Supporting Information

Carbon Nanotube Functionalization with Spontaneous Encapsulation of Ionic Liquids

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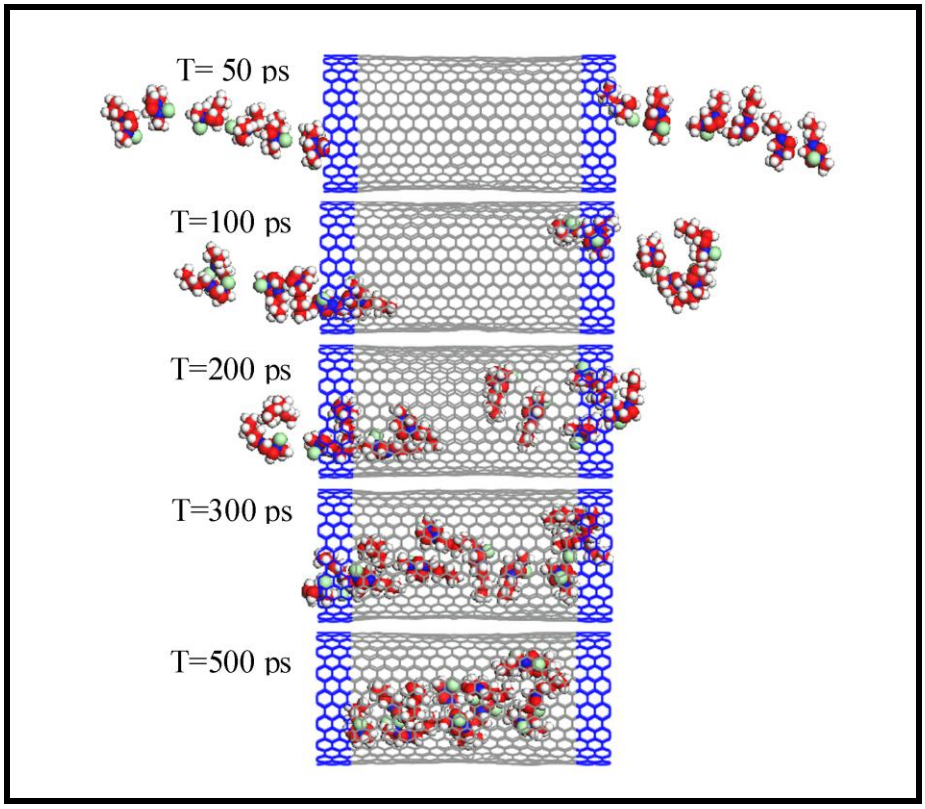

Figure S1

In Figure S1, MD simulation has been performed with the same amount of [Bmim][Cl] initially placed at each end of the SWCNT(16,16) along the direction of the nanotube axis. When the proximal [Bmim] cations pass through both the two ends of the tube at t =50 ps, we have found that deformation of the SWCNT is more serious than that in the one-end encapsulation system, indicating that the interaction between the imidazolium rings and the SWCNT in the two-ended encapsulation system has been intensified. It is also worth mentioning that since the attractive force simultaneously acts on the two strands of [Bmim] cations, the synchronous encapsulation in two directions is more efficient than that in one direction.

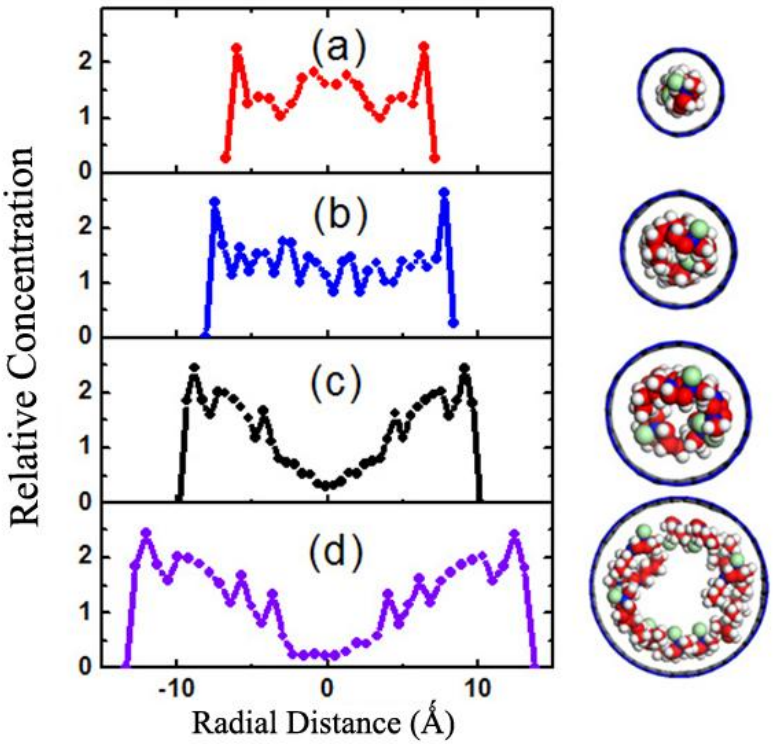

Figure S2

The radial relative concentration and the snapshots of ILs absorbed in different diameters tubes, are given in Figure S1. The ILs distributions inside the nanotubes vary markedly with tube diameter. It is the (8,8) tube with the smallest size that allows the solvent-free ions freely inside the tunnel. As for the (12,12) and (15,15) tubes, ILs attach to the internal surface of the tube, and form a hollow cylinder-like structure. The ILs in (20,20) show ordered hollow monolayer cylindrical structures. Imidazole rings of cations inside the tube mainly parallel to the nanotube surface. The snapshot strongly suggests that as liquid organic electrolyte, ILs can make up a capacity-controlled nanodevice for energy management.