Supporting Information

Phase transitions in nanostructured water confined into carbon nanotube by external electric and magnetic fields: A molecular dynamics investigation

Mohsen Abbaspour,^{*} Hamed Akbarzadeh, Sirous Salemi, Leila Bahmanipour Dep. of Chemistry, Hakim Sabzevari University, Sabzevar, Iran

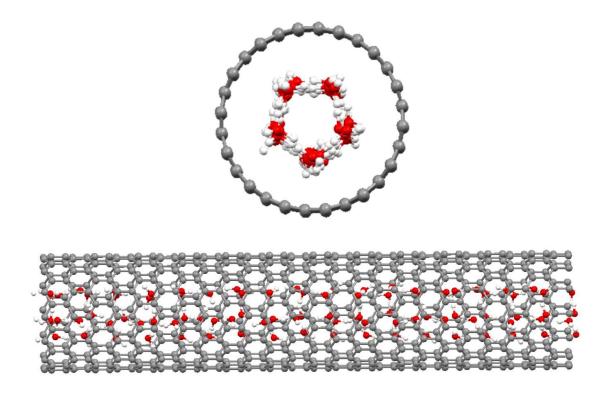


Fig. S1. Snapshots of 90 confined water molecules into (14,0) CNT with the length of 50 Å.

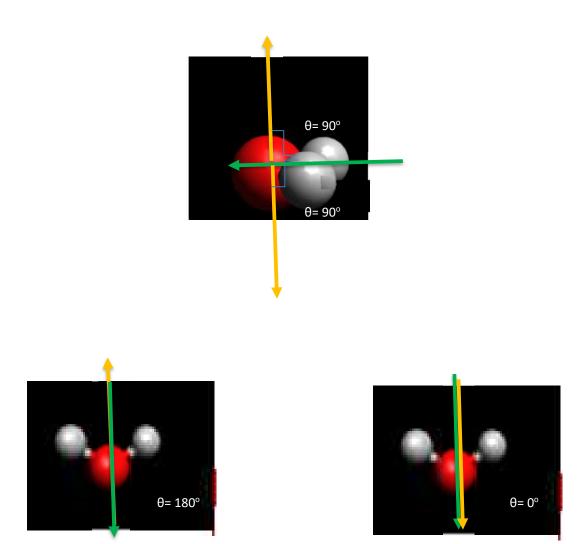


Fig. S2. Definition of the angle between the vector perpendicular to the surface of water molecule in the up or down direction (the yellow arrow as the reference vector) and the dipole moment vector of water molecule (the green arrow as the observed vector). The dipole moment vector passes from the center of mass of the molecule.

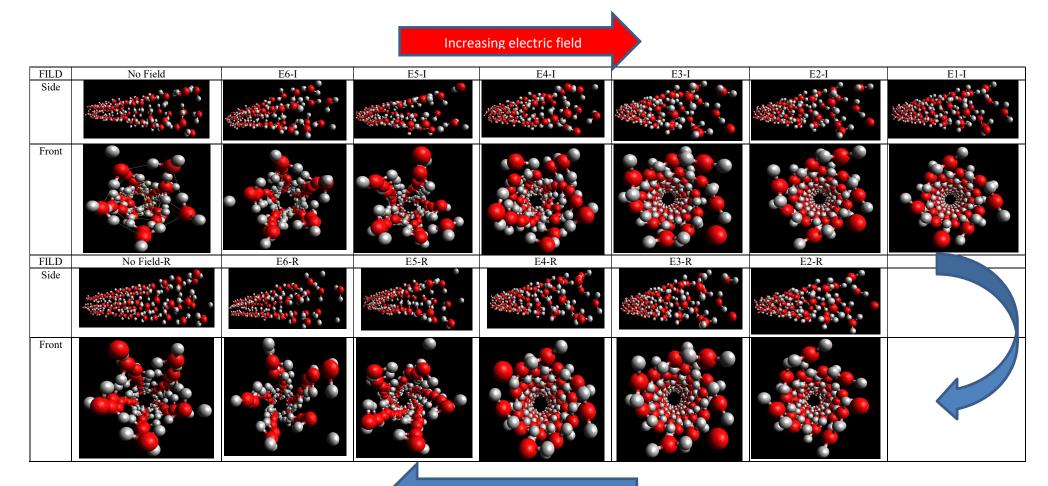


Table 1. The snapshots of confined water into the CNT in the different electric fields in both side and front views.

Decreasing electric field

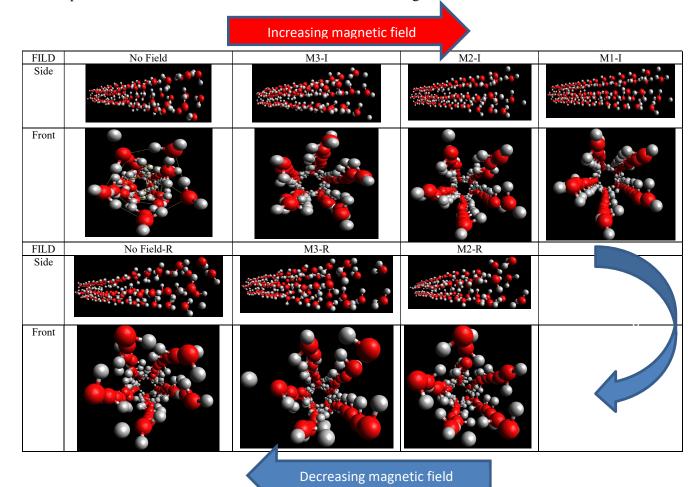


Table 2. The snapshots of confined water into the CNT in the different magnetic fields in both side and front views .