Figures of molecular dynamics simulation of water and ice by TIP5P code

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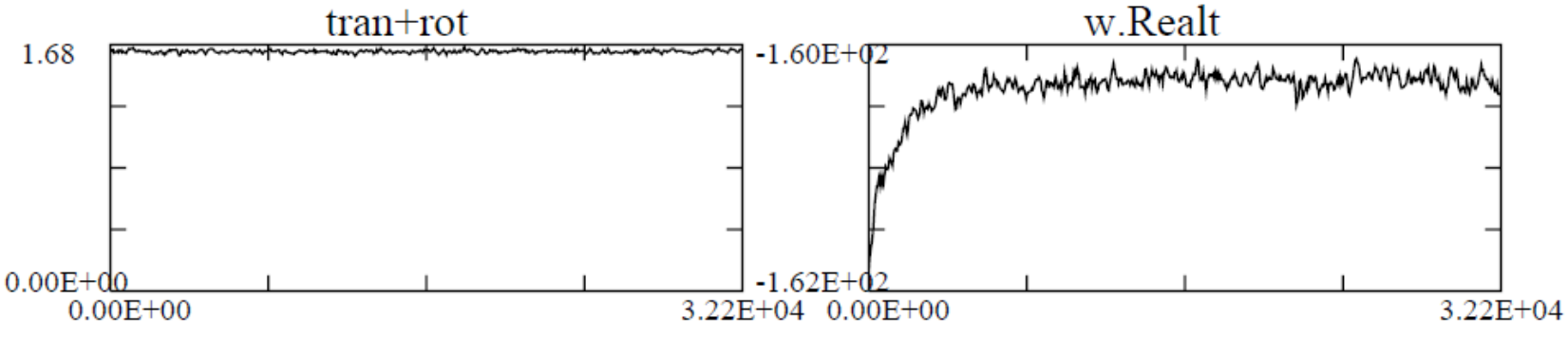
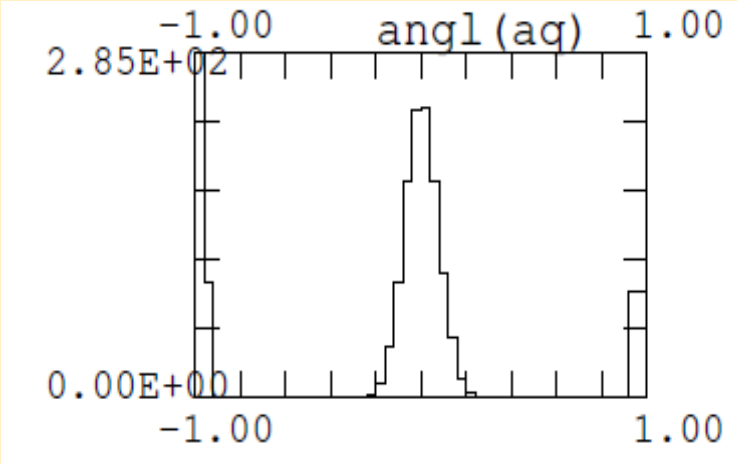
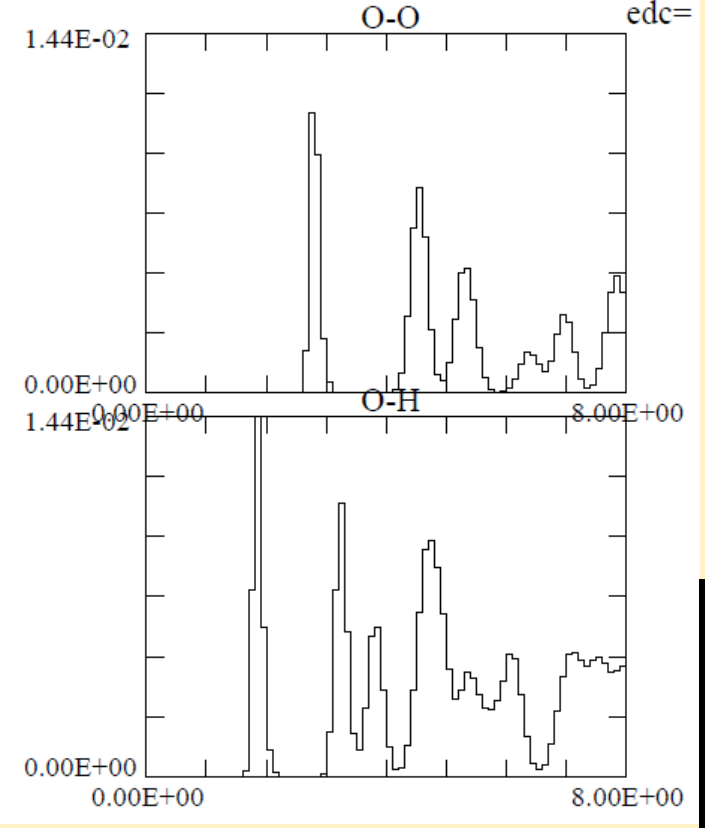
Simulation starting from ice state at 230 K

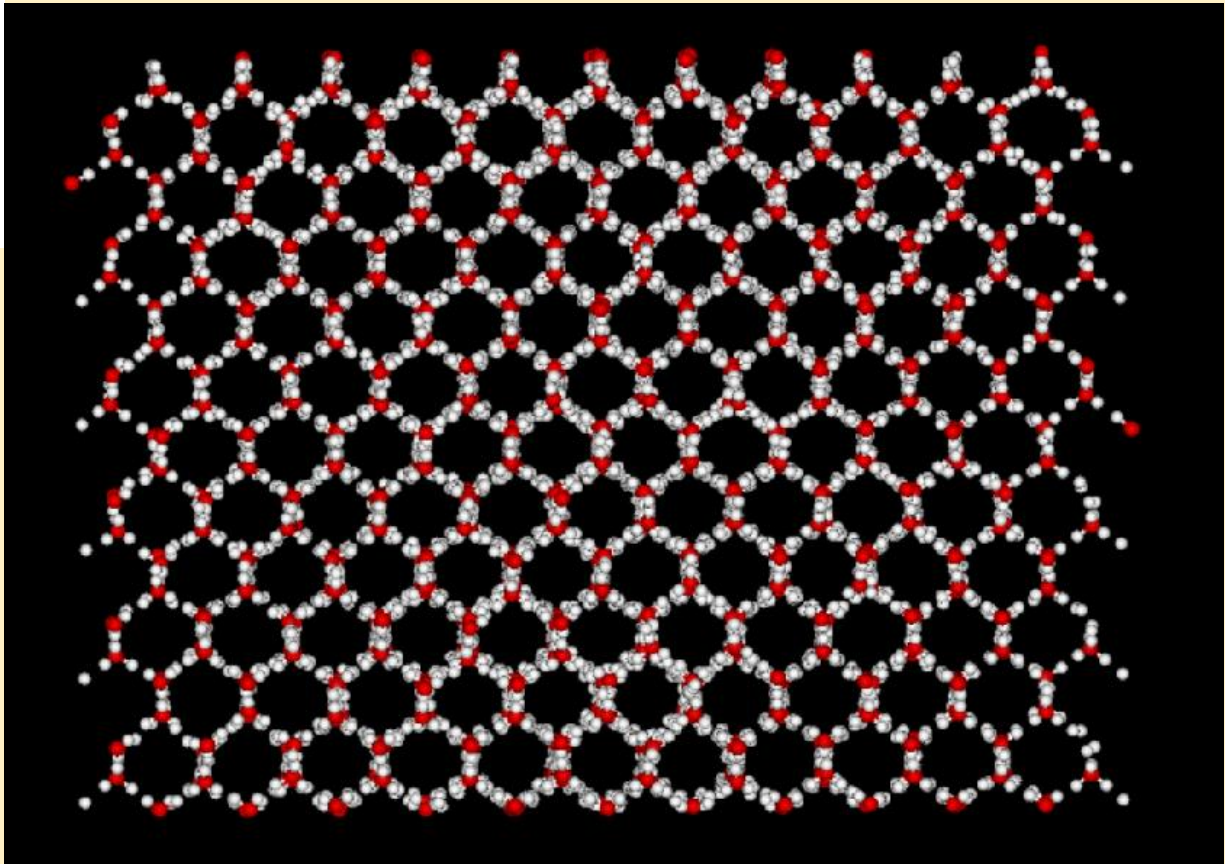


At temperature 230 K of 1728 water molecules, AC electric field 10 GHz in the x-direction with intensity E_0= 10x10^6 V/cm. Left: a) total kinetic energy, b) rotational energy only, c) Coulombic energy, d) Lennard-Jones energy, at time of t=32,200. Right: cosine distribution of water in the x-direction. No oscillations are found at imposed large electric field.

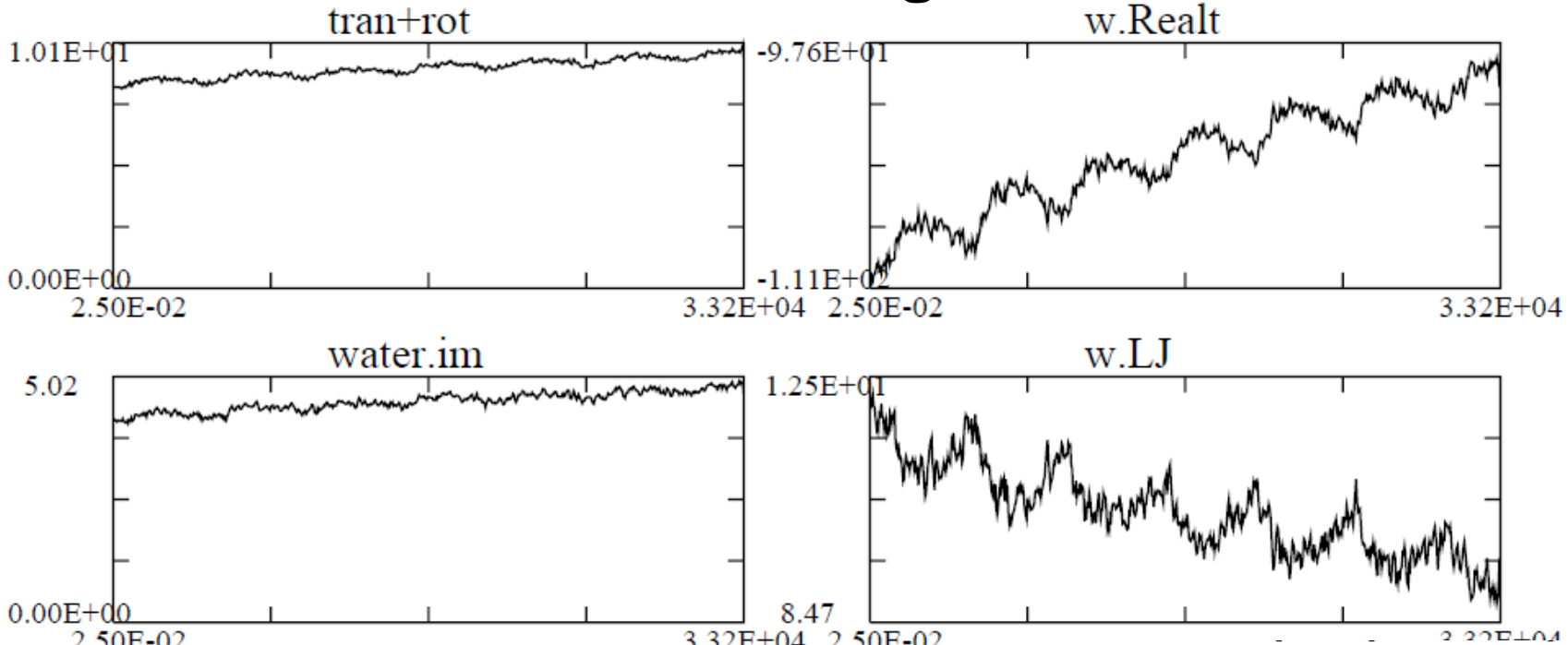




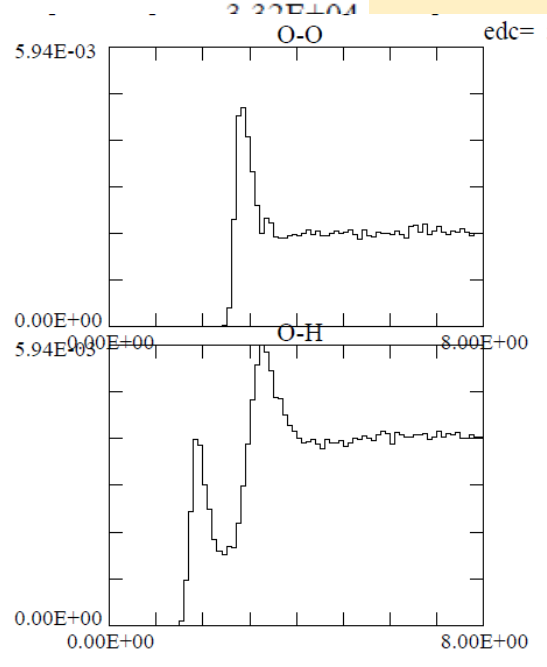
Time t=32,000 of temperature 230 K.
Left: a) pair distribution functions of O–O atoms b) O–H atoms for R=0–8 Angstrom. Peaks are well separated at this temperature.
Right: scatter plot of water molecules where 6–membered rings are formed for frozen ice.

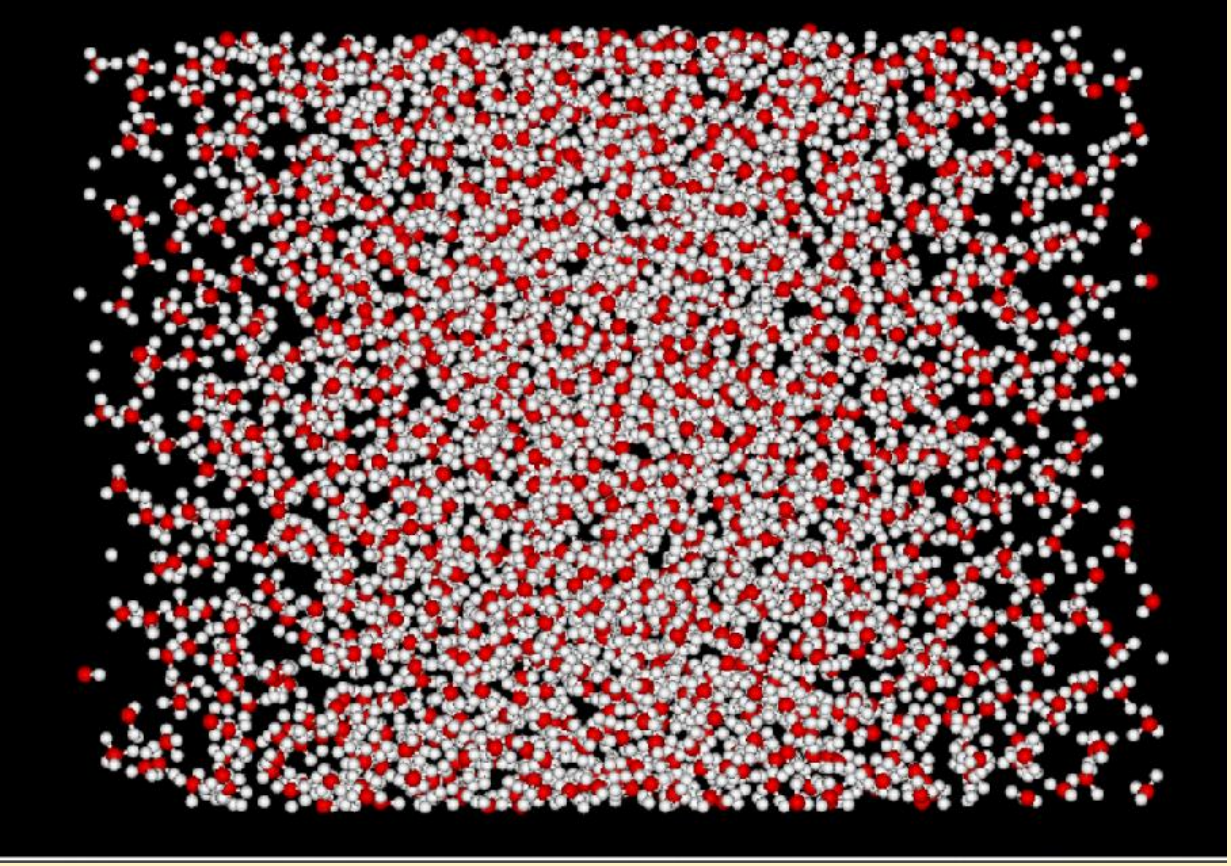


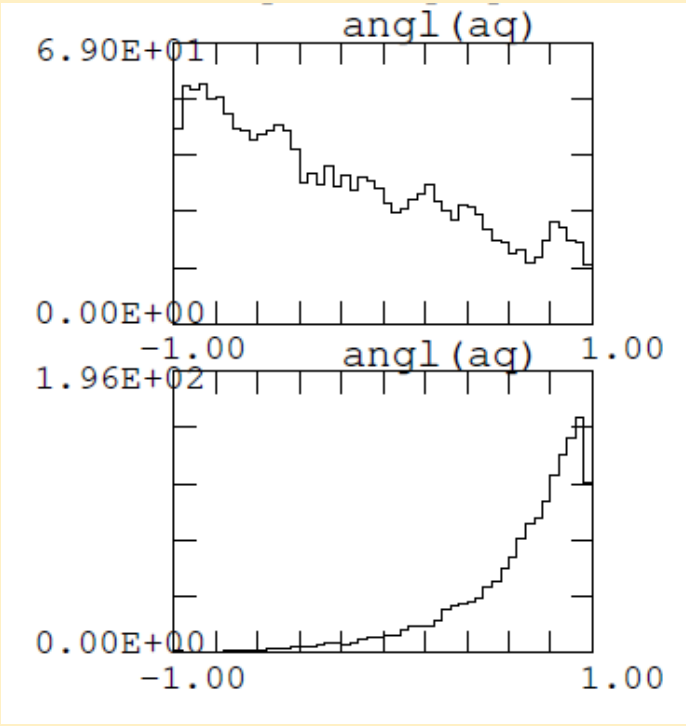
Simulation water state starting from 298 K



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 separated due to water interactions.







At t=33,000 of water molecules.
Left: scatter plot of water, b) x−directional cosine distribution for the cross section x= (−1,1). Due to phase lag of molecules compared to imposed electric field, water is largely heated,