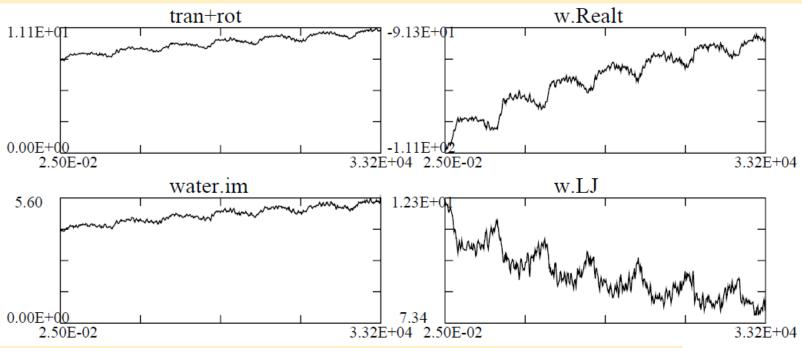
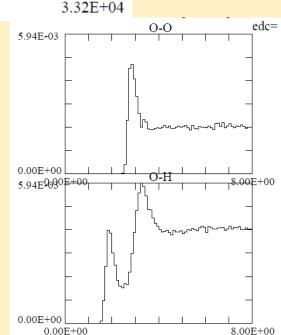
## Molecular Dynamics Simulation of Water and Ice by TIP5P Code

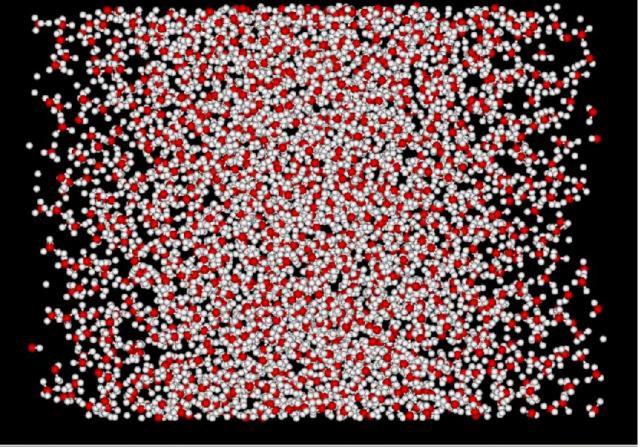
Motohiko Tanaka, Ph.D., Professor Graduate School of Chubu University Kasugai 487-8501, Japan

## \* Simulation water starting from 298 K \*



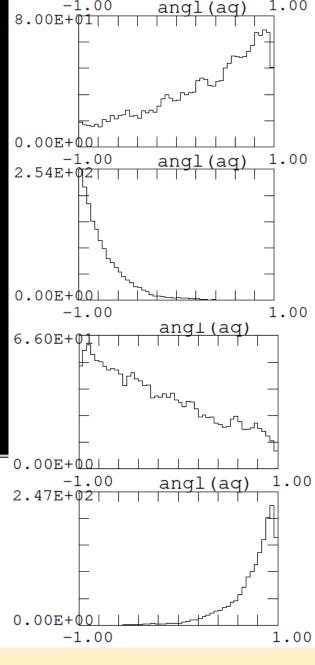
Time t=33,200 starting from 298 K with 1728 water molecules, imposed electric field 10 GHz in x-direction with E\_0= 5x10^6 V/cm (about 3.2 periods). Left: a) Total kinetic energy, b) rotational energy only, c) Coulombic energy, Lennard-Jones energy. Right: Pair distribution functions of a) O-O atoms, 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.



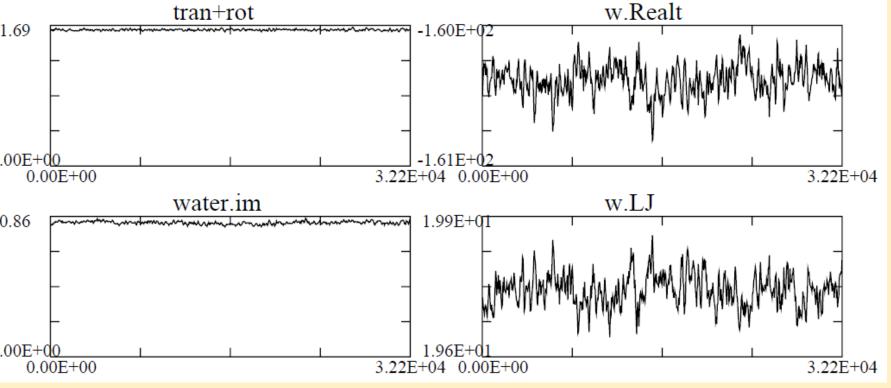


Water molecules at 298 K.

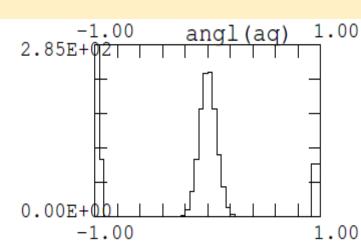
Left: Scatter plot of water at t=32,500, b) x-directional cosine distribution for the cross bins of (-1.0,1.0) at t=27,500 to 32,500. Due to phase lag of molecules compared to imposed electric field, water is largely heated,

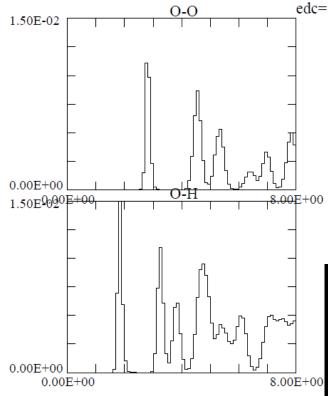


## \* Simulation starting from ice at 230 K \*



At temperature 230 K of 1728 water molecules, AC electric field 10 GHz in the x-direction with intensity E\_0= 5x10^6 V/cm. Left: a) total kinetic energy, b) rotational energy only, c) Coulombic energy, d) Lennard-Jones energy, at time of t=32,300. Right: cosine distribution of water in Bins (-1,1) of the x-direction. No oscillations are really found at the imposed large electric field.





Time t=30,000 of temperature 230 K. Left: a) Pair distribution functions of O-O atoms b) O-H atoms for R=0-8 Angstrom. Peaks are well separated at this temperature. Right: Scatter plot of water molecules where 6-membered rings are formed for frozen ice.

