Supporting Information

Molecular behavior of water on Titanium Dioxide Nanotubes: A Molecular Dynamics Simulation study

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1. Radial distribution function (RDF).

RDFs of water molecules near NTs are calculated to study the local structure of water. The RDFs of oxygen-oxygen (O_w-O_w), hydrogen-hydrogen (H_w-H_w), and oxygen-hydrogen (O_w-H_w) between different water molecules near TiNT, M-TiNT and CNT are displayed in Figure S1a. Both the water molecules inside and in the two water layers outside NTs are computed. It's important to note that the RDFs of water in NTs are not equals to 1 because of the confinement. The location of first peak in the figure shows the closest distance between atom pairs. The first peak of O_w-H_w pair

represents the hydrogen bond length. The RDFs of Ti_{5c}-O_w pair and O_{2c}-H_w pair for water near TiNT are also studied in our work, as shown in Figure S1b. The first peak of O_{2c}-H_w pair represents the hydrogen bond length fromed between the H_w in water molecules and the bridge O_{2c} of TiNT.

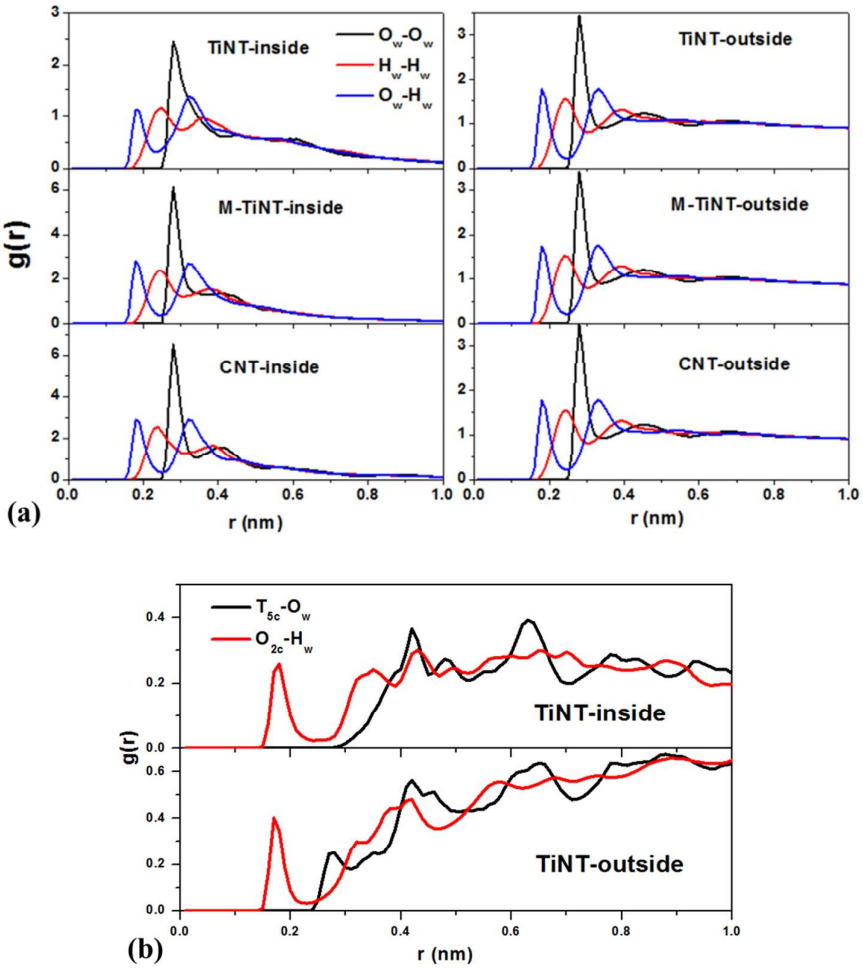

Figure S1. Radial distribution functions (RDFs) of water-water (a) and water-surface (b) pair.

2. Hydrogen bond autocorrelation function ($C_{HB}(t)$).

The hydrogen bond dynamics are computed to investigate the hydrogen bond

breaking dynamics of water near NTs, as shown in Figure 2S. The relaxation time is then obtained by the integration of $C_{HB}(t)$, indicating the stability of the hydrogen bonds.

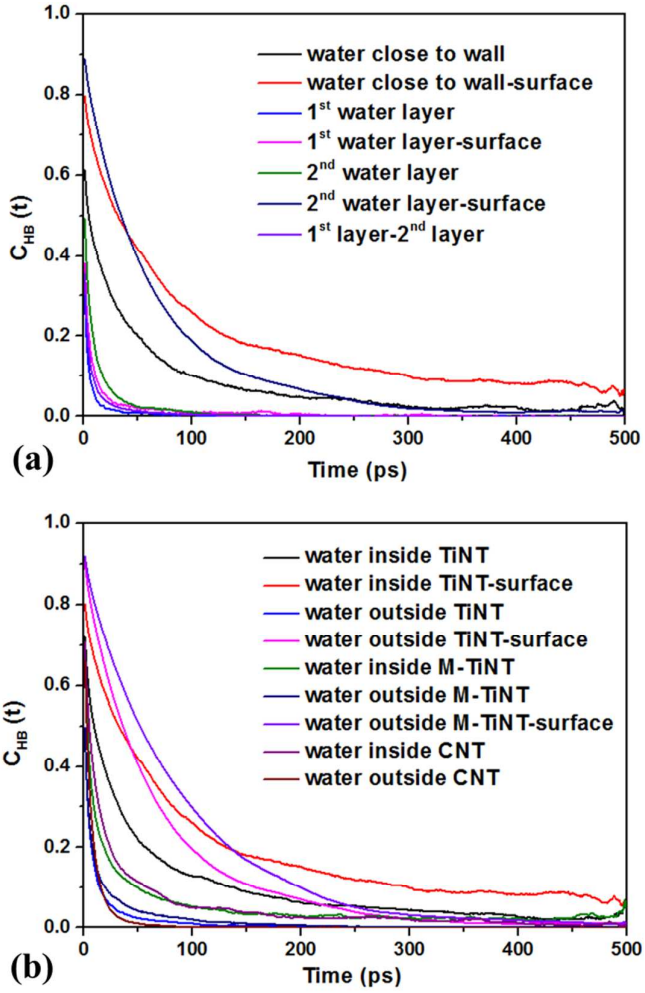

Figure S2. Hydrogen bond autocorrelation function ($C_{HB}(t)$) (a) of water molecules in different layers near the TiNT surface and (b) of water molecules near TiNT, M-TiNT and CNT.