Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary information for:

Deformation of the water nano-droplets on graphene under the influence of DC and AC electric fields

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1. The equilibration phase

In the first step, the droplet was equilibrated for 100 ps. During the equilibration phase, the total energy was monitored and is shown in figure S1. As can be seen the systems nearly equilibrated after about 30 ps. The obtained results, after 100 ps equilibration phases, then were used as the initial conditions to consider the water droplet spreading on the graphene under the influence of the external electric fields as well as the initial conditions of the free drops.

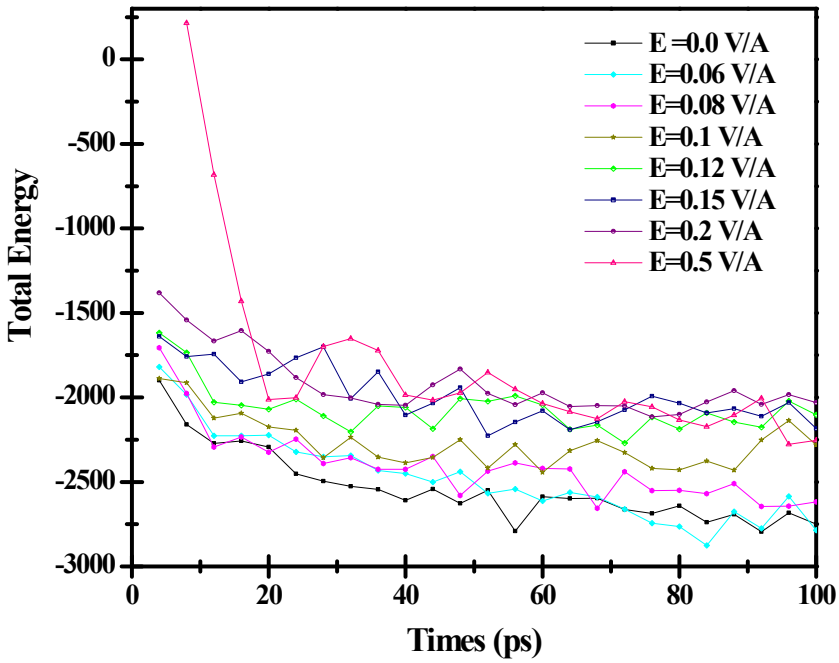

Figure S1 The total energy distribution of the system as a function of times

2. The water droplets response to the various constant and oscillating electric fields

The water molecules interactions were computed with the aid of the transferable intermolecular potential 4 points (TIP4P) model as well as the transferable intermolecular potential 3 points (Tip3p) and the extended single point charge (SPC/E) water models in the simulations. The average of *cos(θ)* as a function of simulation time in the presence of the various constant electric fields are shown in panels of figures 2 and S2.

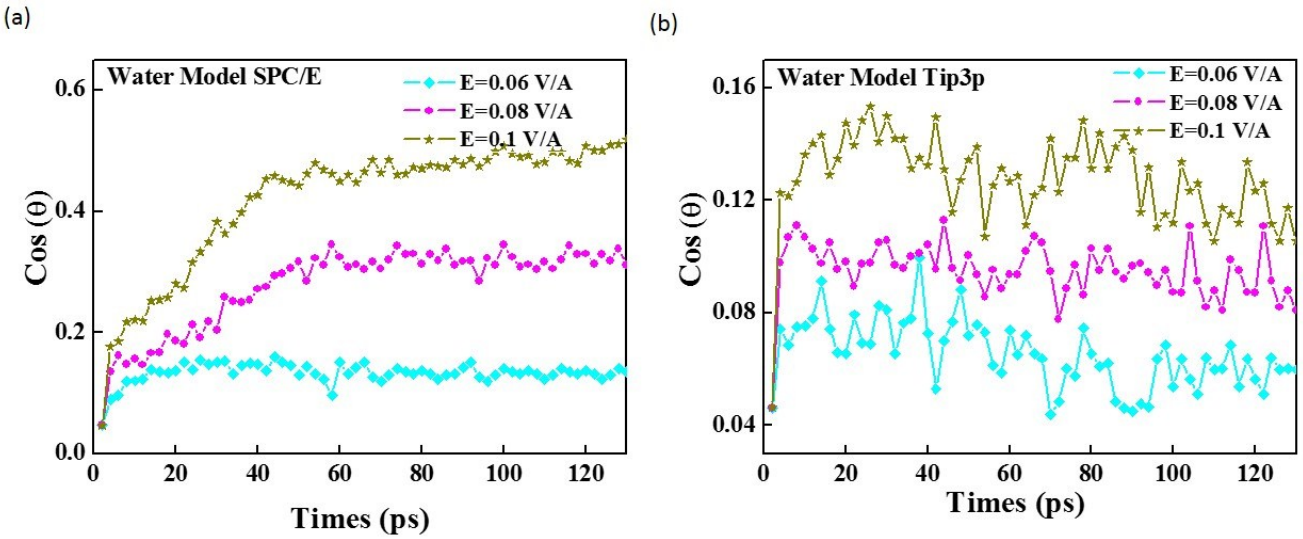

Figure S2 The average of Cos(θ) as a function of time for the droplet on graphene under the application of different electric fields for various water model : (a) SPC/E, (b) Tip3P; where θ is the angle between the water dipoles and an applied field.

The average of *cos(θ)* as a function of simulation time in the presence of the various oscillating electric fields are shown in panels of figures 7 and S3.

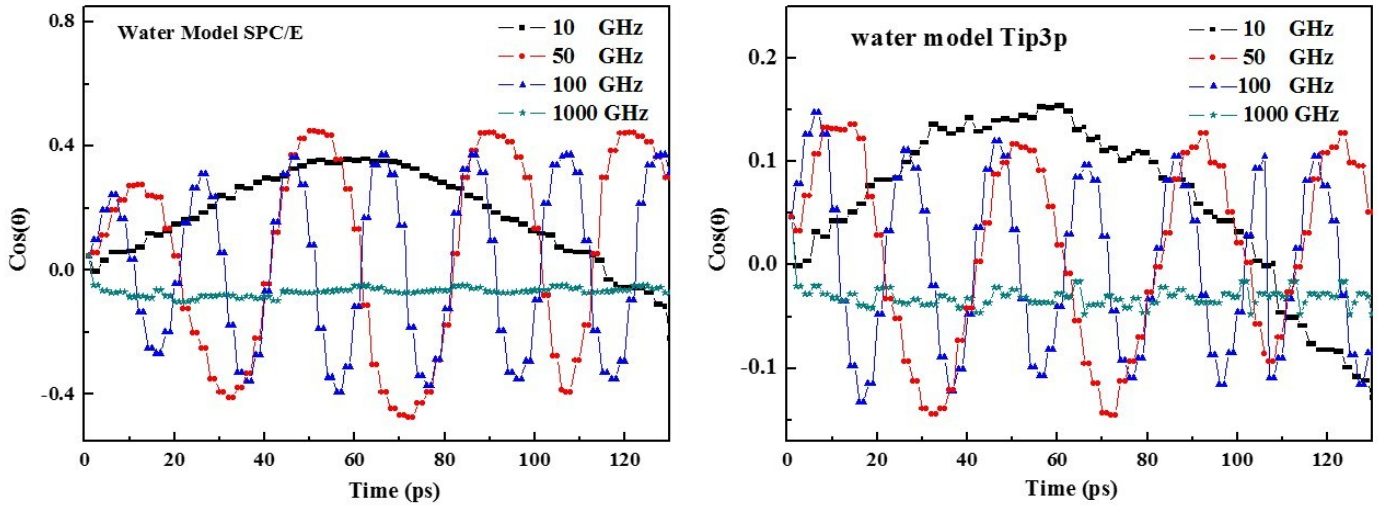

Figure S3 The average of Cos(θ) as a function of time for the droplet on graphene under the application of different oscillation electric fields for various water model : (a) SPC/E, (b) Tip3P; where θ is the angle between the water dipoles and an applied field.