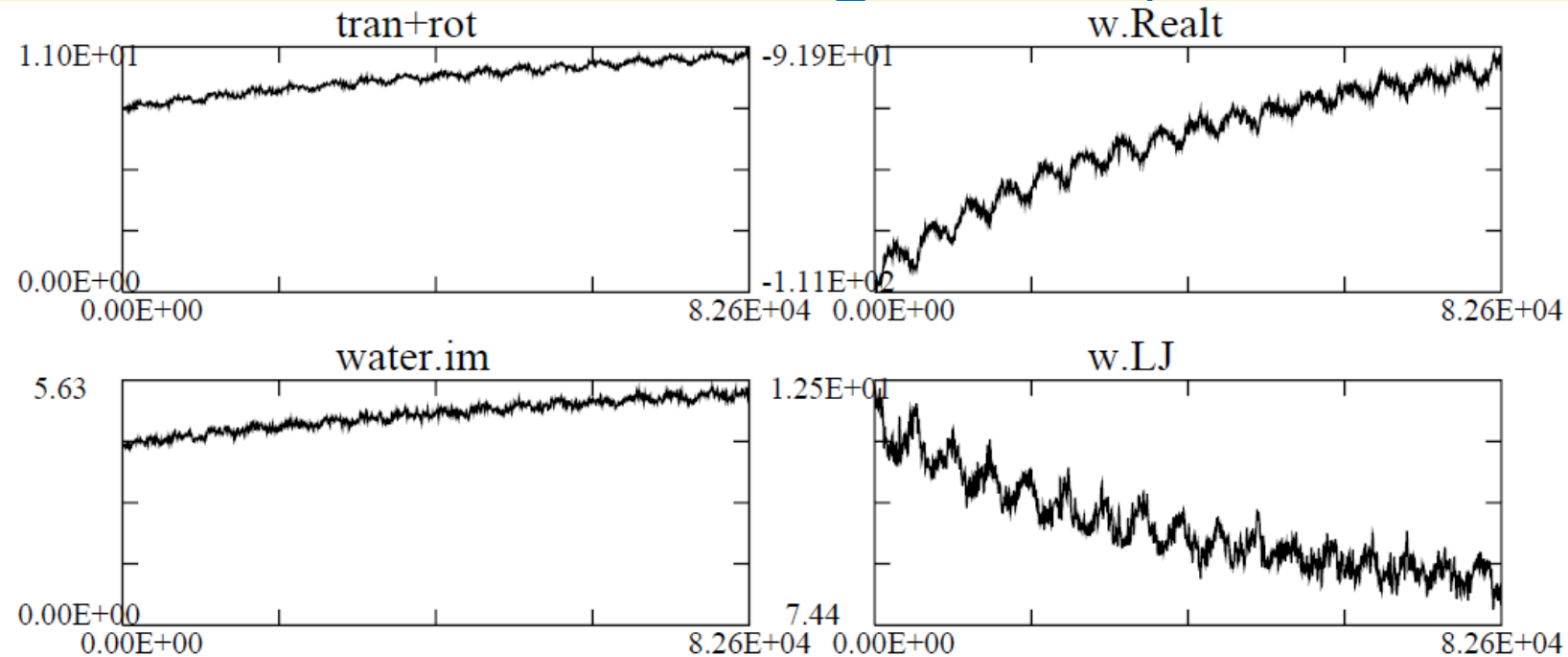


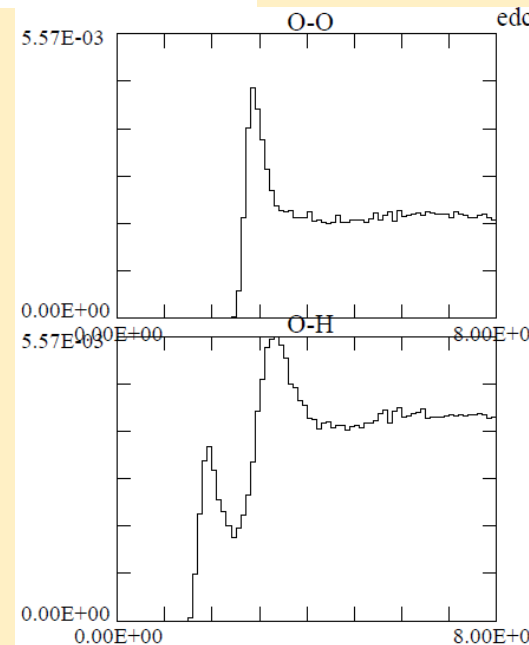
# ***Molecular Dynamics Simulations of Water and Ice by TIP5P Code***

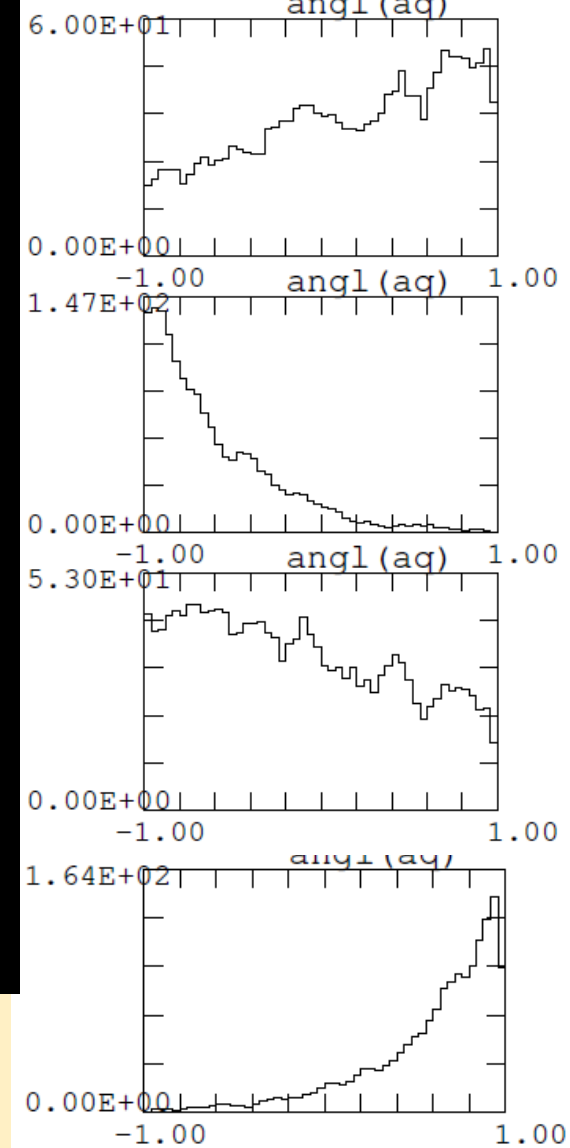
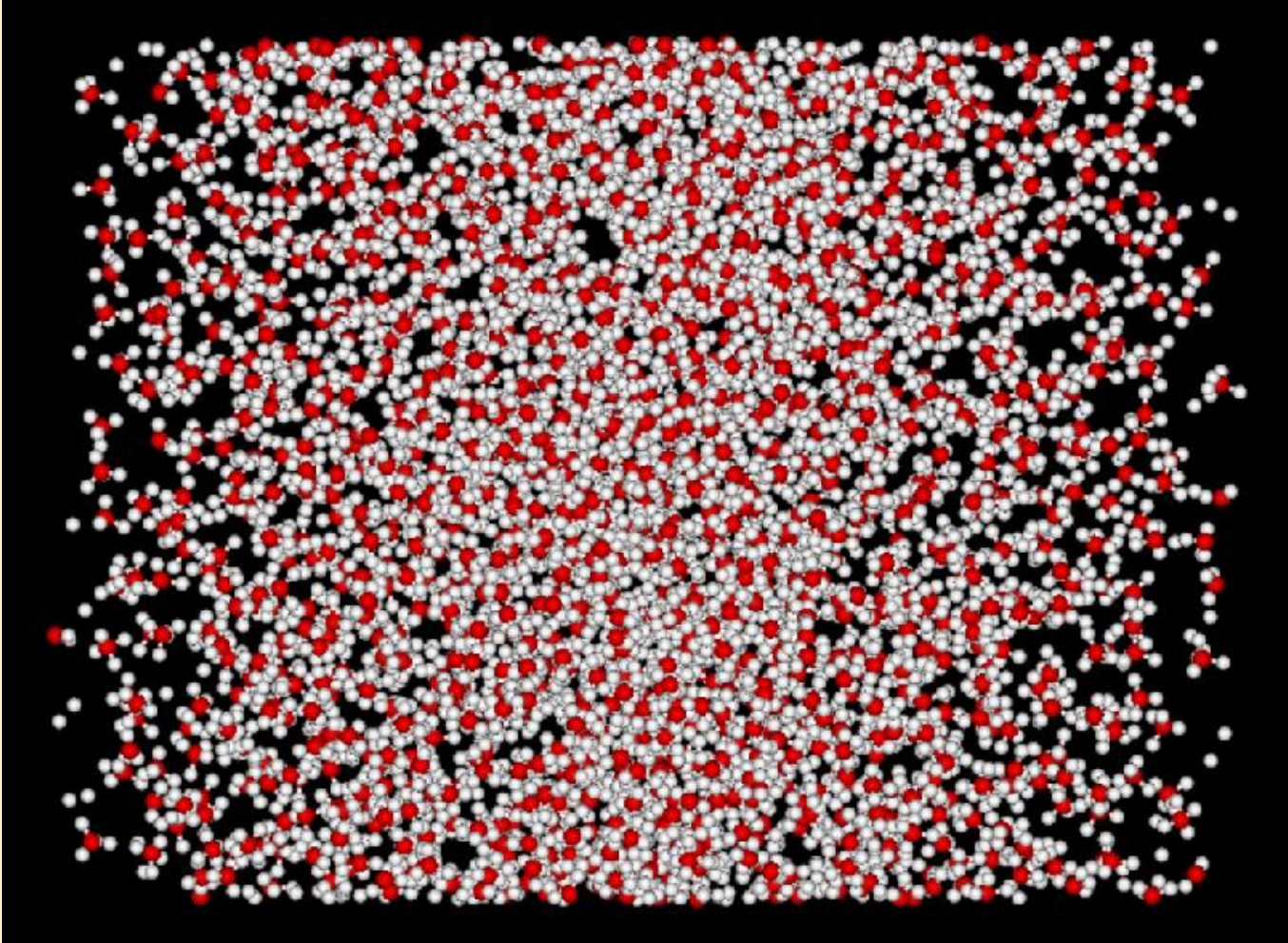
*Motohiko Tanaka, Ph.D., Professor  
Graduate School of Chubu University  
Kasugai 487-8501, Japan*

# Simulation water starting at 298 K, NVE



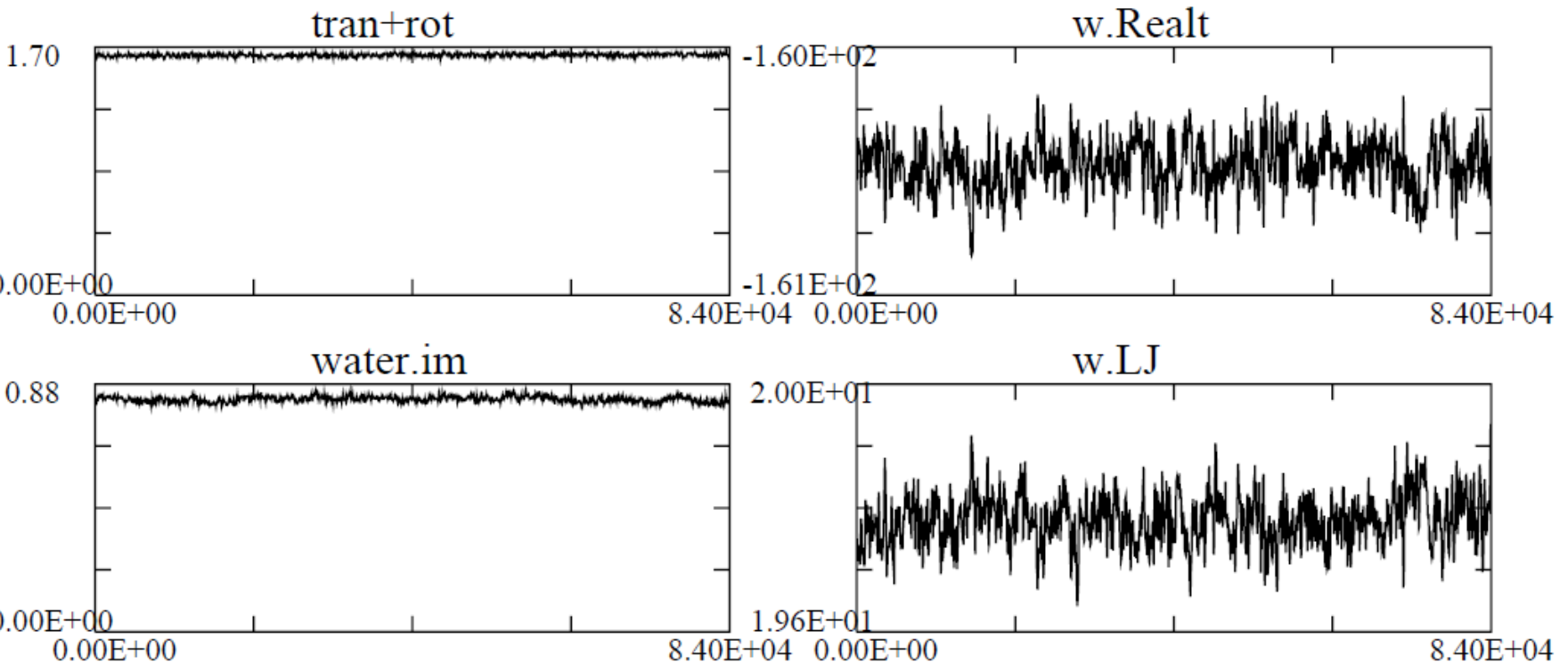
The time  $t=82,600$  starting from 298 K with 1728 water molecules, imposed electric field 10 GHz in x-direction with  $E_0 = 5 \times 10^6$  V/cm and NV run (by 8.3 periods). Left: a) Total kinetic energy, b) rotational energy only, c) Coulombic energy, Lennard-Jones energy. The final temperature is about 405 K. Right: Pair distribution functions of a) O-O atoms, b) O-H atoms in  $R=0-8$  Angstrom. O and H atoms are thus mixed showing heavy water interactions. Compare with the frozen ice of 230 K.



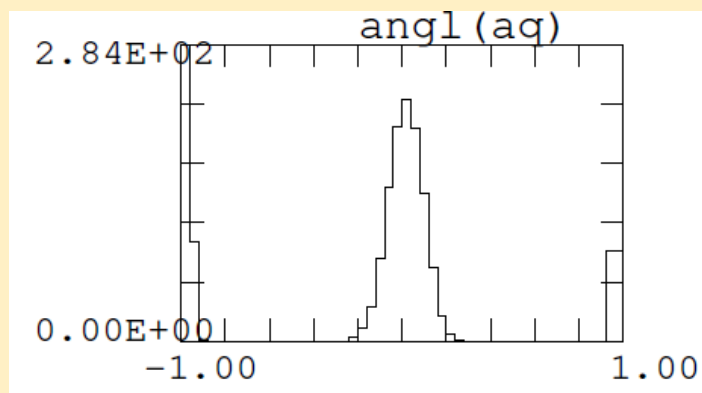


Water molecules starting 298 K.  
 Left: Scatter plot of water at  $t=80,000$ , b) x-directional cosine distribution for the cross bins of  $(-1.0, 1.0)$  at  $t=72,500$  to  $80,000$ . Due to phase lag of molecules compared to imposed electric field, water is largely heated,

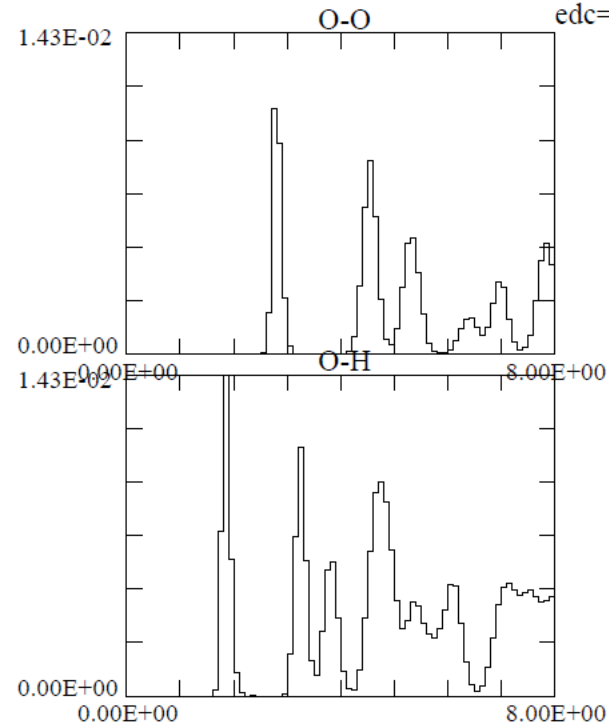
# Simulation starting at ice 230 K, NVE



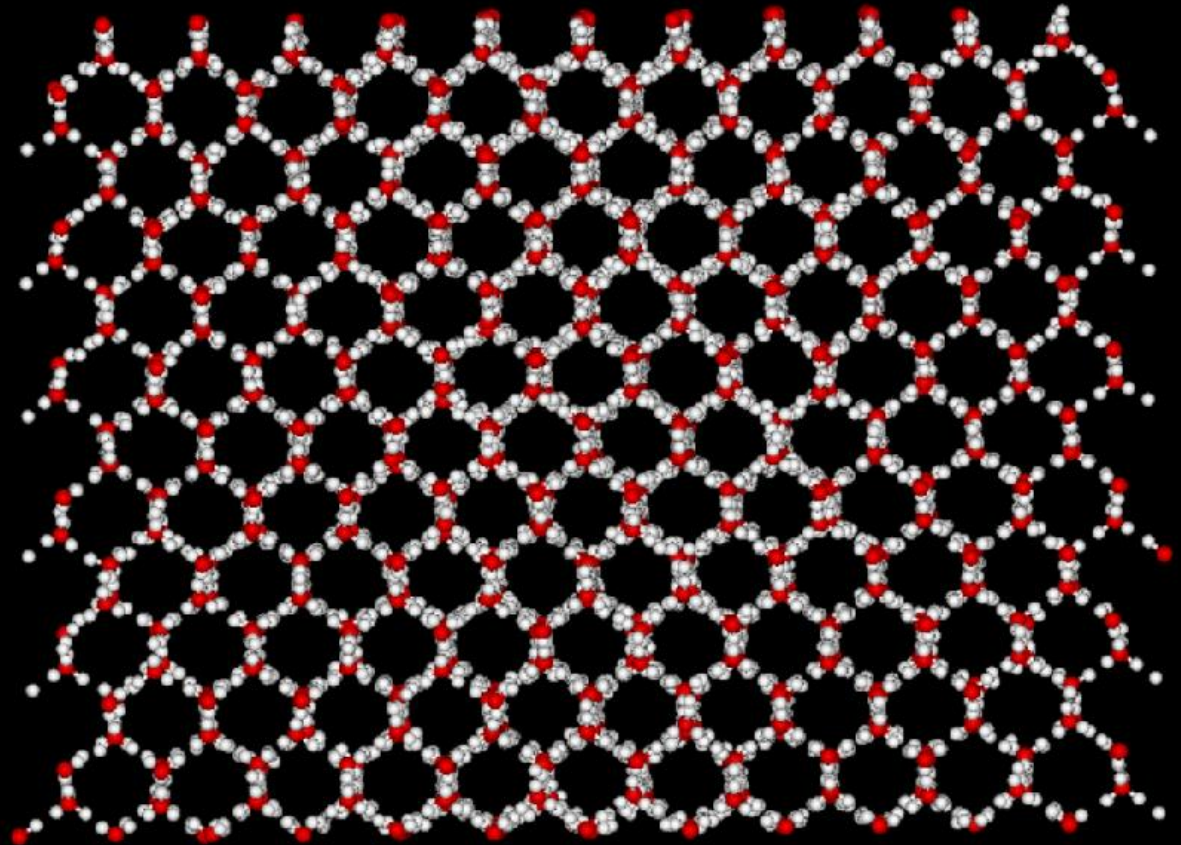
At temperature 230 K of 1728 water molecules, AC electric field 10 GHz in the x-direction with intensity  $E_0 = 5 \times 10^6$  V/cm. Left: a) total kinetic energy, b) rotational energy only, c) Coulombic energy, d) Lennard-Jones energy, at the time of  $t=84,000$ . Right: cosine distribution of water in Bins  $(-1,1)$  of the x-direction. No oscillations are really found at the imposed electric field.







Time  $t=80,000$  of the temperature 230 K.  
Right: Scatter plot of water molecules where ice is frozen by 6-membered water clusters.



# References

1. “Classical Mechanics”, H. Goldstein, C. Poole, J. Safko, 3rd Edition, Pearson Education Inc., England, 2003.
2. “Microwave heating of water, ice and saline solution: Molecular dynamics study”, M.Tanaka and M.Sato, J.Chem.Phys., 126, 034509 1-9 (2007).
3. “Microwave heating of water and ice by TIP5P code”, M. Tanaka, <https://github.com/Mtanaka77/> (May 2023).
4. “Microwave heating and collapse of methane hydrate by molecular dynamics simulations, M. Tanaka, M. Sato, and S. Nakatani, arXiv.1909.01024, Cornell University, 2019, USA