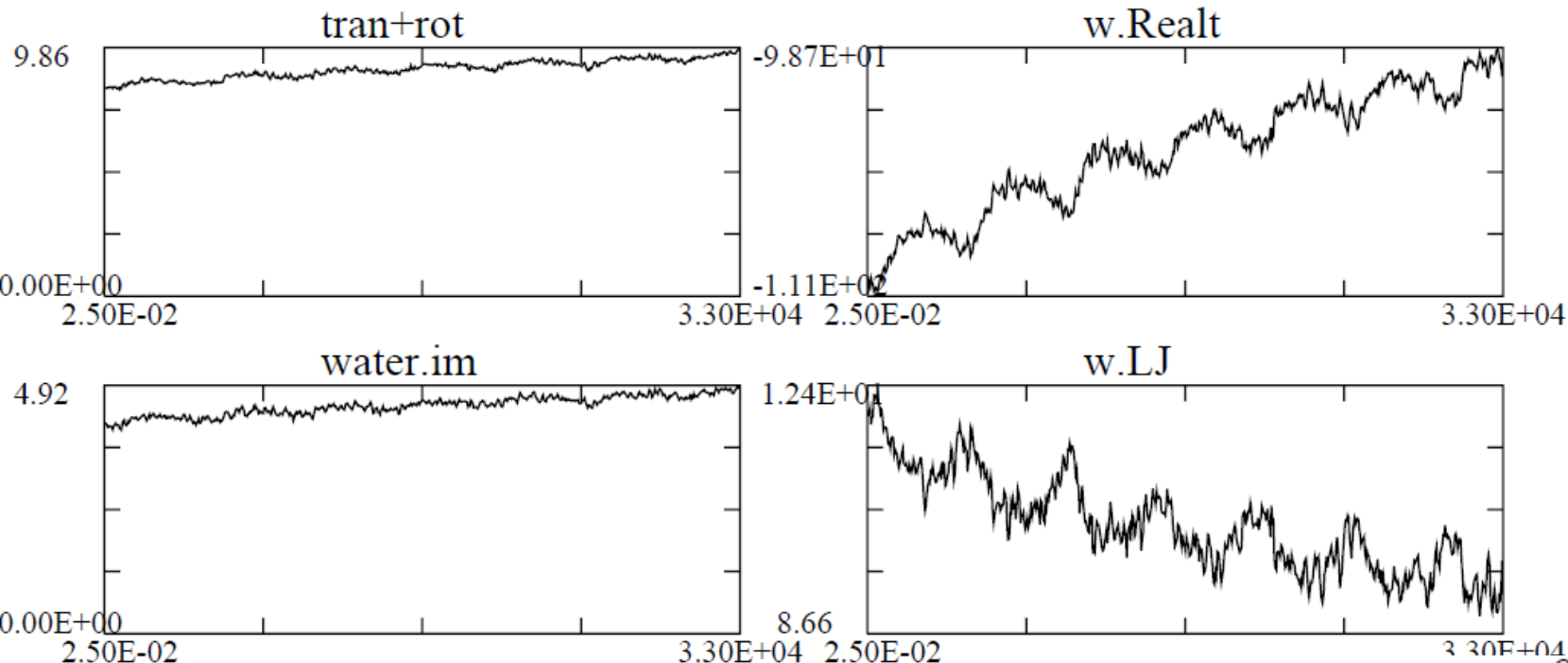


# ***Molecular Dynamics Simulation of Water and Ice by TIP5P Code***

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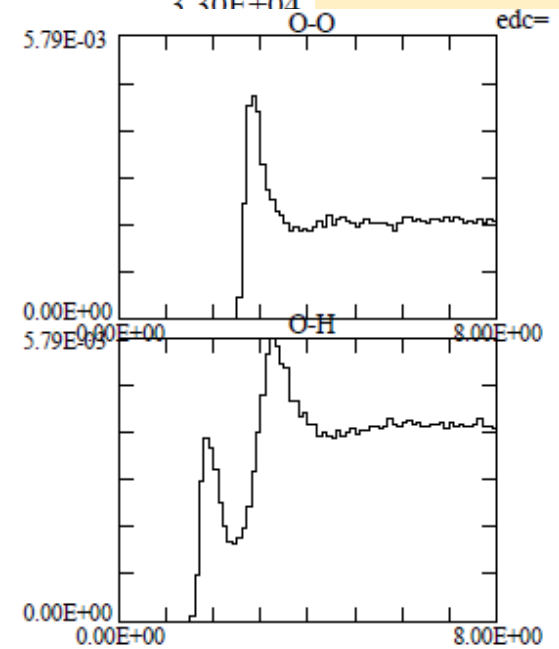
# \* Simulation water starting from 298 K

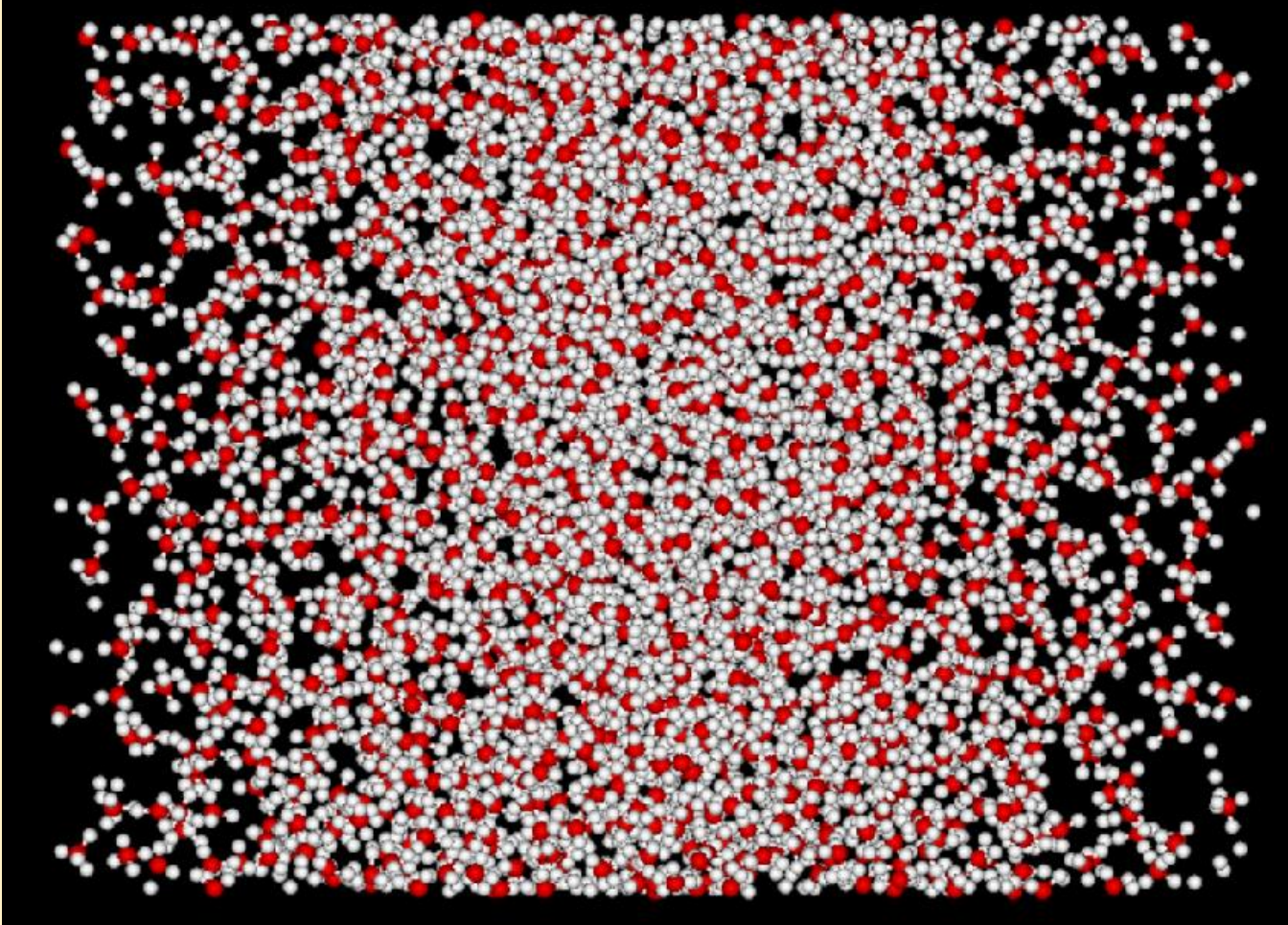


Time  $t=33,000$  starting from 298 K with 1728 water molecules, imposed electric field 10 GHz in x-direction with  $E_0 = 5 \times 10^6$  V/cm (by 3.3 periods).

Left: a) Total kinetic energy, b) rotational energy only, c) Coulombic energy, Lennard-Jones energy. The final temperature is about 365 K.

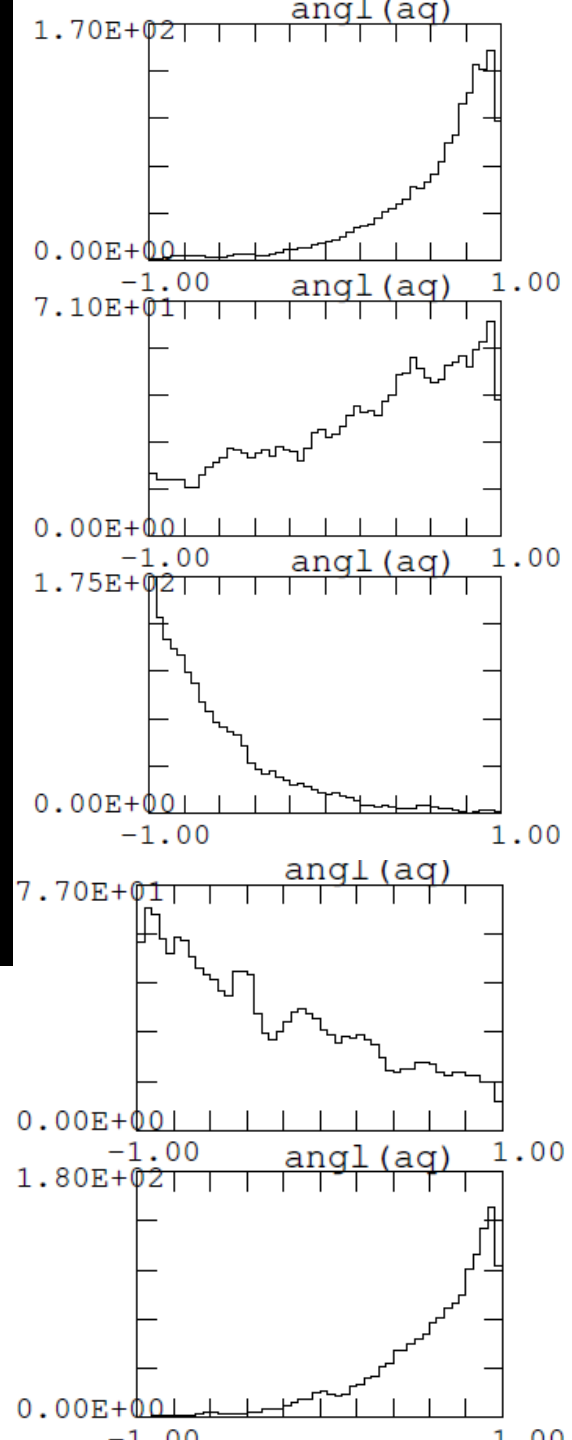
Right: Pair distribution functions of a) O-O atoms, b) O-H atoms in  $R=0-8$  Angstrom. O and H atoms are thus mixed showing heavy water interactions. Compare with the frozen ice of 230 K.



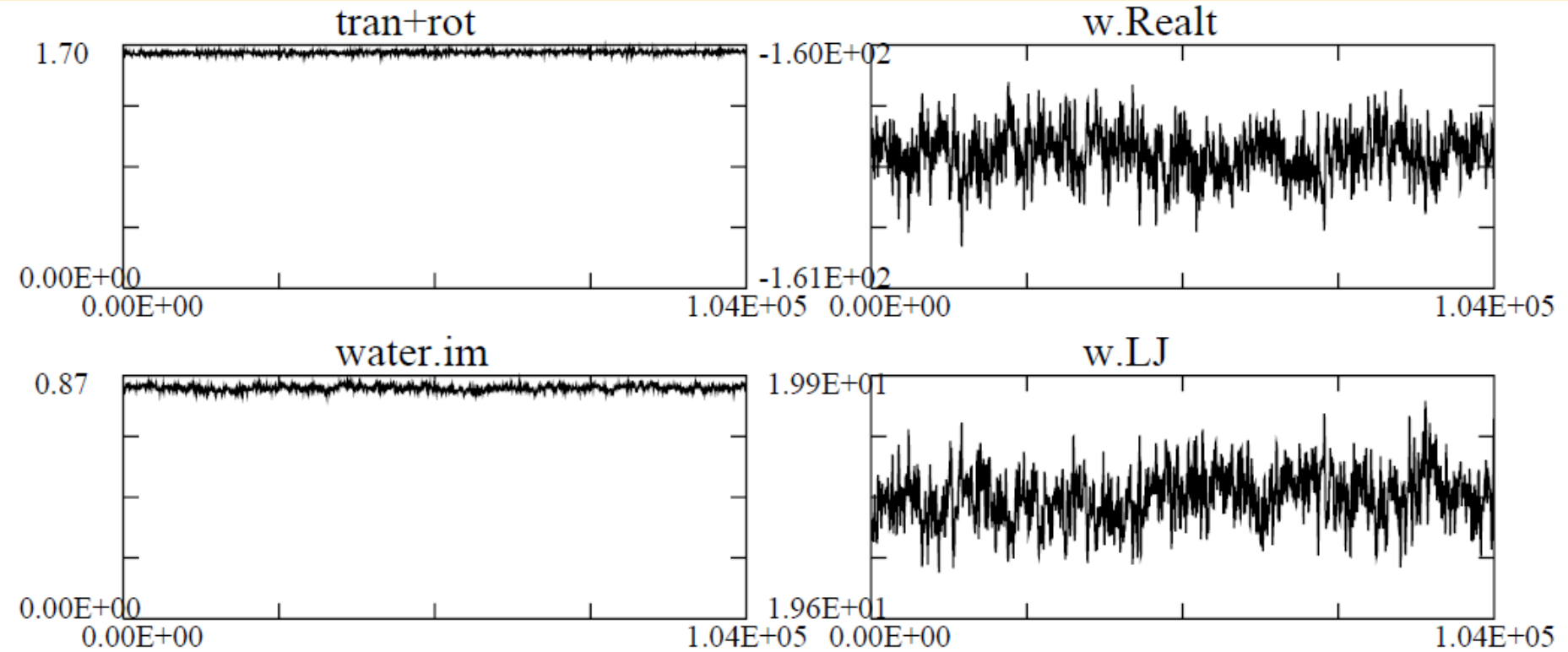


Water molecules at 298 K.

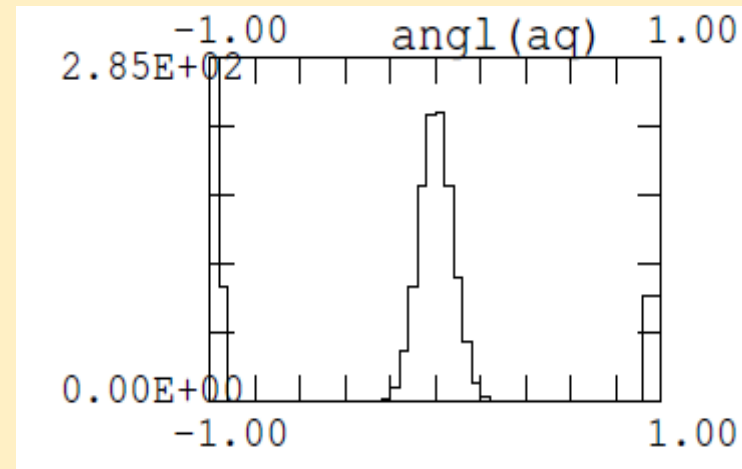
Left: Scatter plot of water at  $t=32,500$ , b) x-directional cosine distribution for the cross bins of  $(-1.0, 1.0)$  at  $t=22,500$  to  $32,500$ . Due to phase lag of molecules compared to imposed electric field, water is largely heated,



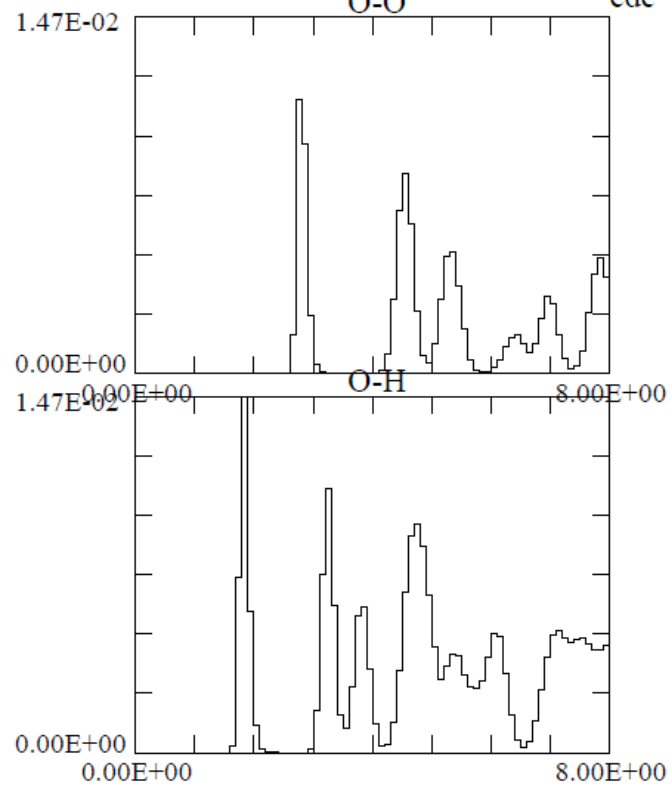
## \* Simulation starting from ice at 230 K



At temperature 230 K of 1728 water molecules, AC electric field 10 GHz in the x-direction with intensity  $E_0 = 5 \times 10^6$  V/cm. Left: a) total kinetic energy, b) rotational energy only, c) Coulombic energy, d) Lennard-Jones energy, at the time of  $t=104,000$ . Right: cosine distribution of water in Bins  $(-1,1)$  of the x-direction. No oscillations are really found at the imposed electric field.







Time  $t=104,000$  of the 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.

