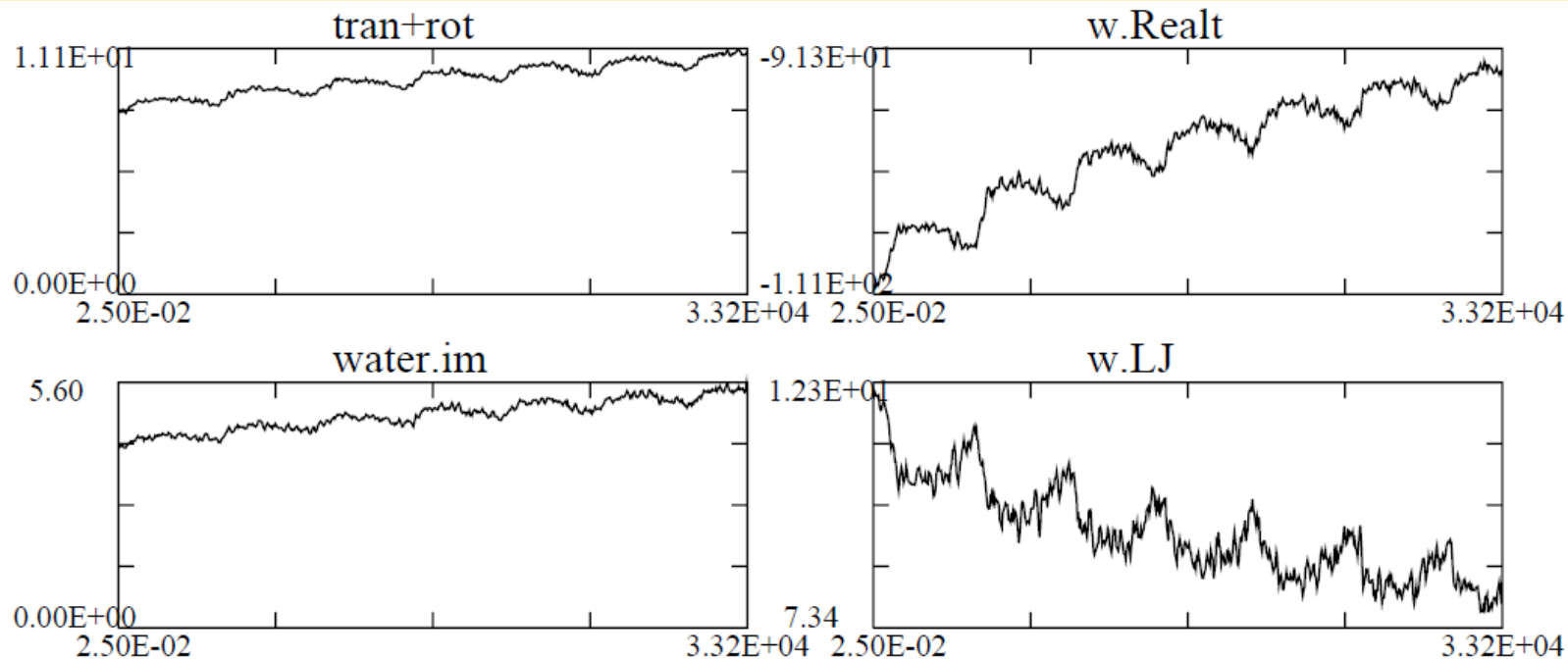


# ***Molecular Dynamics Simulation of Water and Ice by TIP5P Code***

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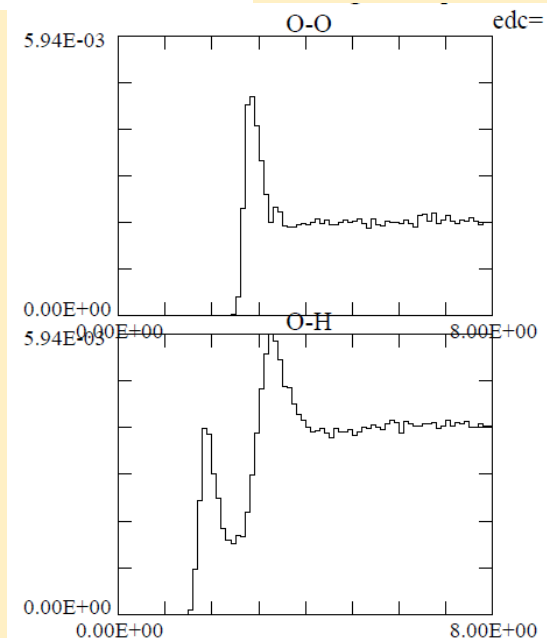
# \* Simulation water starting from 298 K \*

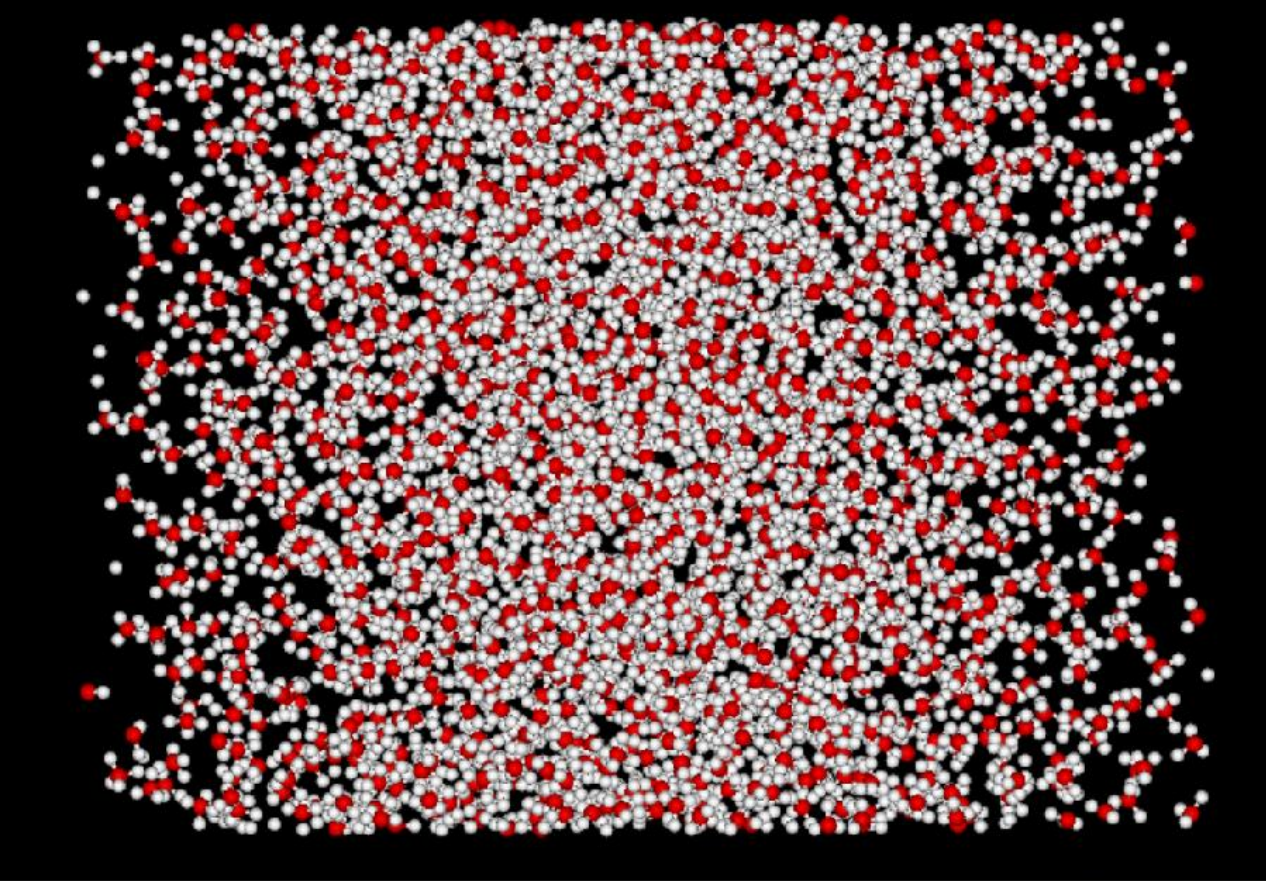


Time  $t=33,200$  starting from 298 K with 1728 water molecules, imposed electric field 10 GHz in x-direction with  $E_0 = 5 \times 10^6$  V/cm (about 3.2 periods).

Left: a) Total kinetic energy, b) rotational energy only, c) Coulombic energy, Lennard-Jones energy.

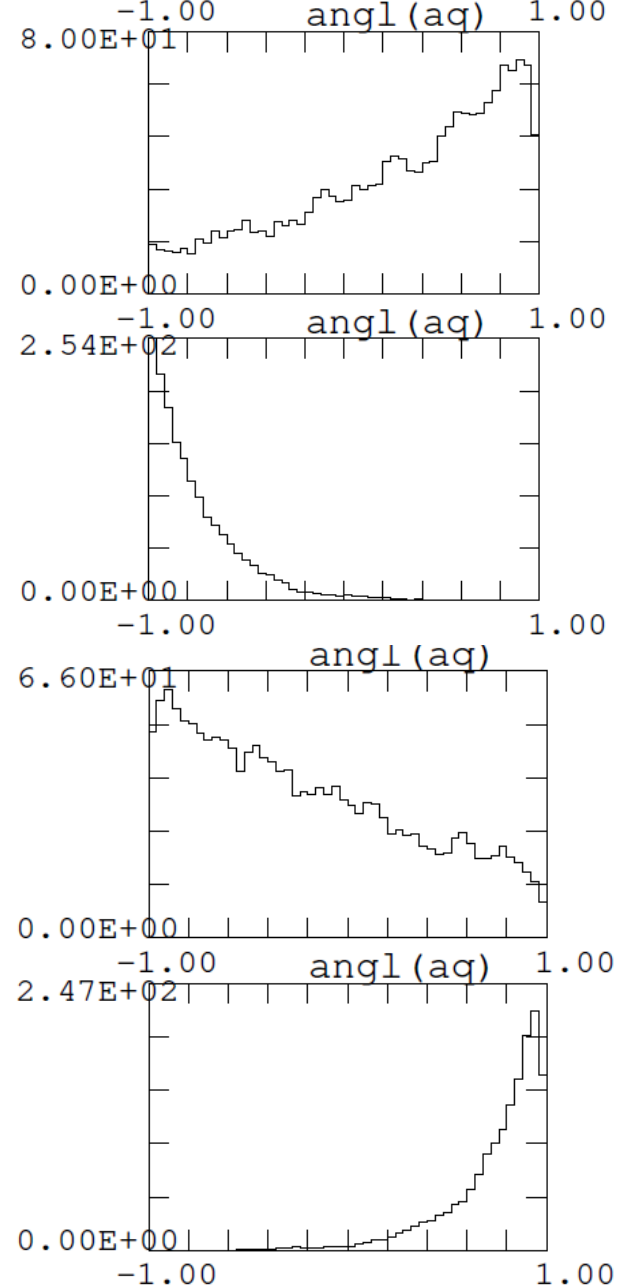
Right: Pair distribution functions of a) O-O atoms, b) O-H atoms in  $R=0-8$  Angstrom. O and H atoms are thus mixed showing heavy water interactions. Compare with the frozen ice of 230 K.



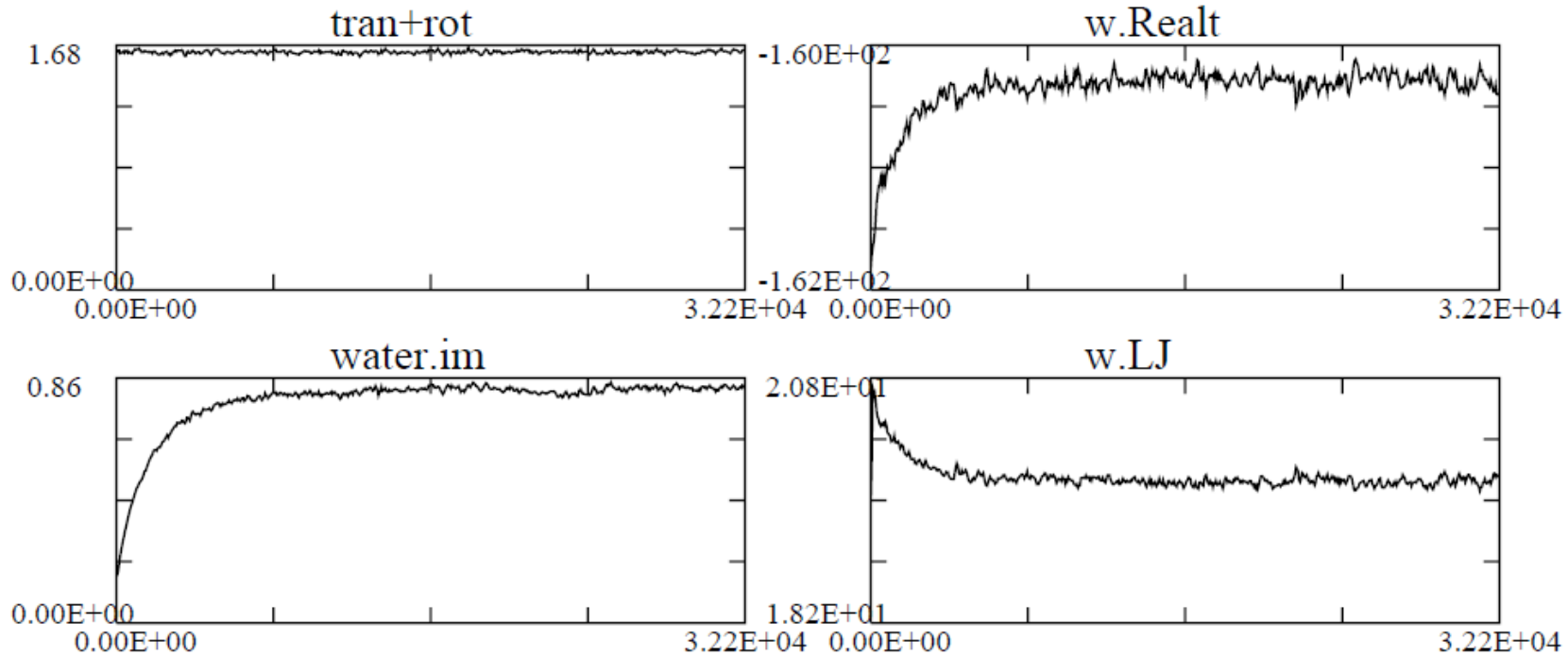


Water molecules at 298 K.

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  $E_0 = 10 \times 10^6$  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 really found at imposed large electric field.

