Molecular Dynamics Simulations of Water and Hydrate Molecules by TIP5P Code

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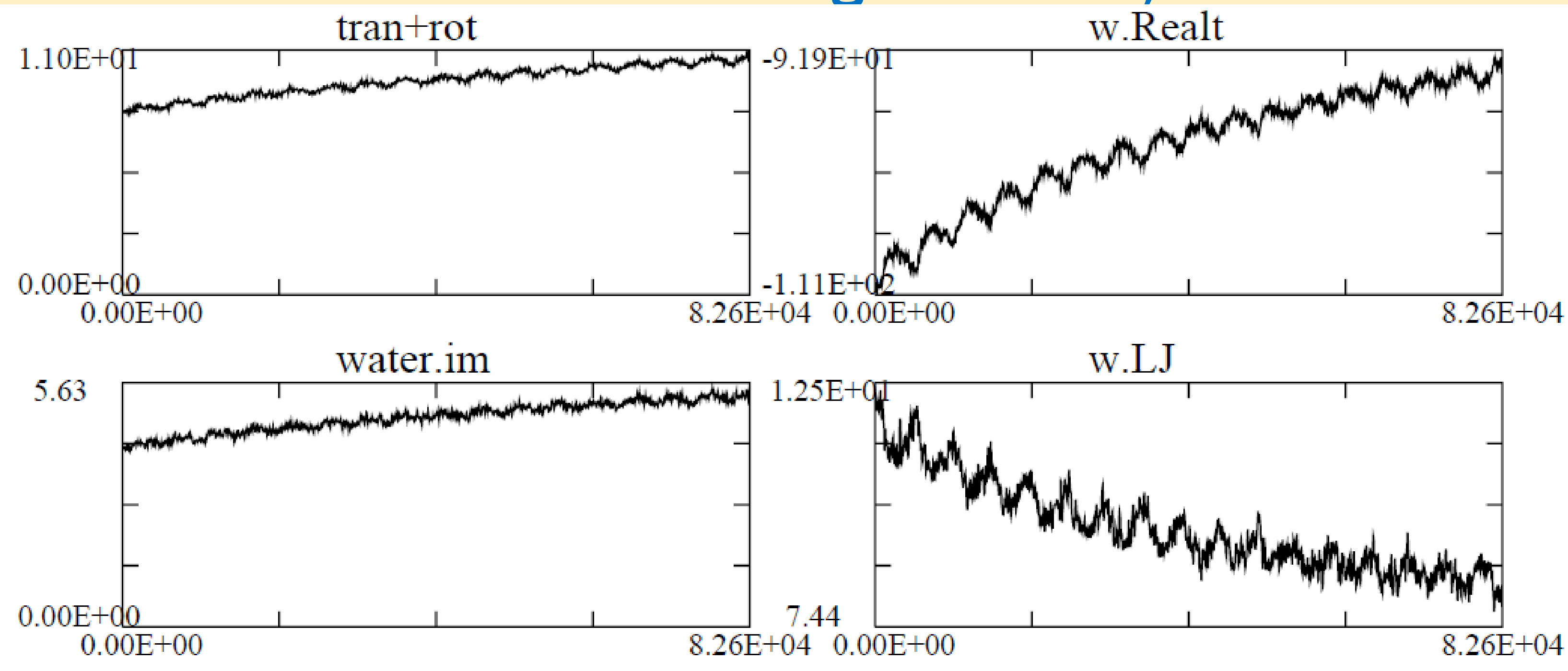
Dielectric constant of water and ice

Water dielectric constant in temperature. It changes slowly for less than 273 K, and after phase transition it becomes rapidly for > 273 K. (Eyring et al., PNAS, 1966).

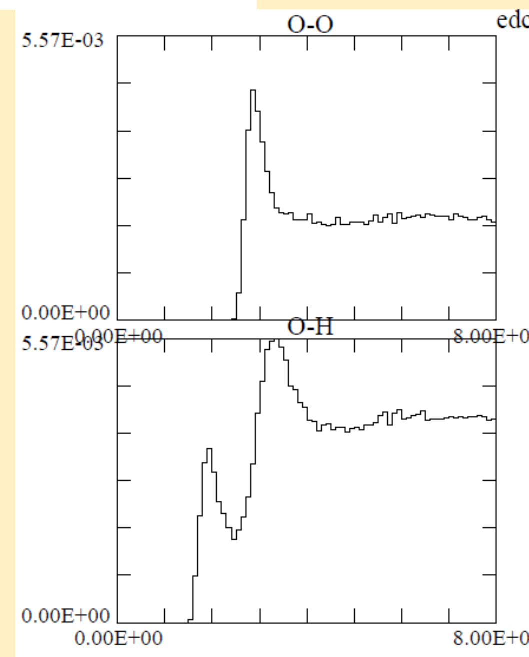
Water T (K),	Dielectric constant of liquid	
273 K	88	<- 298 K, $\varepsilon = 80$
373 K	56	
473 K	35	

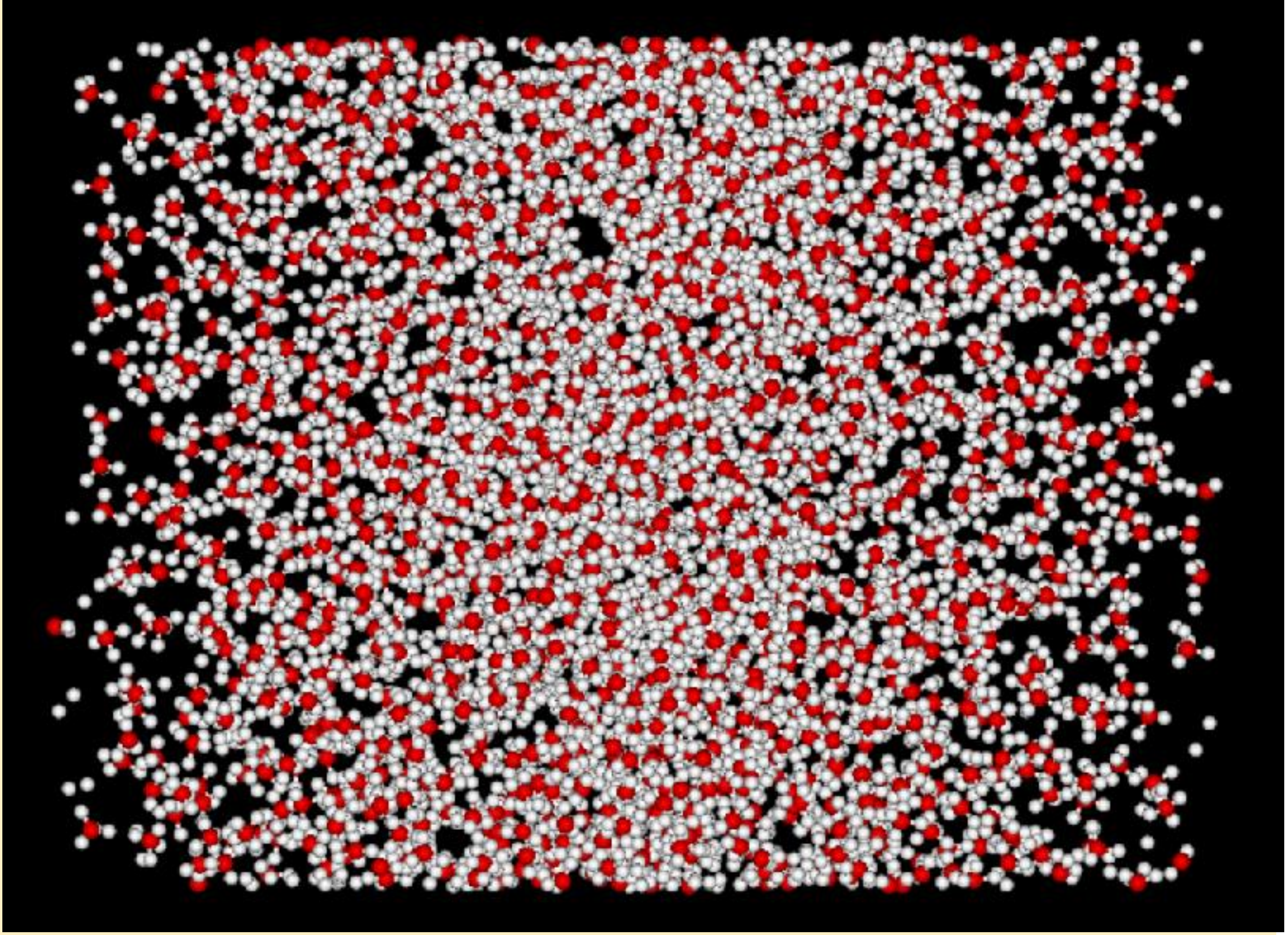
Ice I, T (K),	Dielectric constant	
273 K	91.5	
262.3 K	95.0	
252.2 K	97.4	
241 K	100	
228.4 K	104	<- 230 K, $\varepsilon = 104$
216.3 K	114	

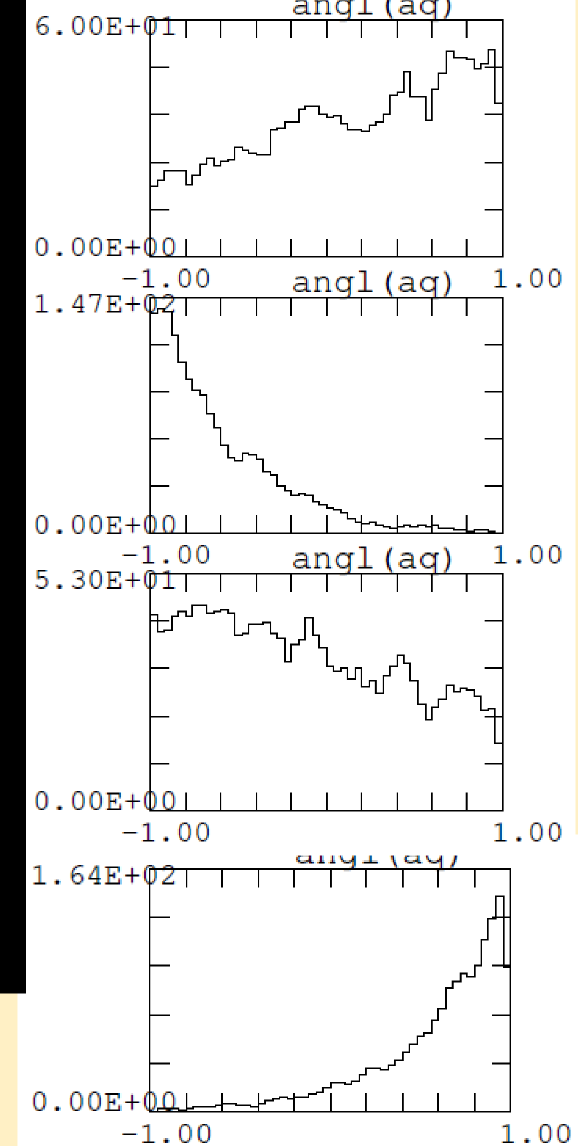
Simulation water starting at 298 K, NVE



The time t=82,600 starting from 298 K with 1728 water molecules, imposed electric field 10 GHz in x–direction with E_0= 5x10^6 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.

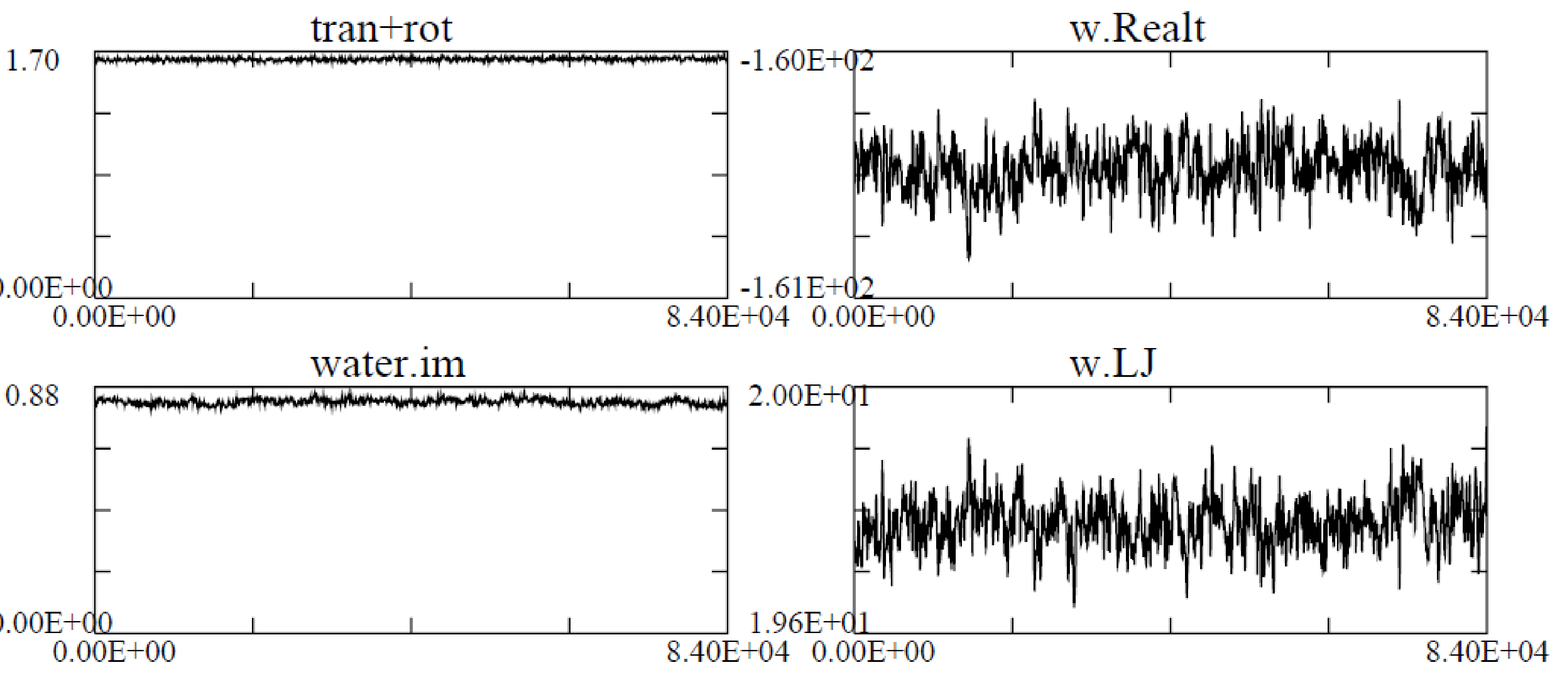




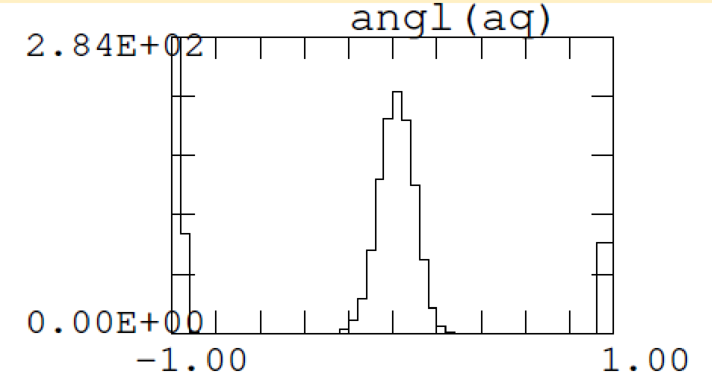


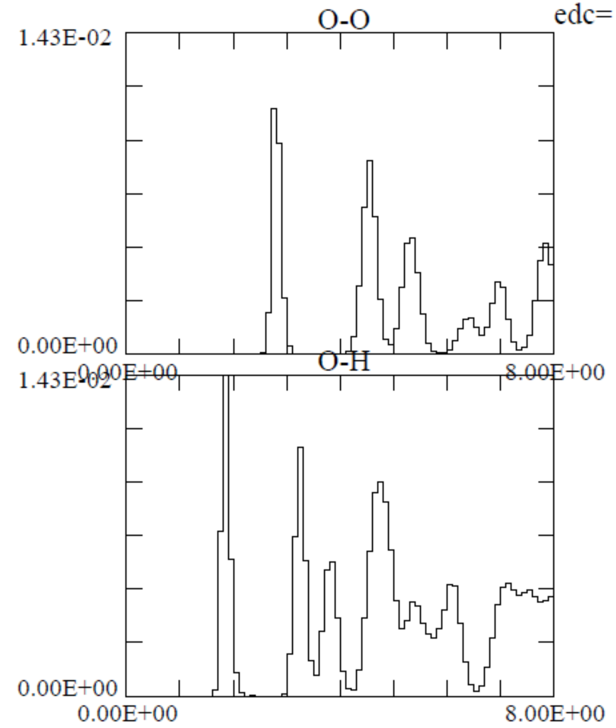
Water molecules starting 298 K.
Left: Scatter plot of water at t=80,000, b) x-directional cosine distribution for the cross bins of (-1.0,1.0) at t=72,500 to 80,000. Due to phase lag of molecules compared to imposed electric field, water is largely heated,

Simulation starting at ice 230 K, NVE

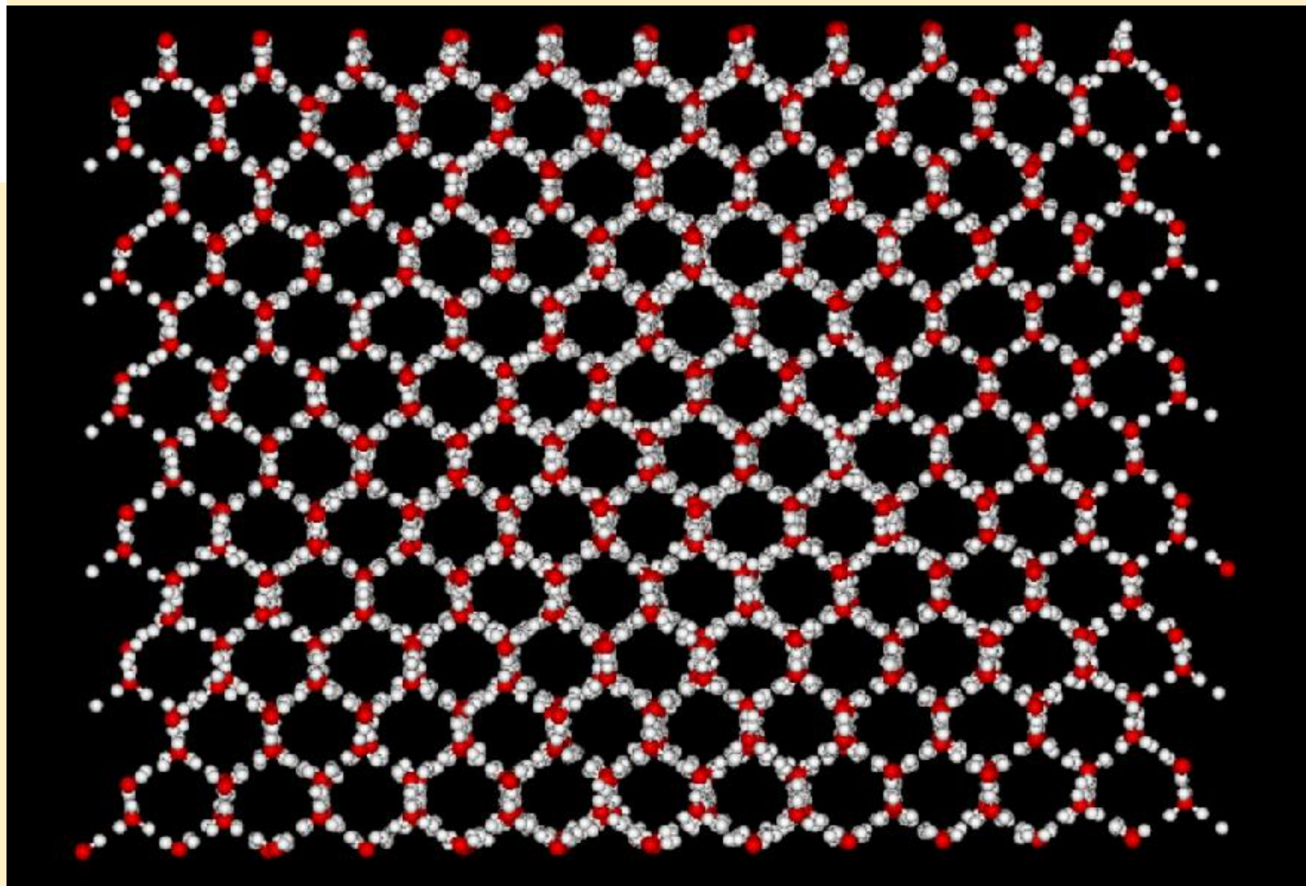


At temperature 230 K of 1728 water molecules, AC electric field 10 GHz in the x-direction with intensity E_0= 5x10^6 V/cm. Left: a) total kinetic energy, b) rotational energy only, c) Coulombic energy, d) Lennard-Jones energy, at the time of t=84,000. Right: cosine distribution of water in Bins (-1,1) of the x-direction. No oscillations are really found at the imposed electric field.



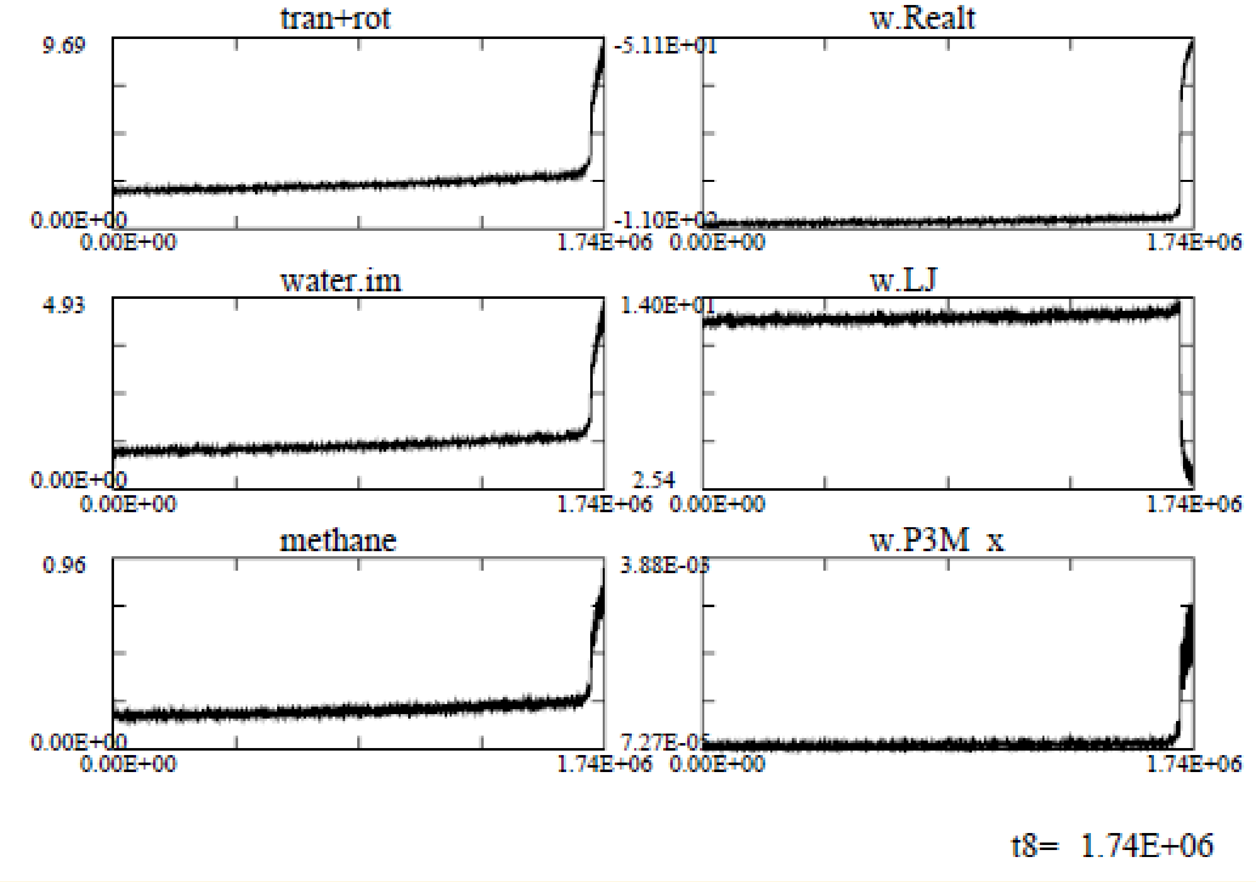


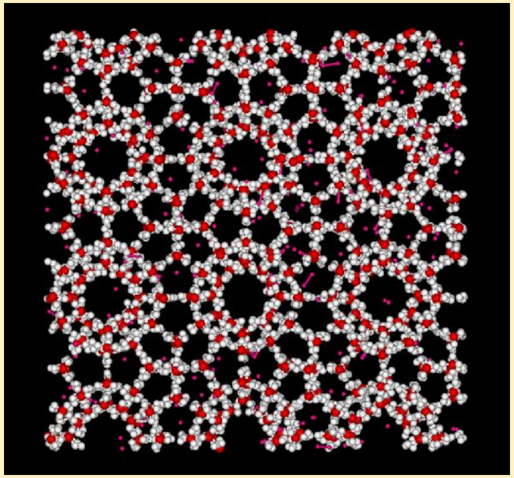
Time t=80,000 of the temperature 230 K.
Left: a) Pair distribution functions of O–O atoms
b) O–H atoms for R=0–8 Angstrom. Peaks are well separated at this temperature.
Right: Scatter plot of water molecules where ice is frozen by 6–membered water clusters.

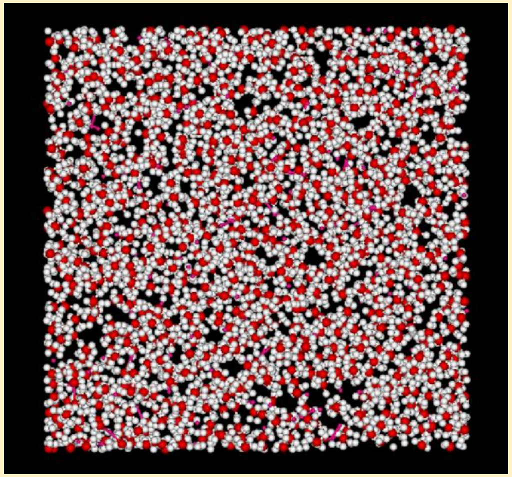


Methane Hydrate at T>273 K

Microwaves at 10 GHz are excited for methane hydrate at T>273 K by the TIP5P-Ewald code. The collapse of molecules is shown here.







Energy of water and methane, and that of Coulombic and LJ potentials (top), and scatter plots at t= 1.70 x 10^6 and after sudden collapse at t=1.74 x 10^6 (right).

References

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