The Abdus Salam
International Centre
for Theoretical Physics

Molecular Dynamics of

WATER CLUSTERS

Represented by

NGUYEN VU LINH

SIMULATION DIRECTORY STRUCTURE

Directory for MD simulations of water clusters.

- HOME/MDTutorial/Exercises/Exc1

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  - final_exam-Temp

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  - compile_different_deltaT.sh

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FINDING EQUILIBRIUM REGION

Total energy, temperature, and potential energy at 300 K.

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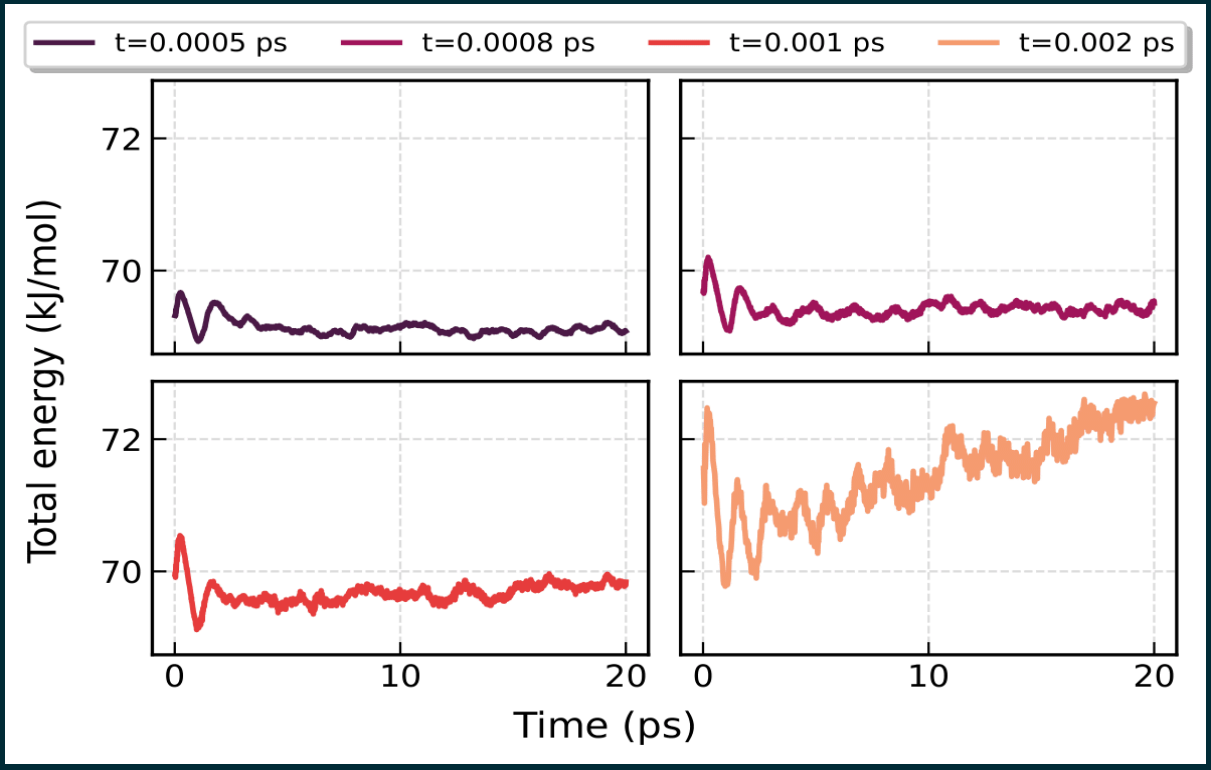

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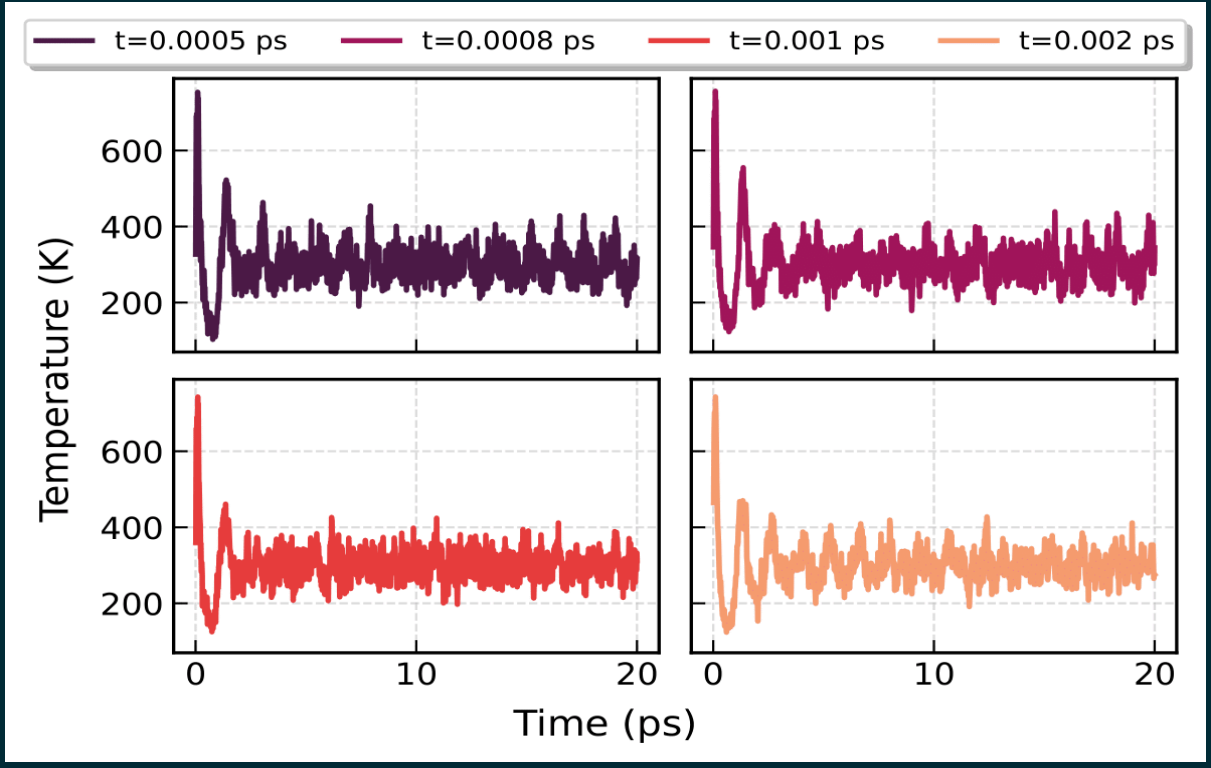

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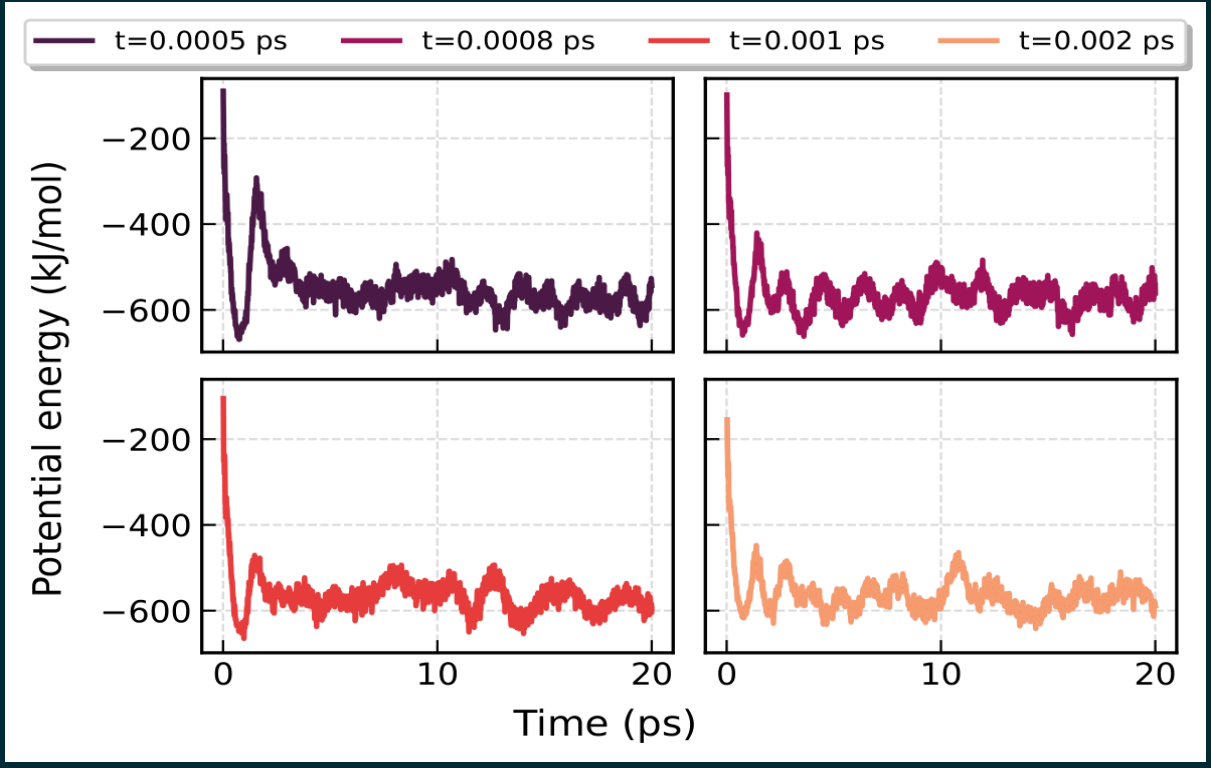

RADIAL DISTRIBUTION FUNCTION

$$g(r) = \frac{dN_r}{4\pi r^2 dr\,\rho}$$

Radial distribution function of O-O, O-H, and O-H pairs.

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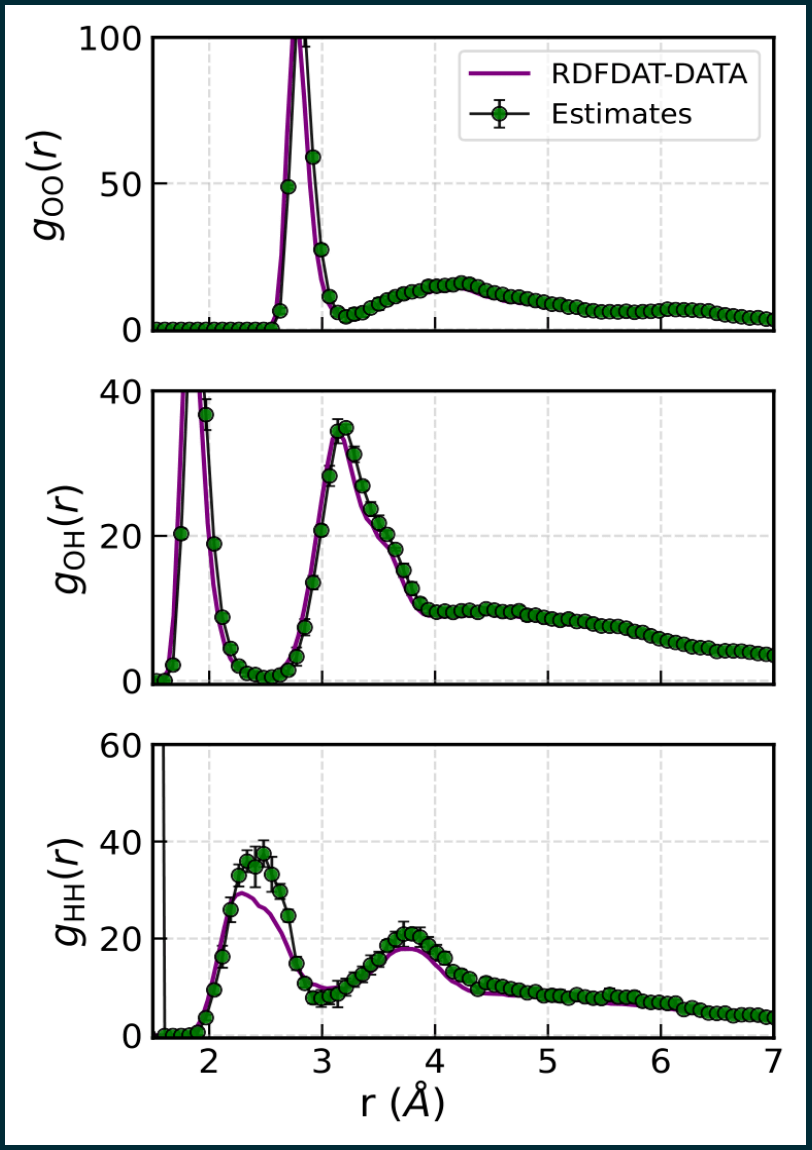

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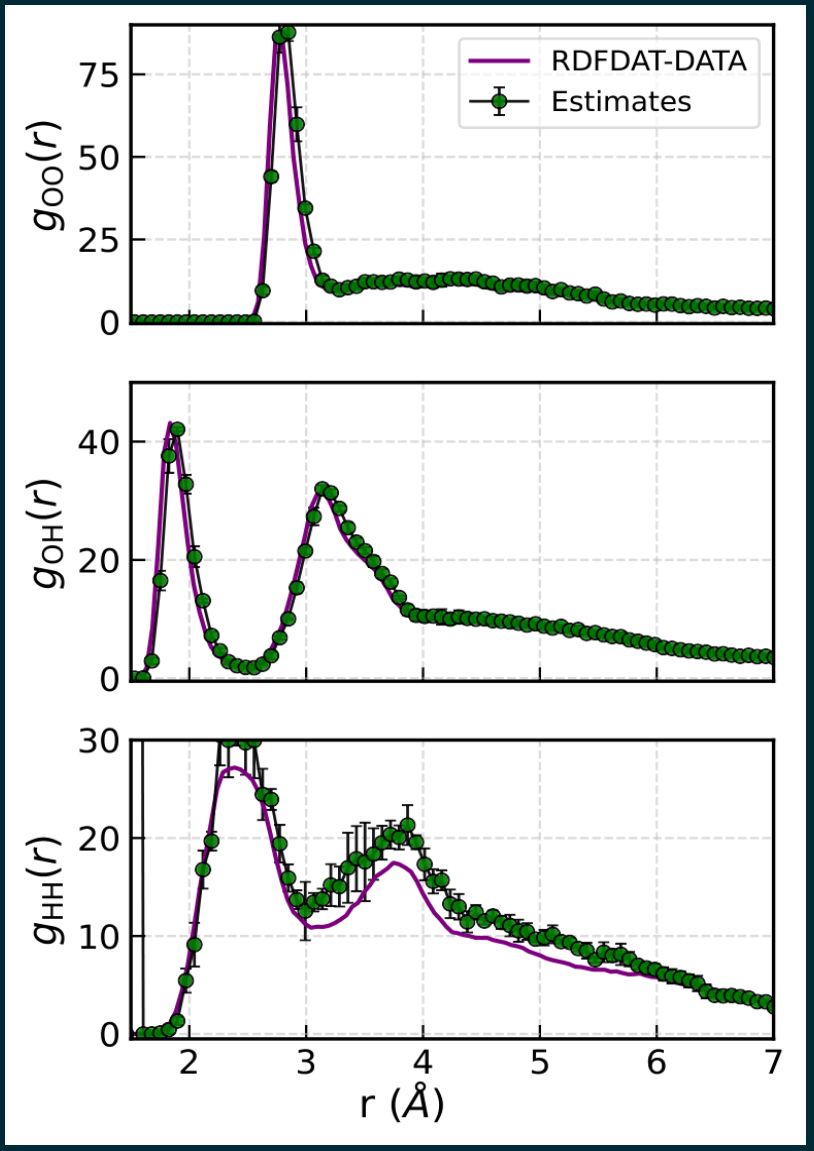

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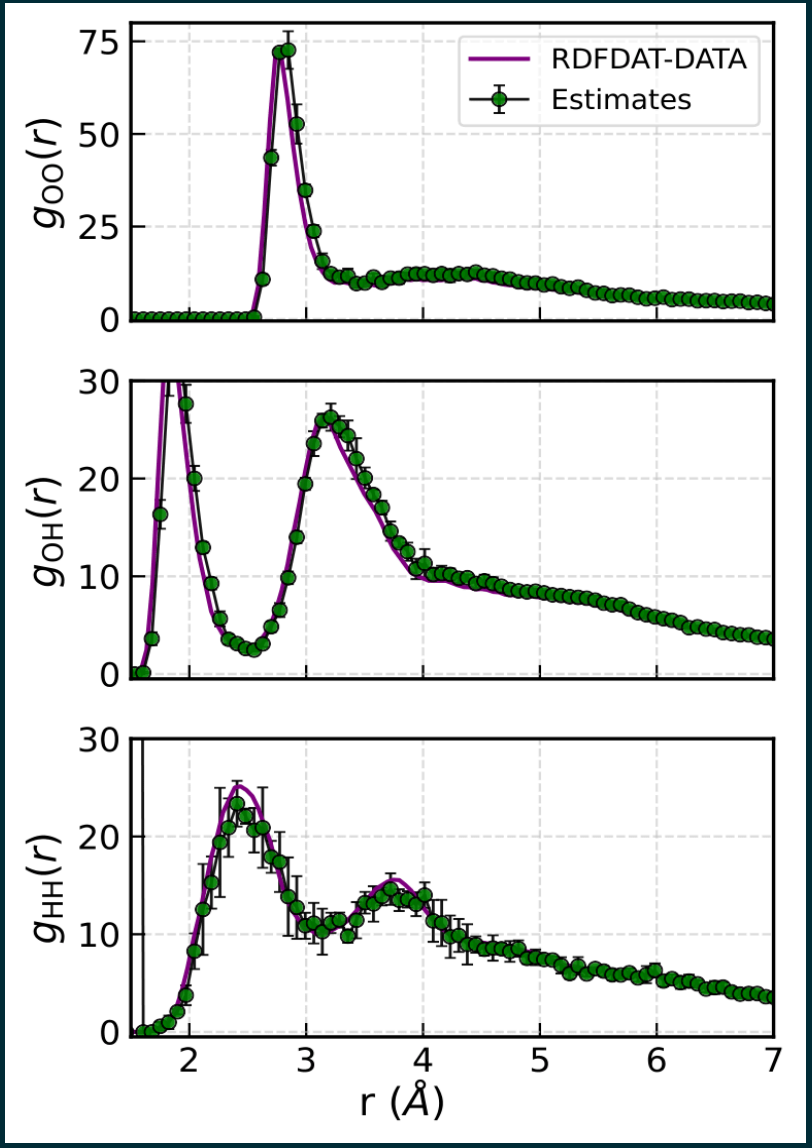

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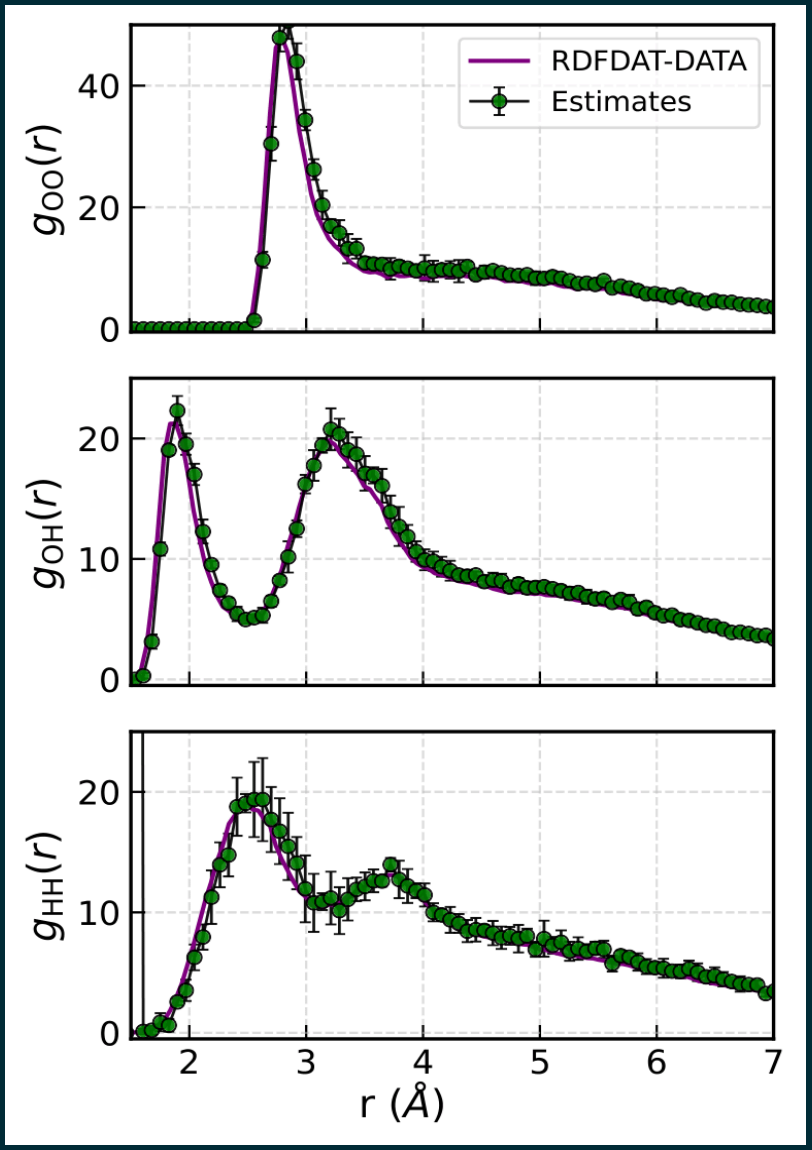

DIPOLE MOMENT

Dipole moment of water molecules

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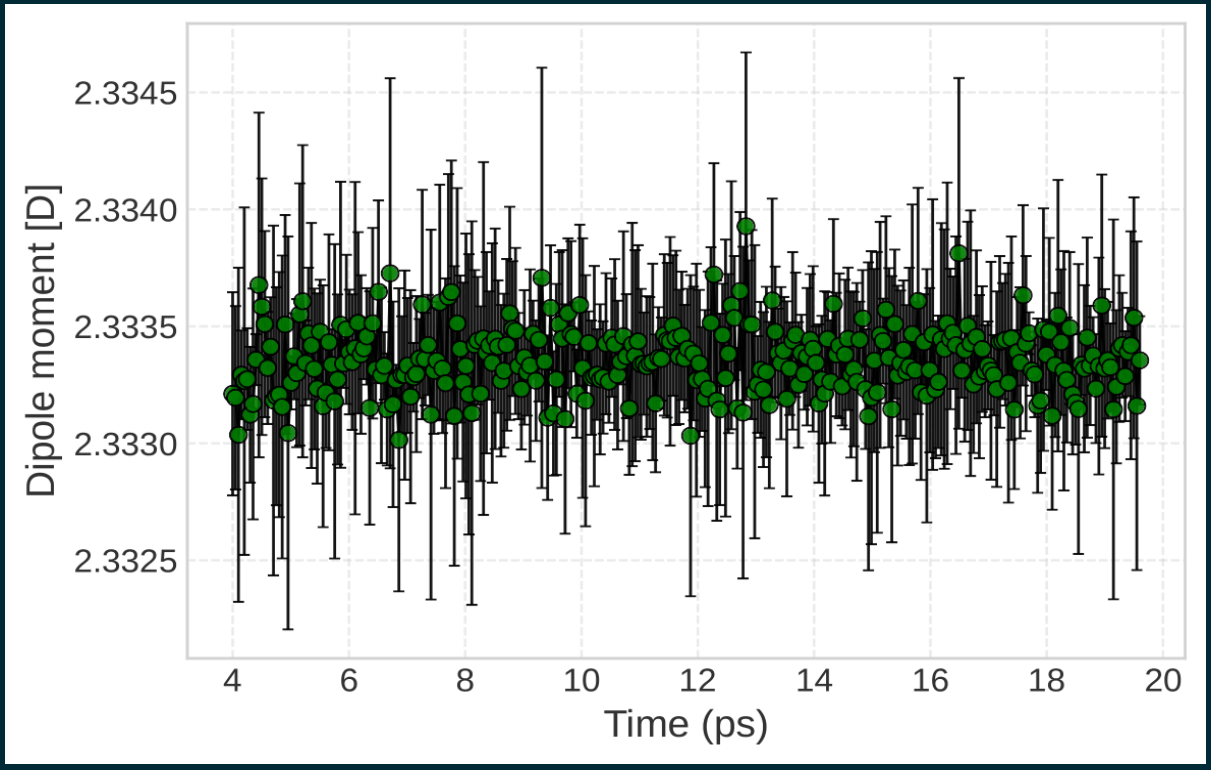

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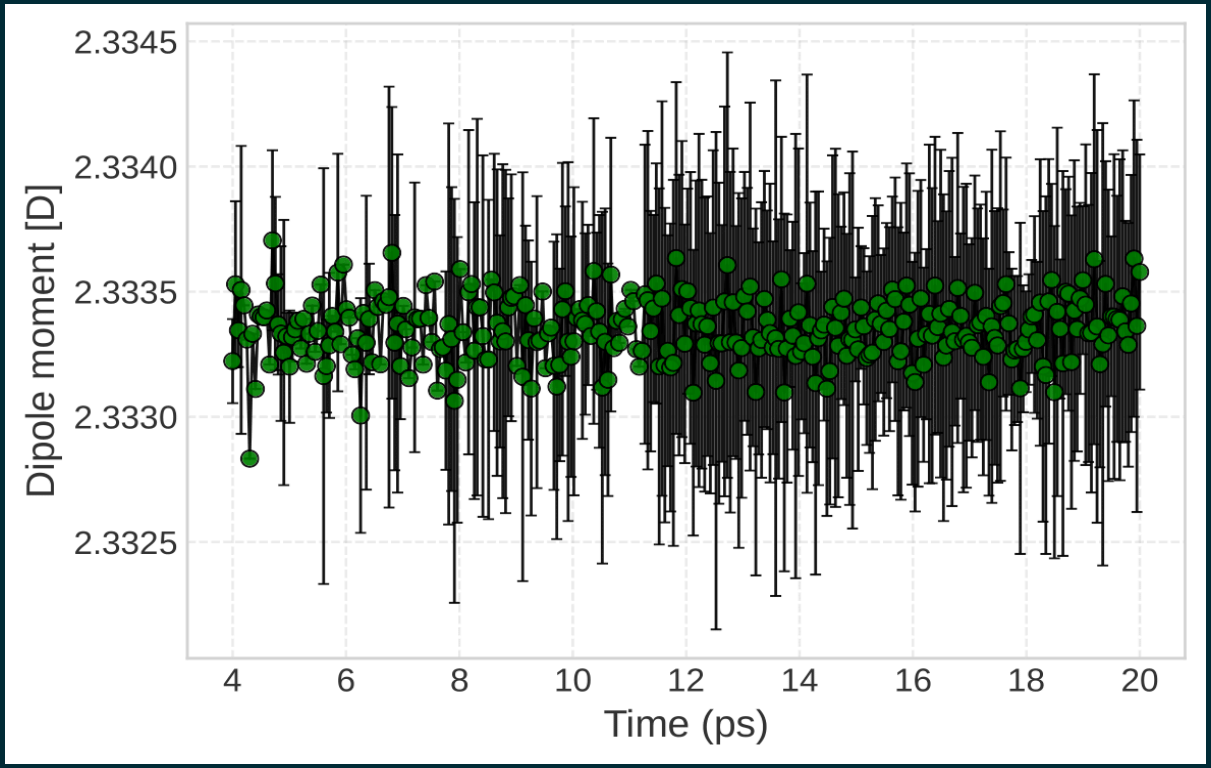

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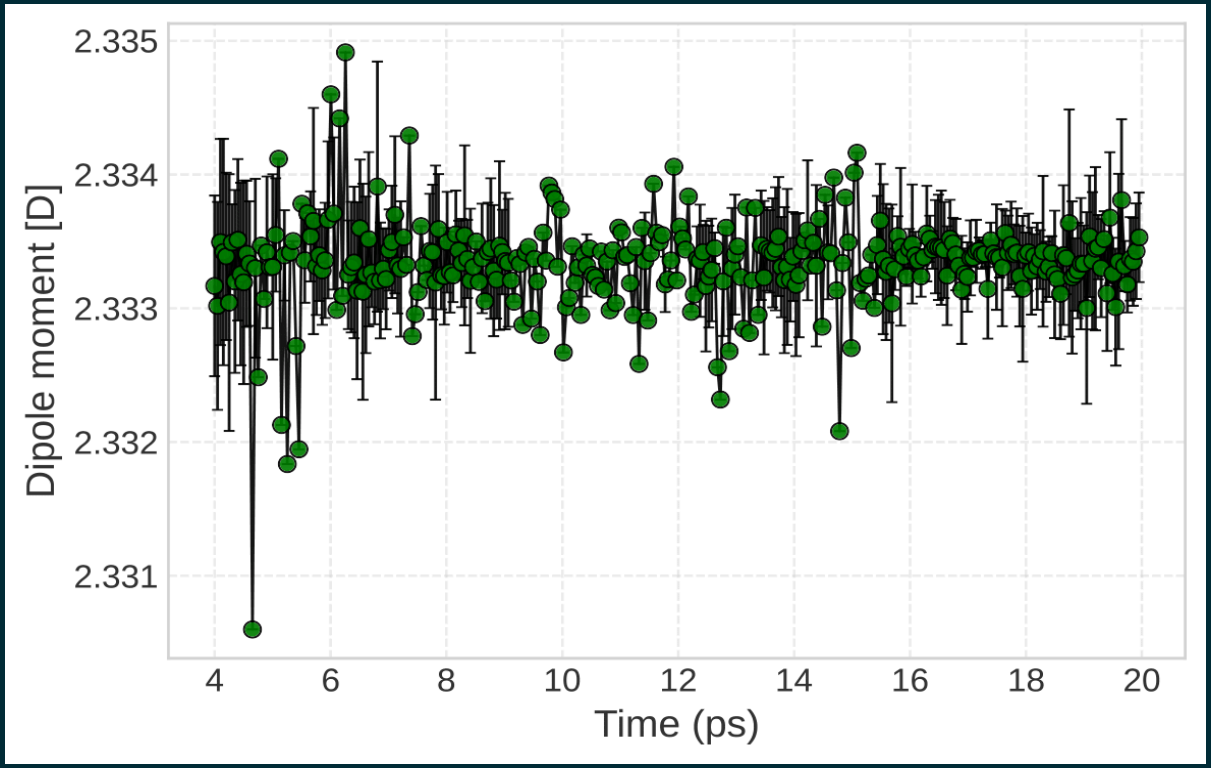

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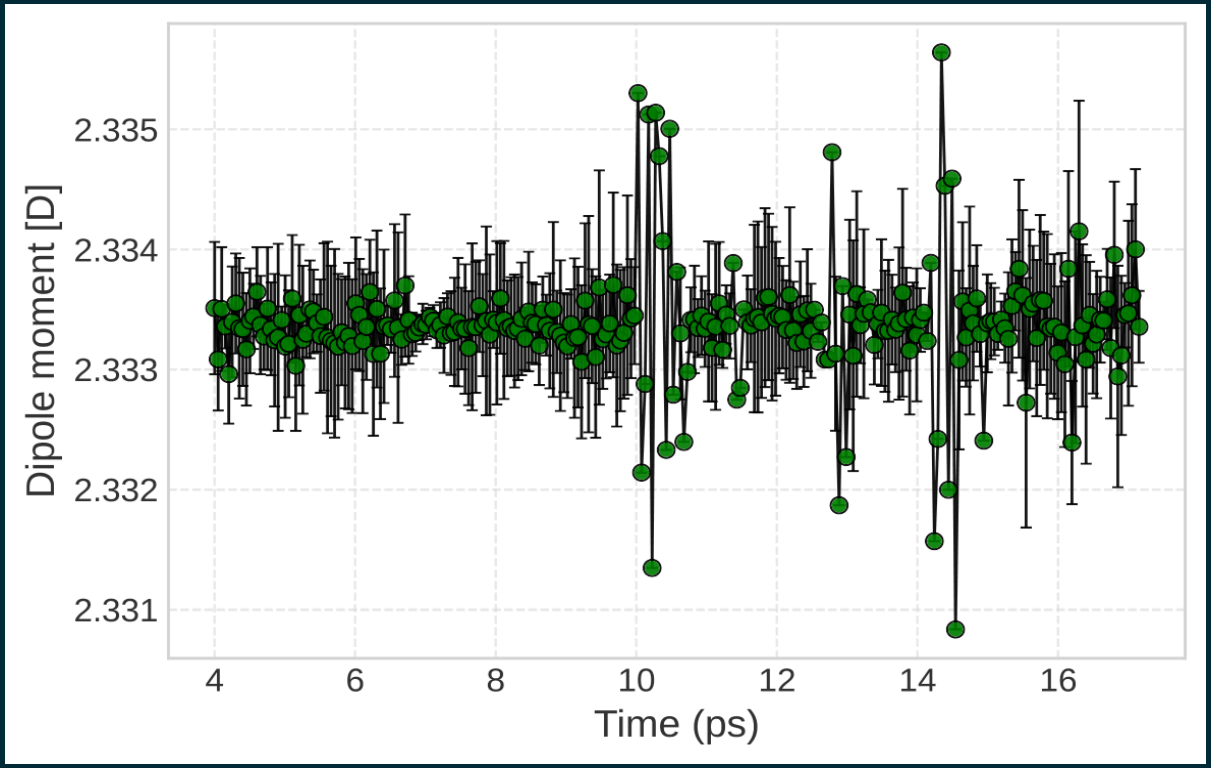

Dipole fluctutation of water molecules

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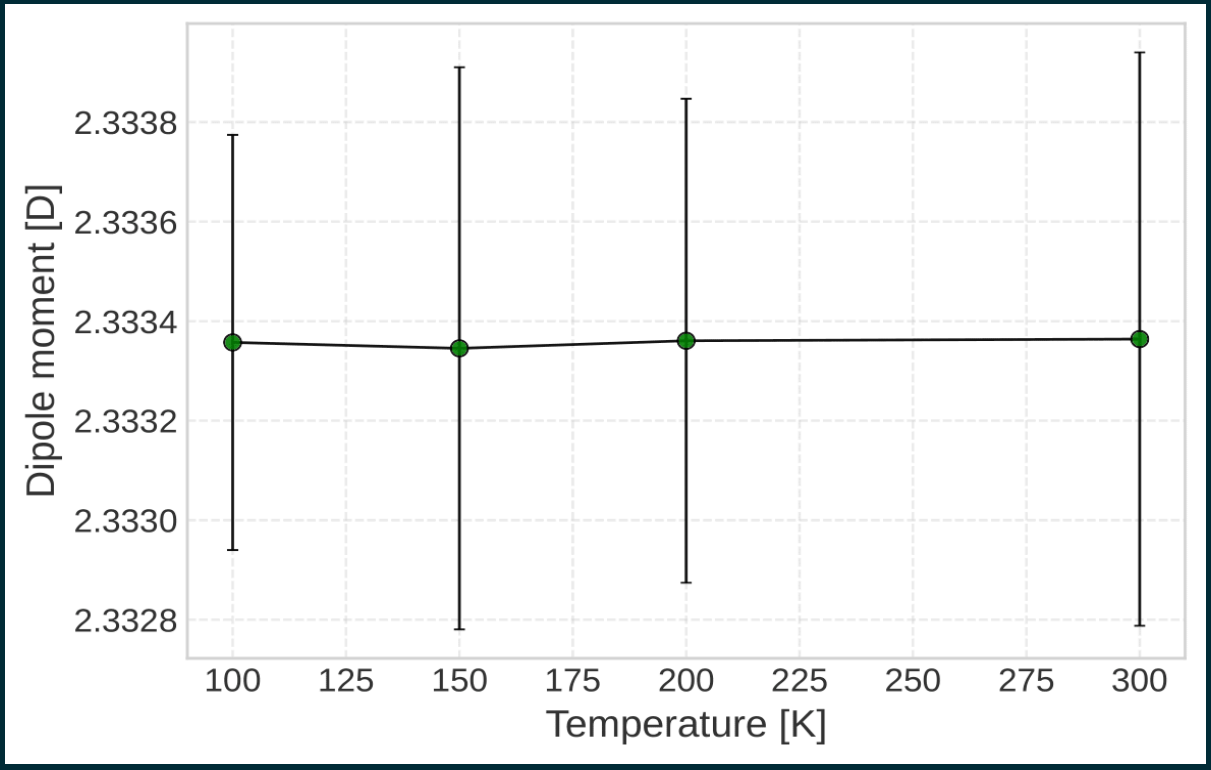
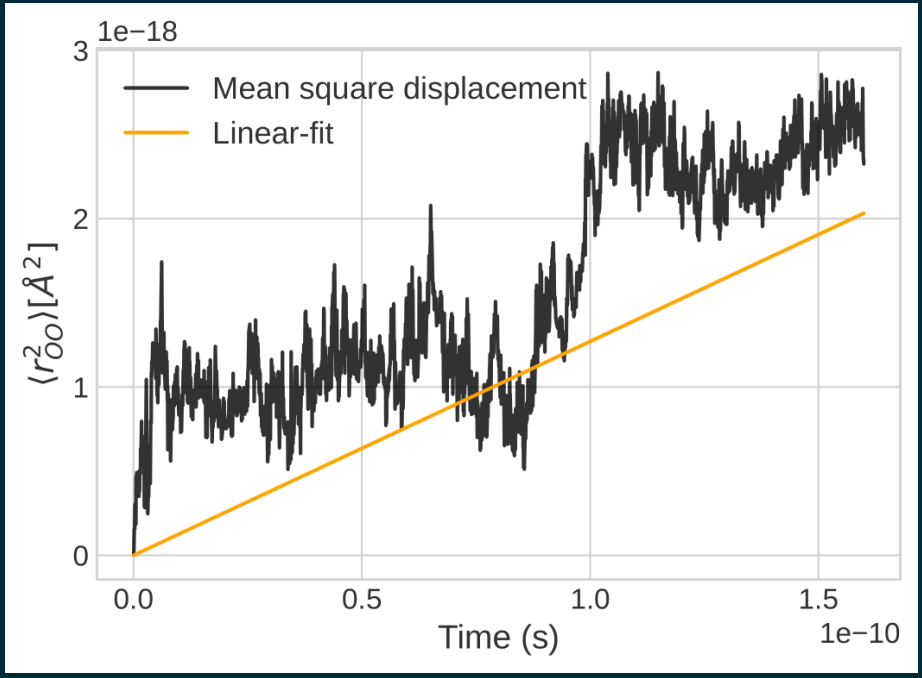
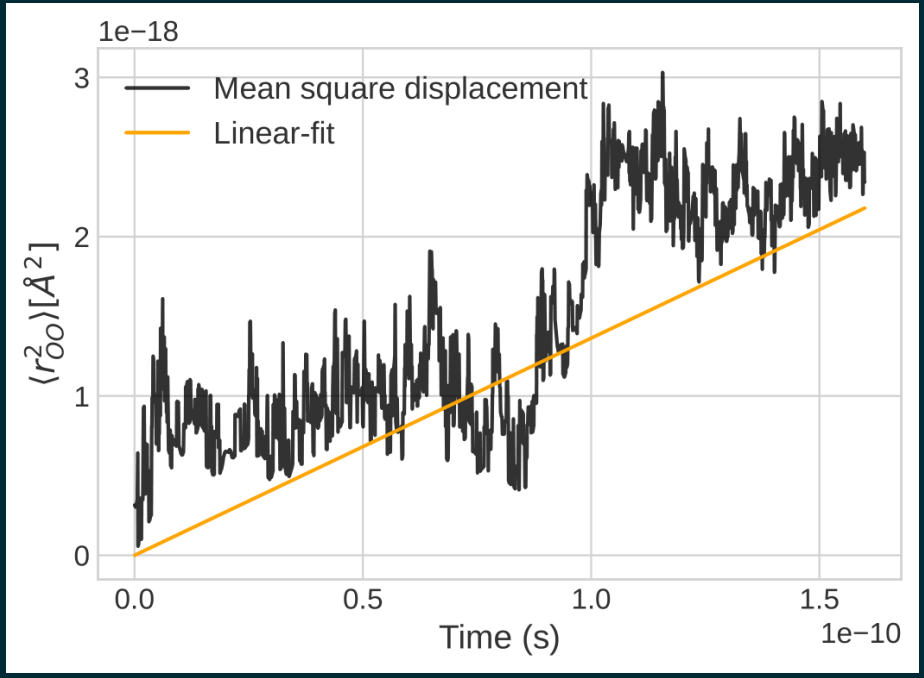


DIFFUSION CONSTANT AT 300 K

Hydrogen



Oxygen