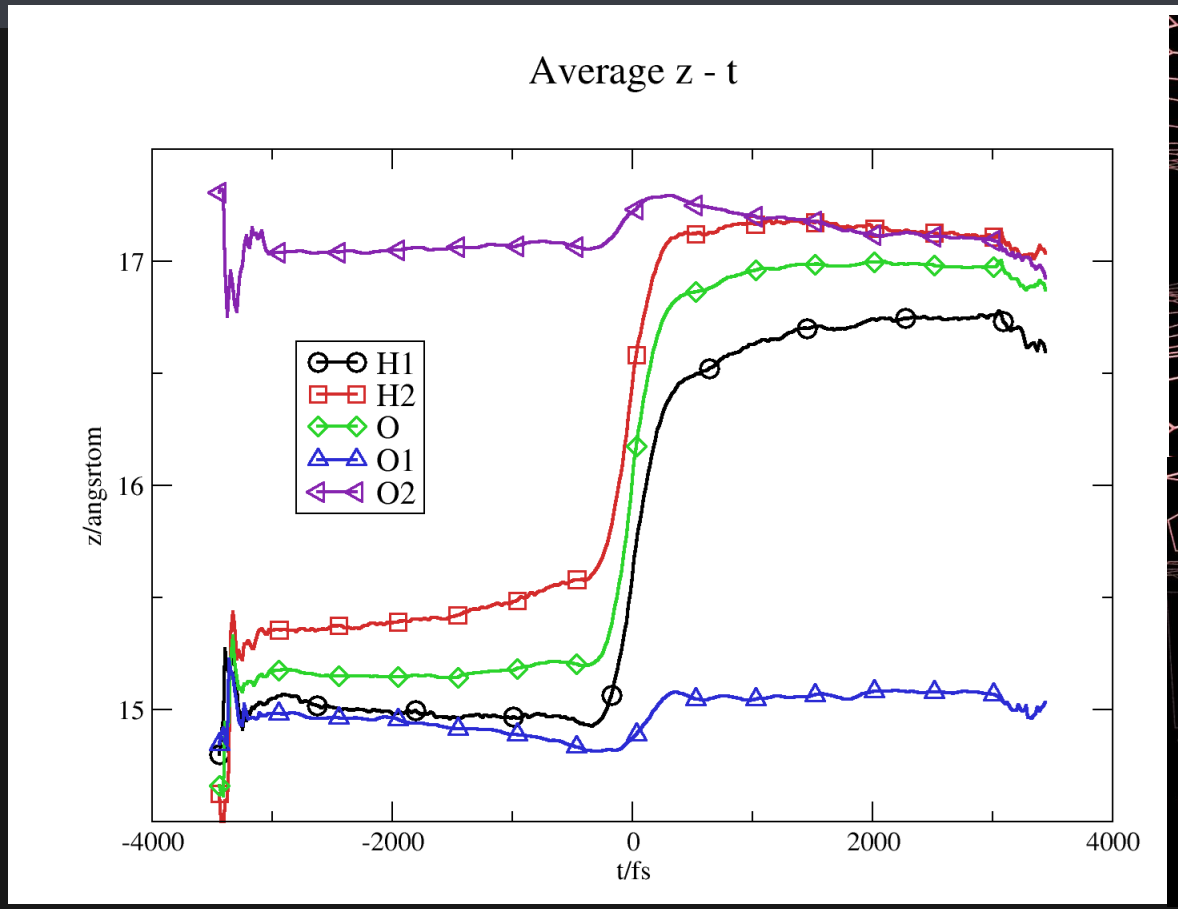


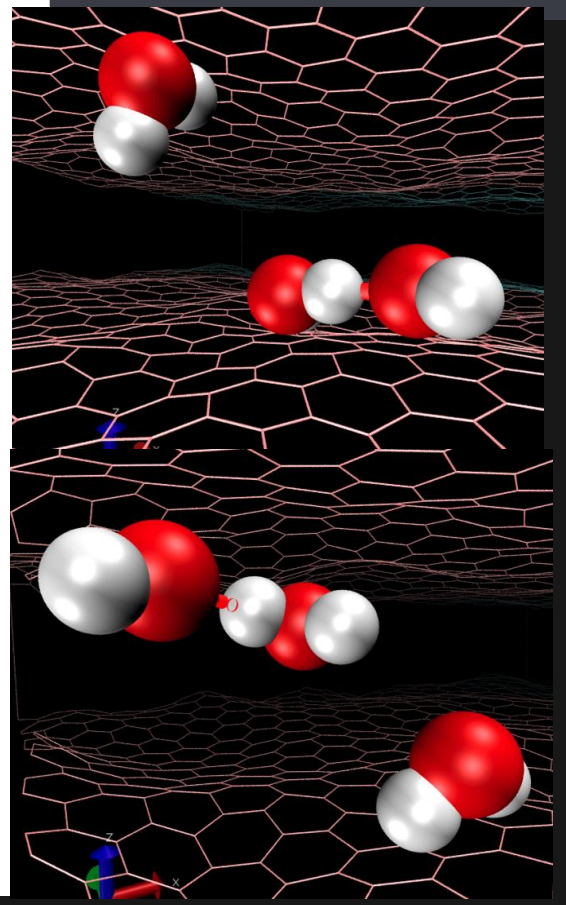
TIME EVOLUTION: REFERENCE STATE



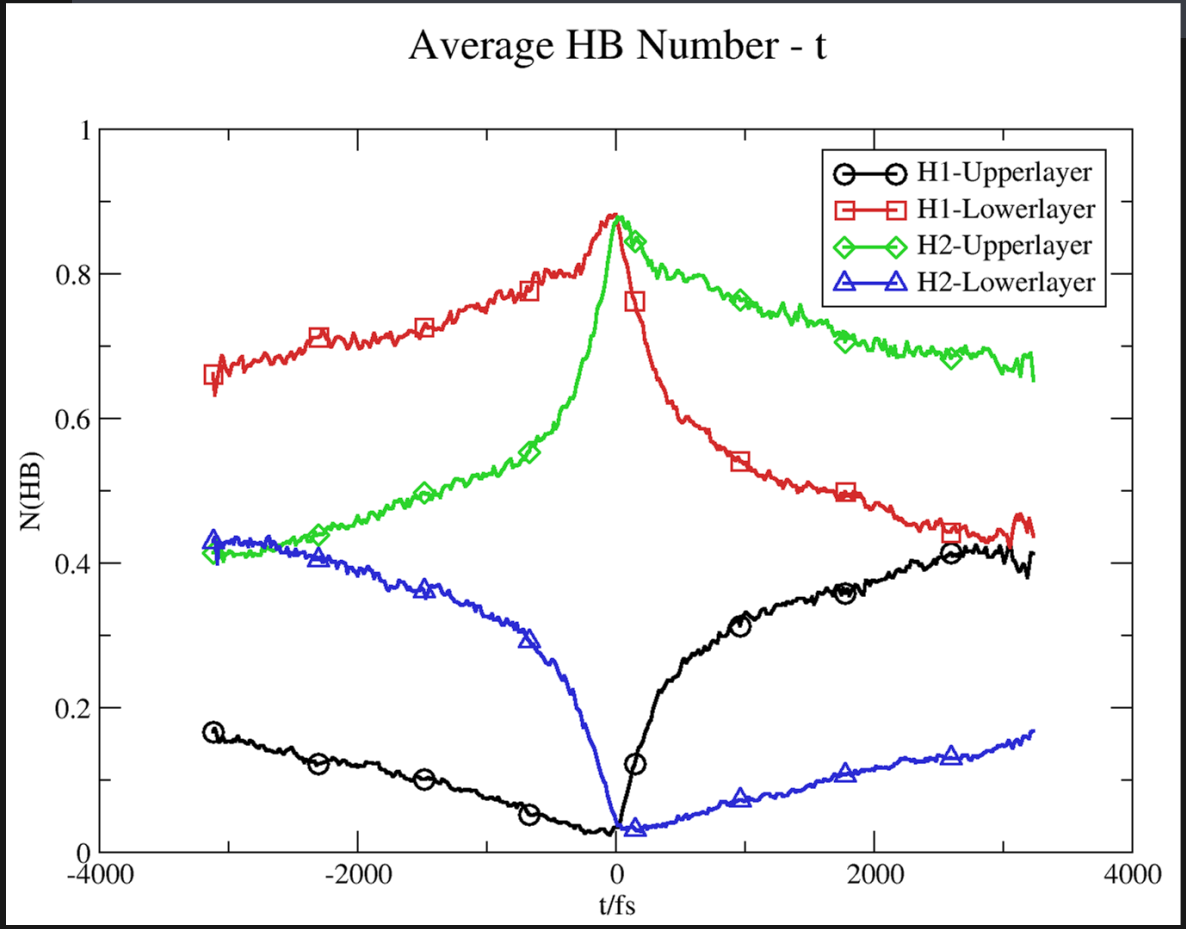
- Detectable in about 70% of successful jumping trajectories
- Having determined the reference state, we analyzed time evolution of CVs including z-coordinates, H Bonds and bond orientations along the transition path of jumping events.

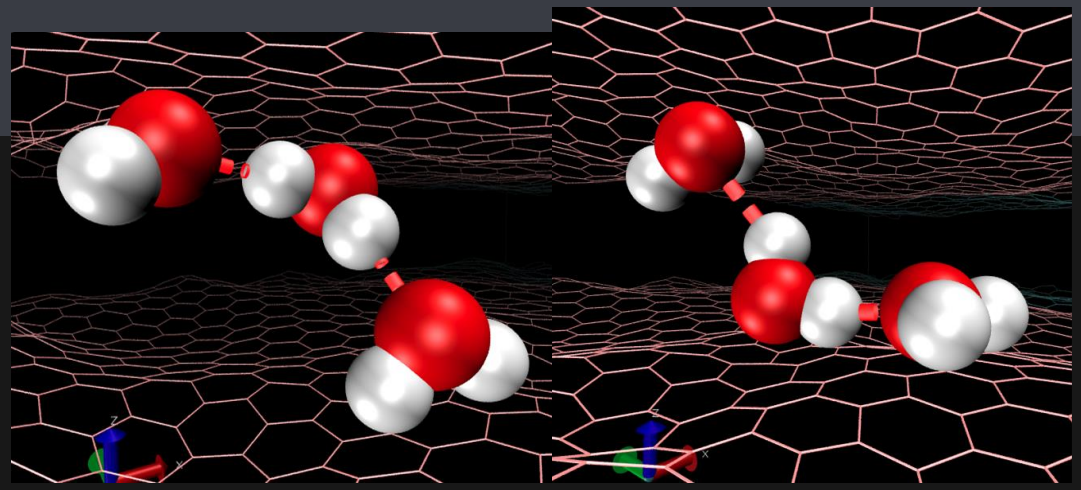
TIME EVOLUTION: Z





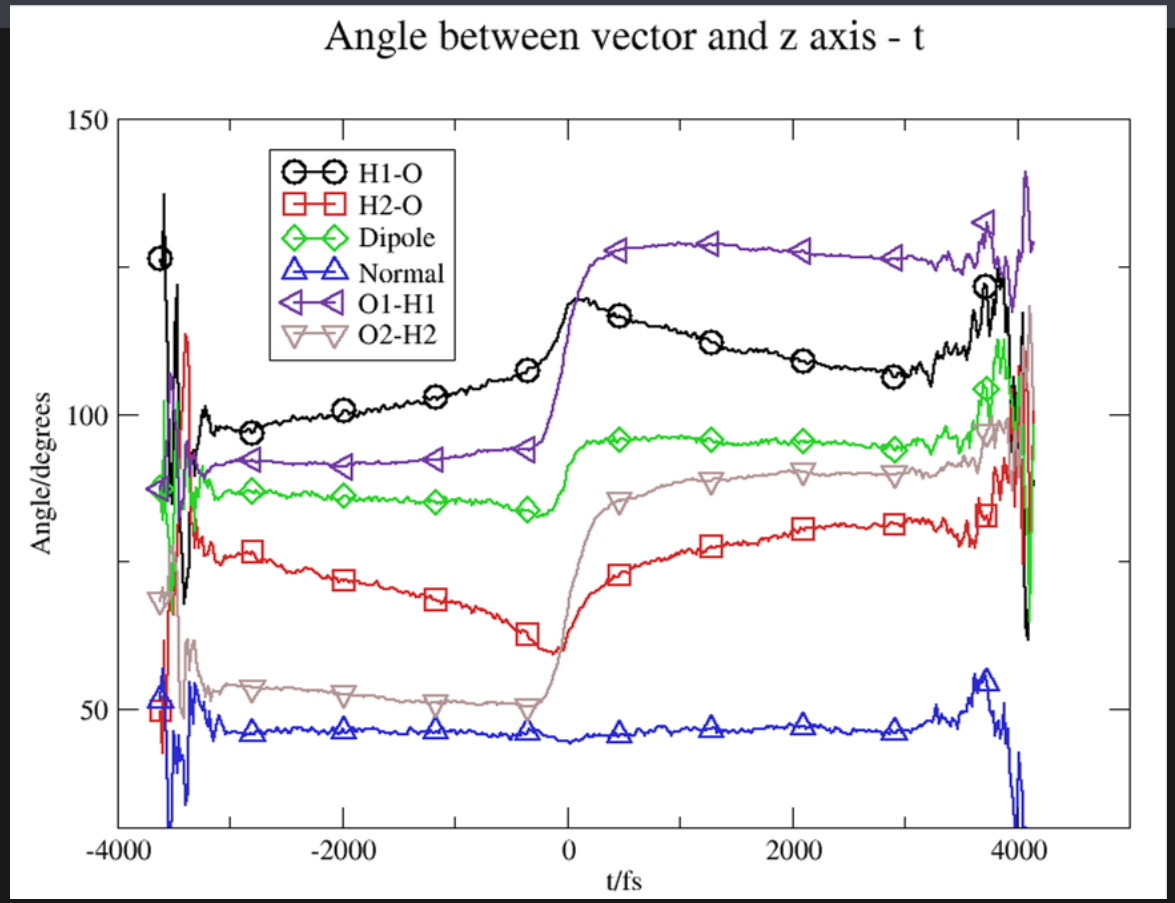
TIME EVOLUTION: H–BOND



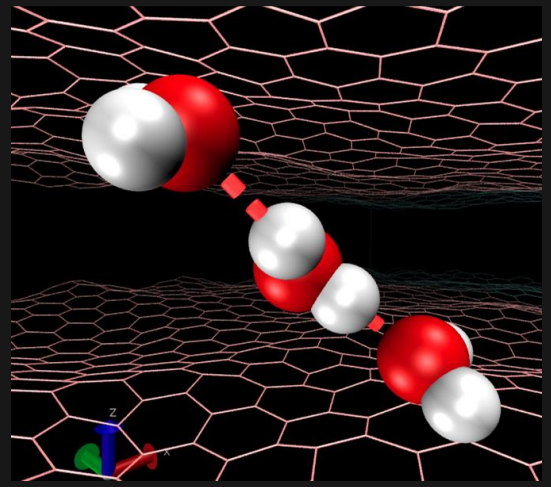


- Concerted interlayer H-Bond exchange

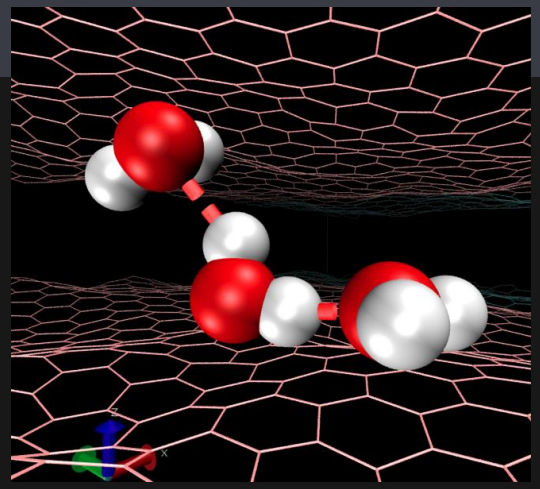
TIME EVOLUTION: ORIENTATION

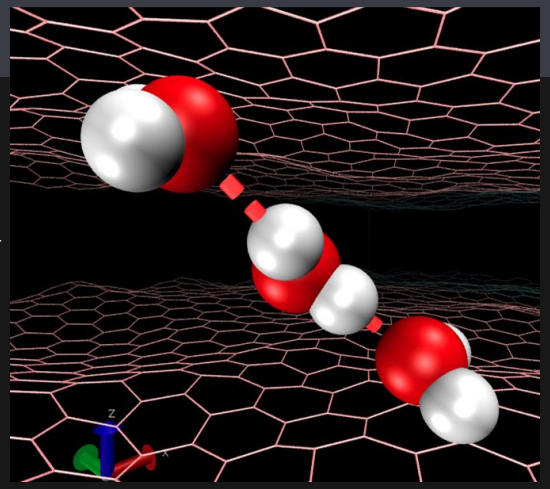


- Time Scale:
  - Dipole-- z evolution
  - OH-- H Bond evolution

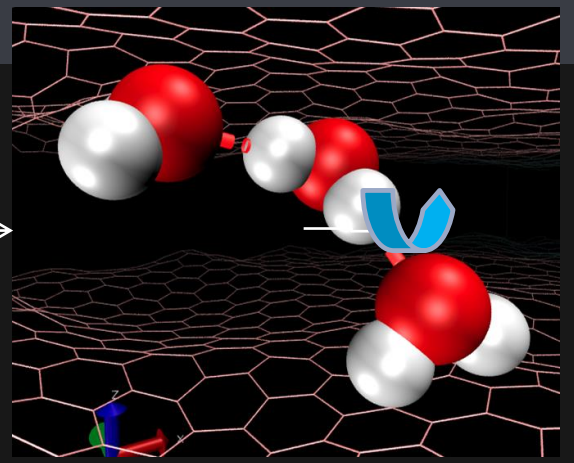


MECHANISM: SUMMARY

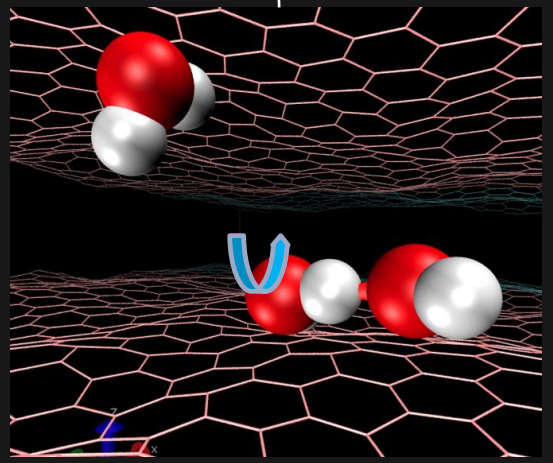


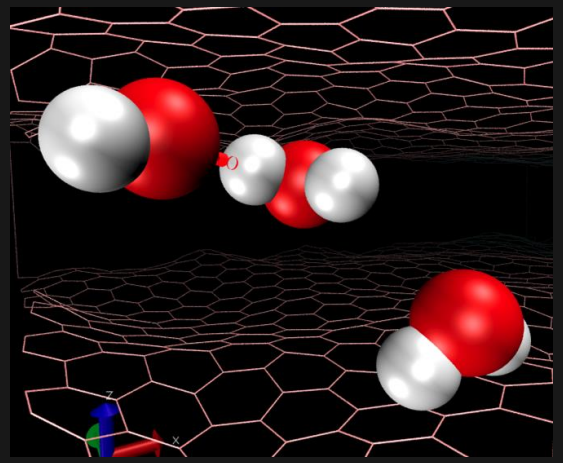


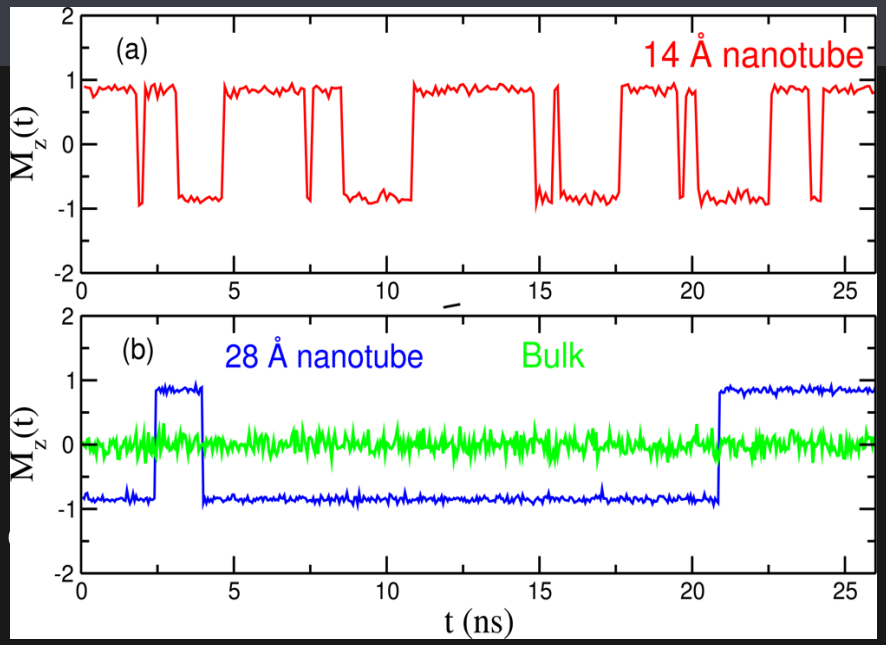
"Transition State"



Angle Jump

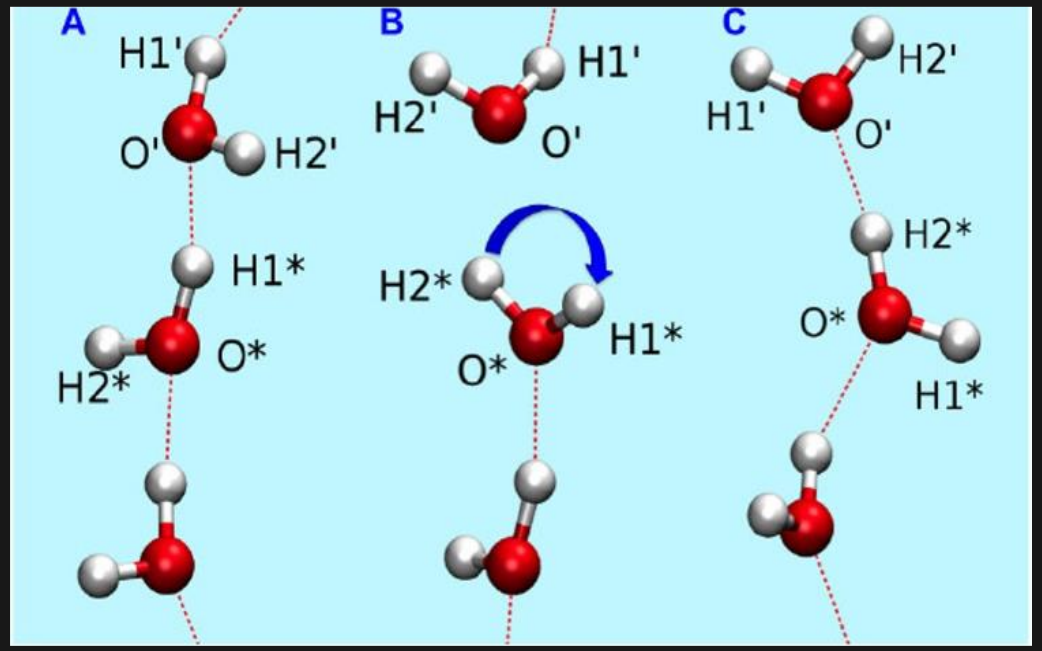






Time evolution of the average dipole projection along the nanotube axis.

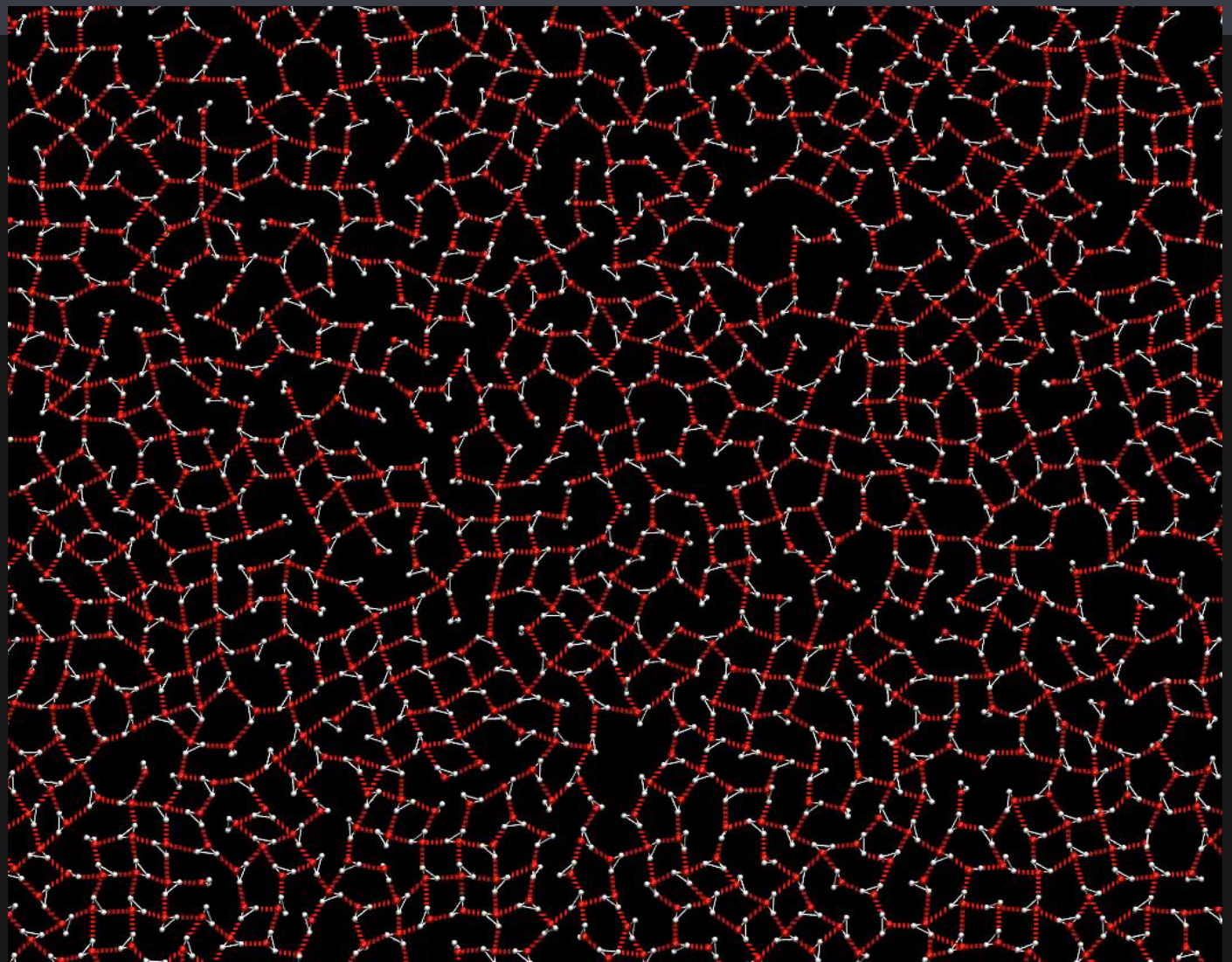
Similarity with water in nanotube

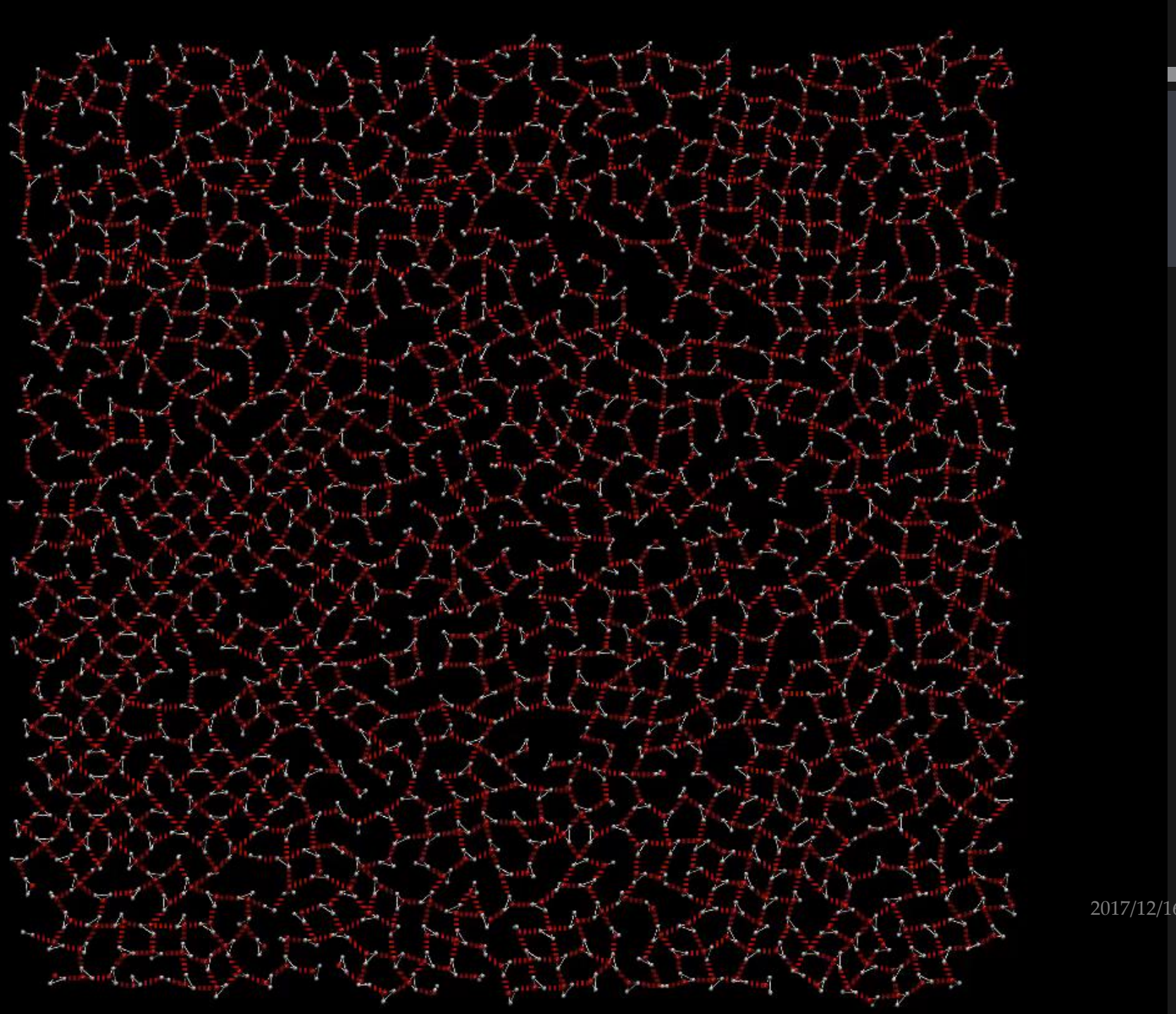


CHALLENGES

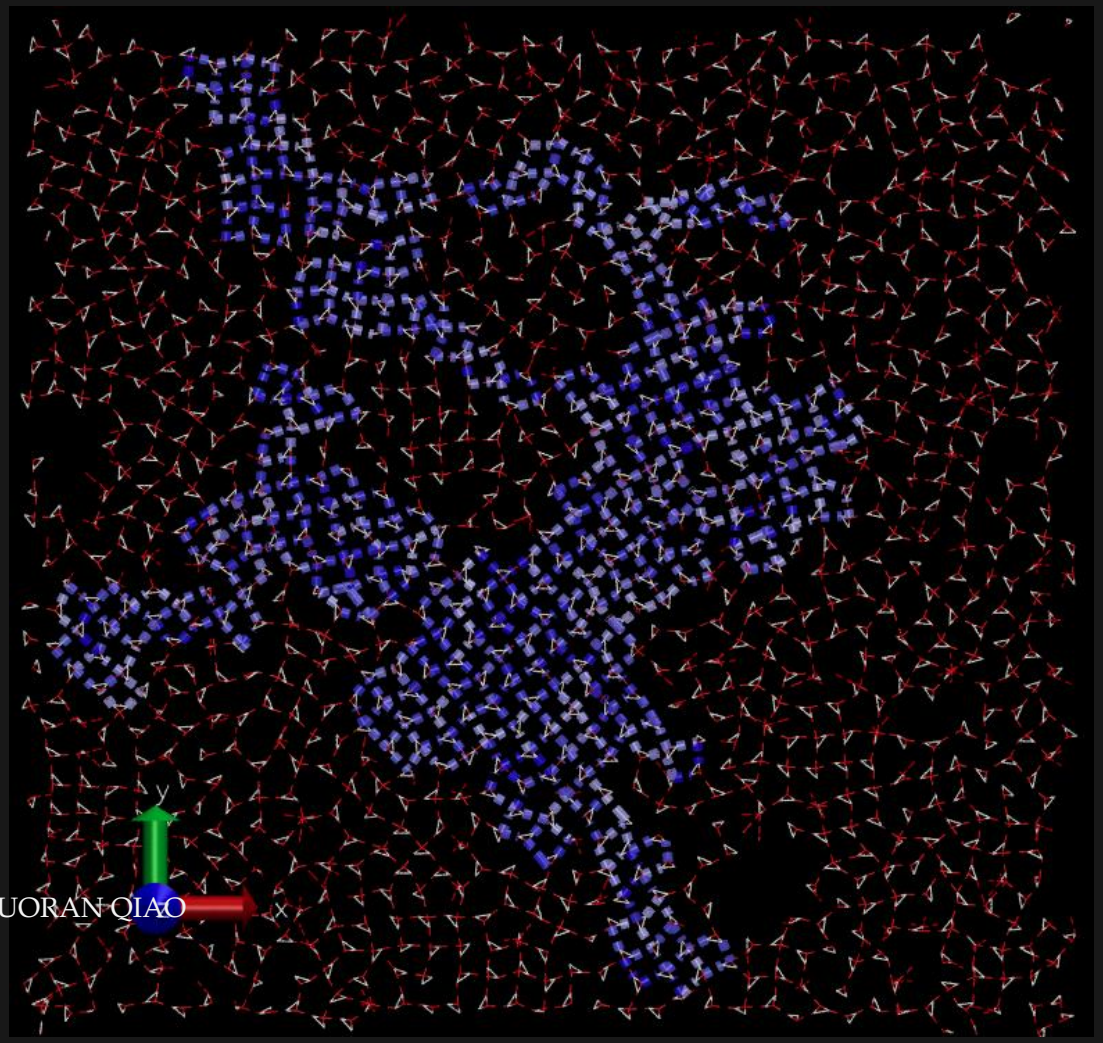
- Correlation with cavity fluctuations
- Energy transfer mechanisms

DYNAMICS OF WATER CLUSTERS& NUCLEATION

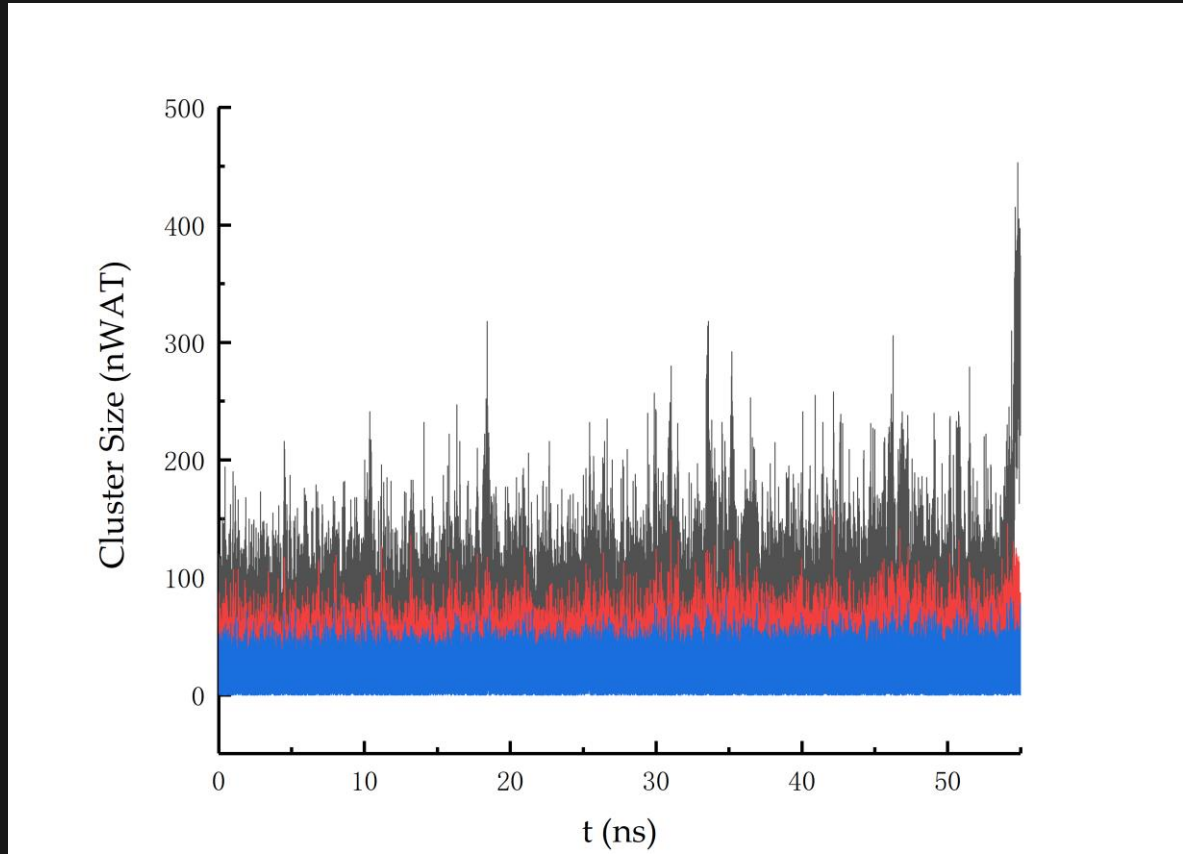




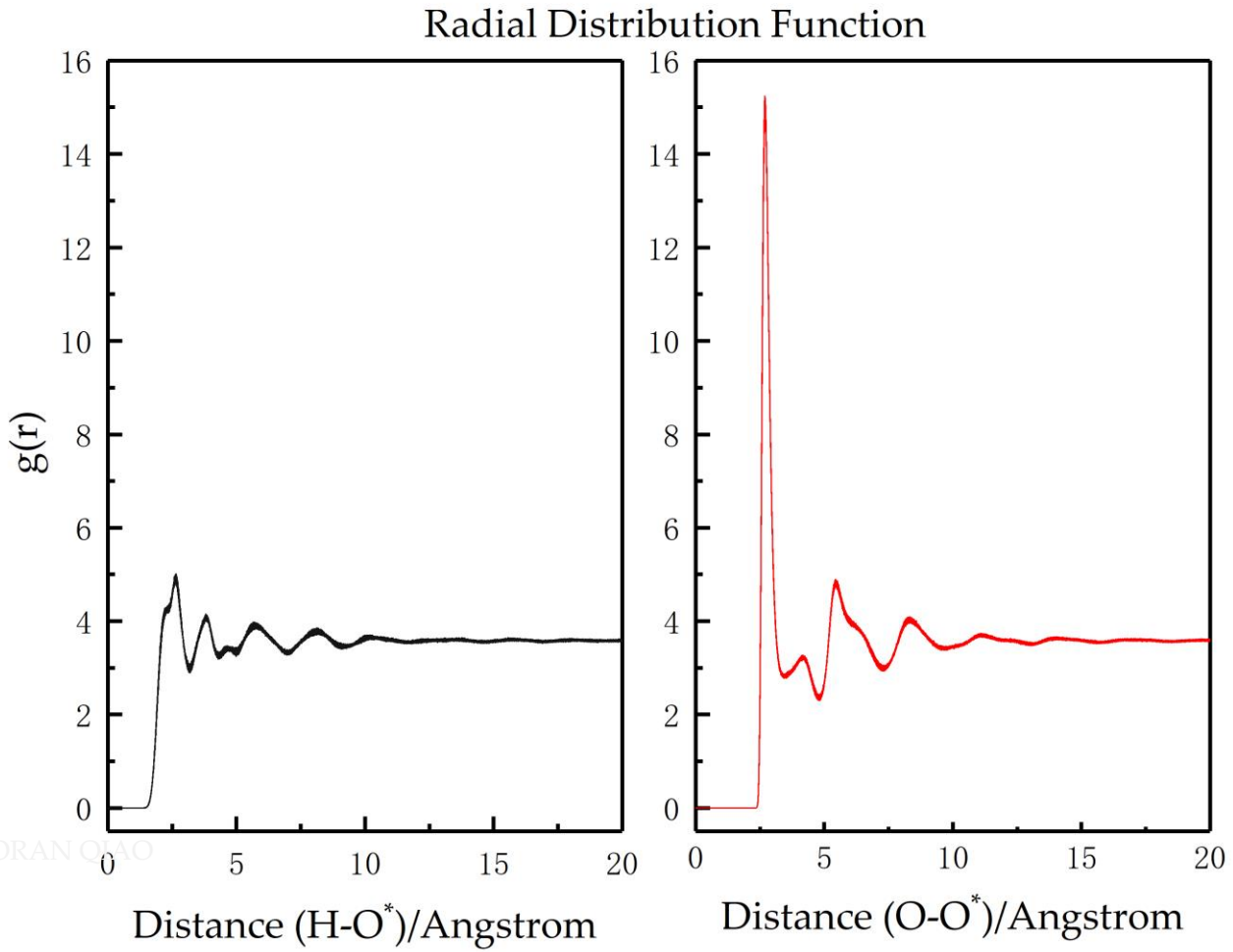
CLUSTERS IN "ICE-LIKE" WATER

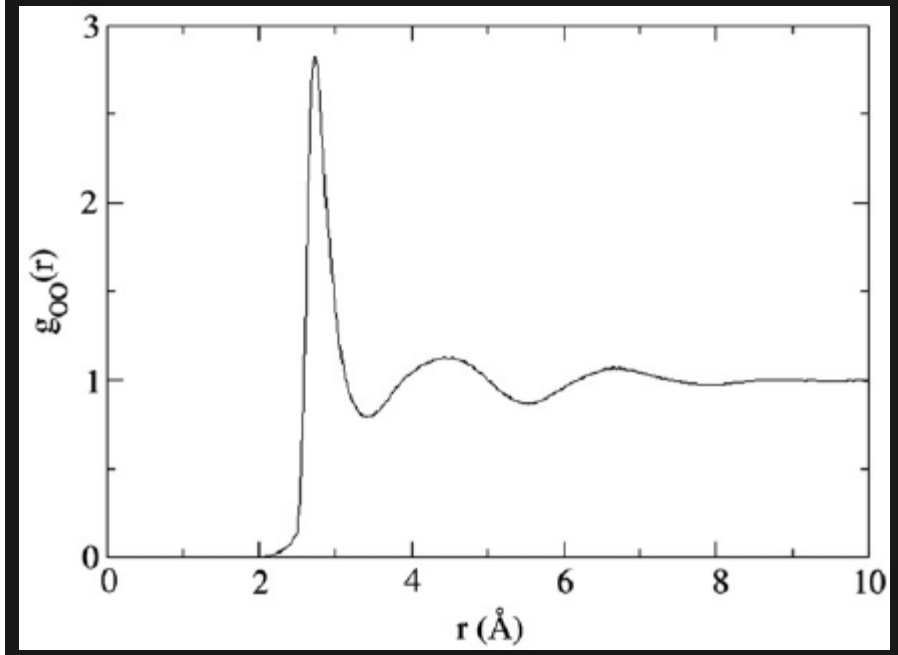


Max cluster size evolution

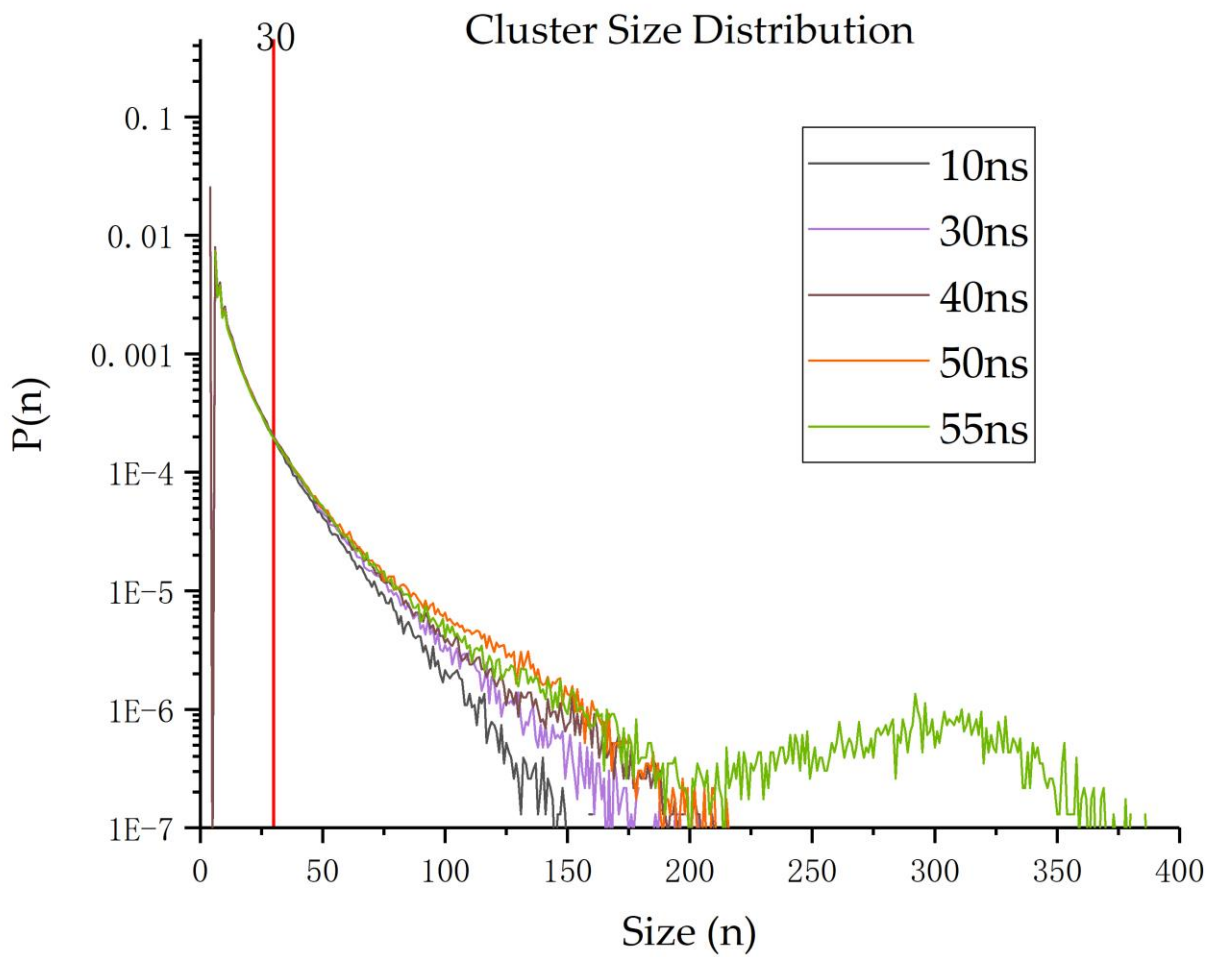


RADIAL DISTRIBUTION FUNCTION

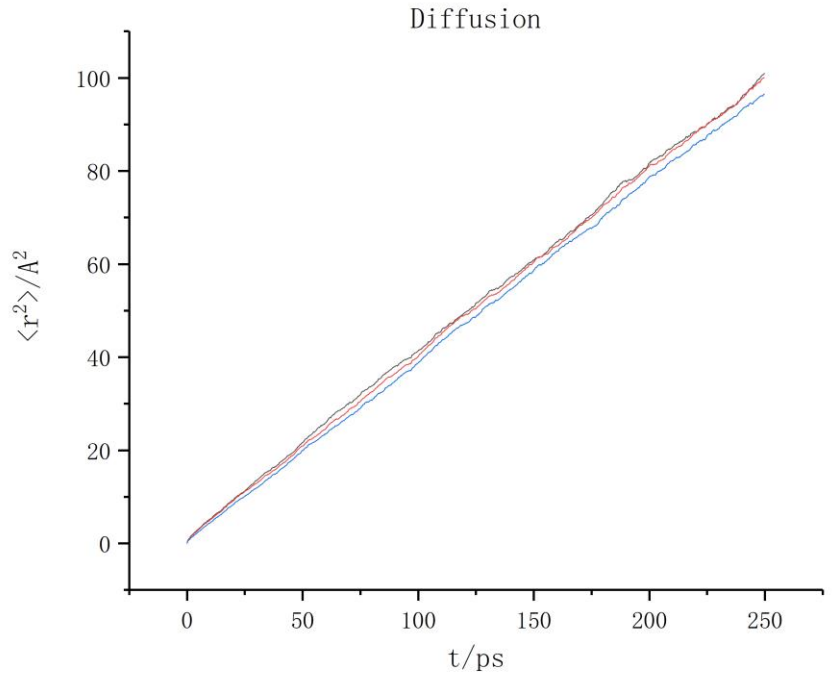


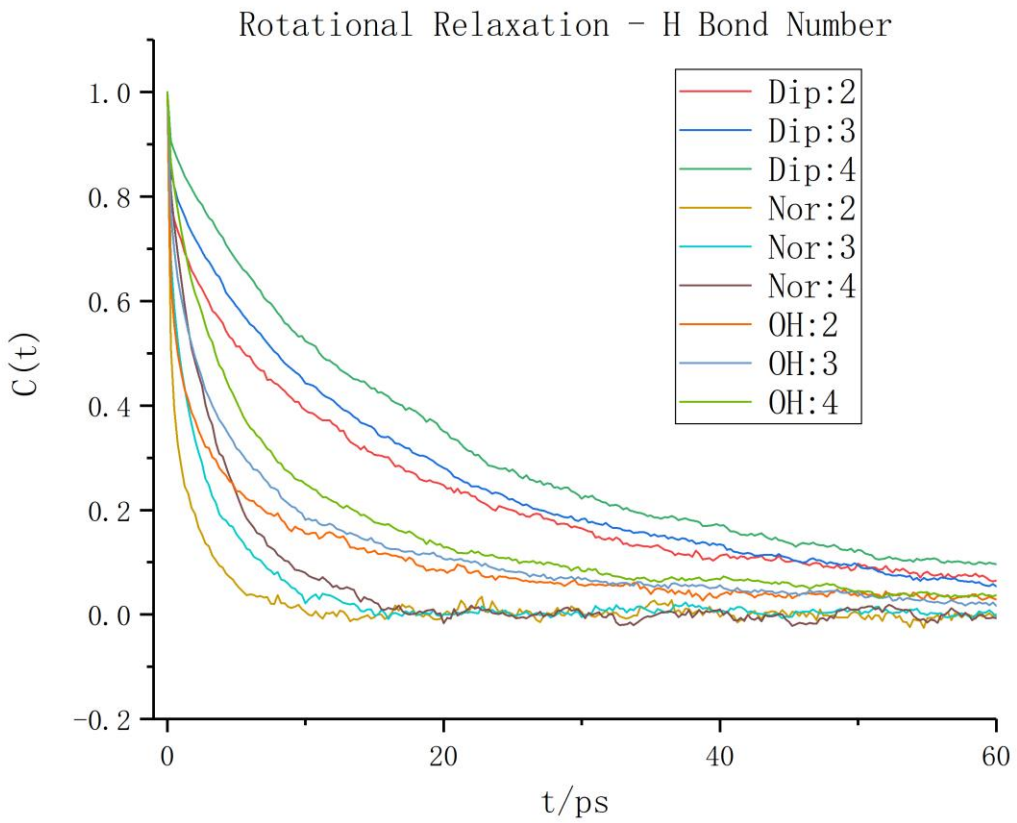


CLUSTER SIZE DISTRIBUTION



DIFFUSION& ROTATIONAL RELAXATION – H BOND NUMBER

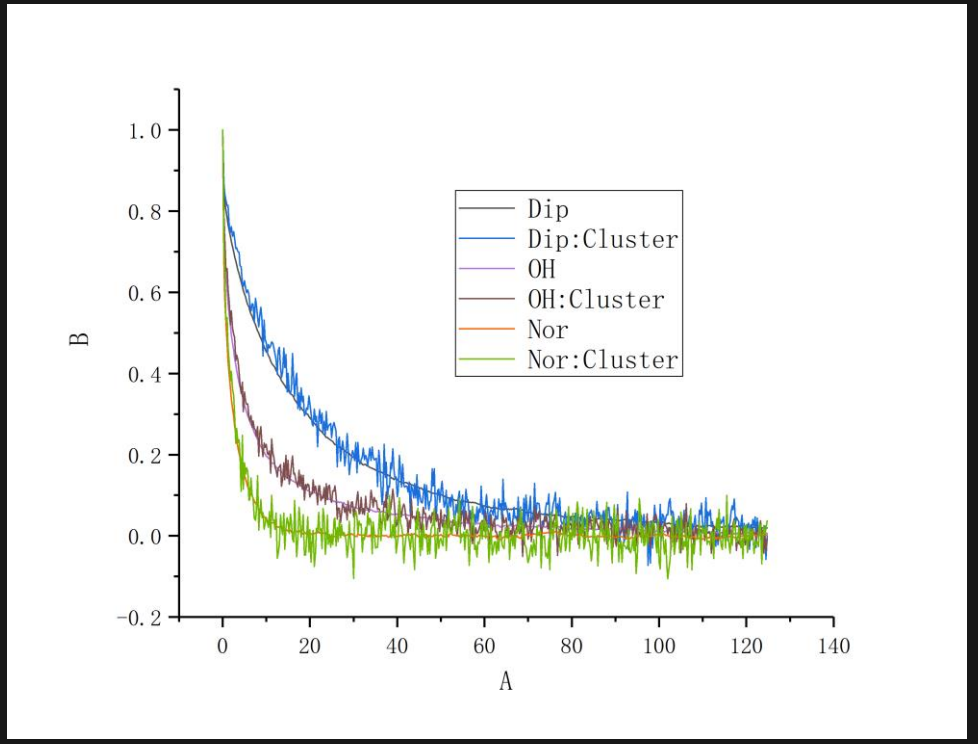




CHALLENGES

No significant difference of relaxation time scale between clusters& free water molecules

Definition of clusters



THANKS FOR YOUR ATTENTION!