Electronic Supplementary Information (ESI)

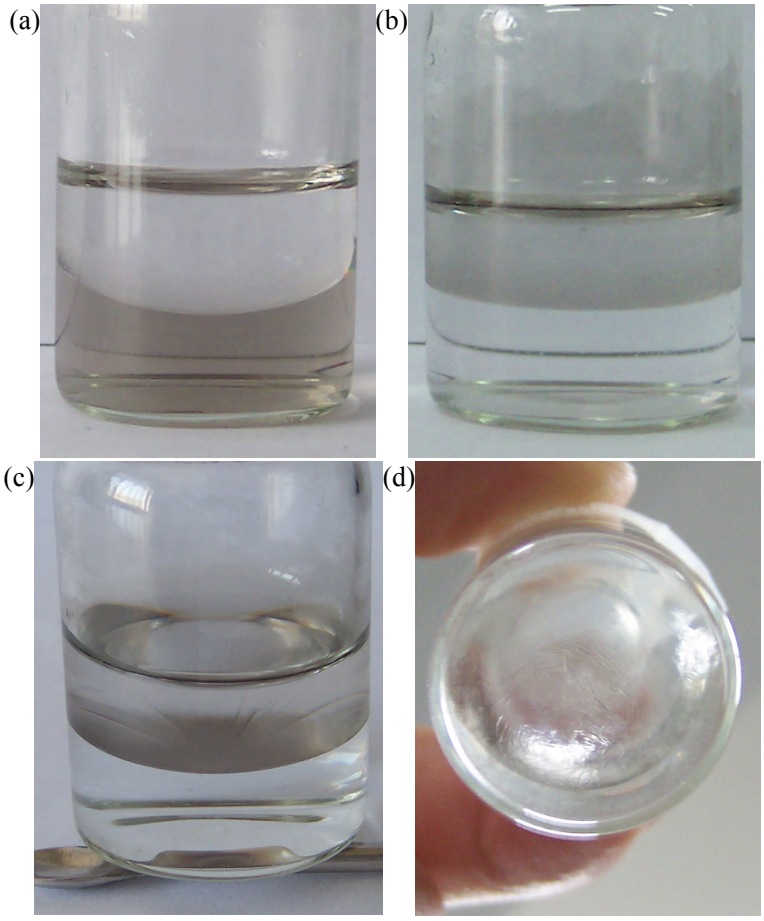

Figure S1. (a) Aqueous of SWNTs-Im covered with toluene; (b)-(d) the SWNTs-Im was extracted from the aqueous phase and self-assembled into a film at the toluene/water interface, (b) the front view, (c) top front view, and (d) bottom view.

From the front view (Fig. S1b), it was noted that the film crept up the glass wall of the vial. This indicated that there was a strong driving force for the formation of a self-assembled monolayer at the interface[1]. If one tilted the vial, from the top front view, a film with at the interface was clearly seen with slight wrinkle and did not break into pieces (Fig. S1c). Owing to the interfacial reflectance, the film appeared black. And from the bottom view, it could be seen that the thin film was liquid-like: homogeneous, transparent, and almost colorless, as shown in Fig. S1d.

Theoretical simulation details

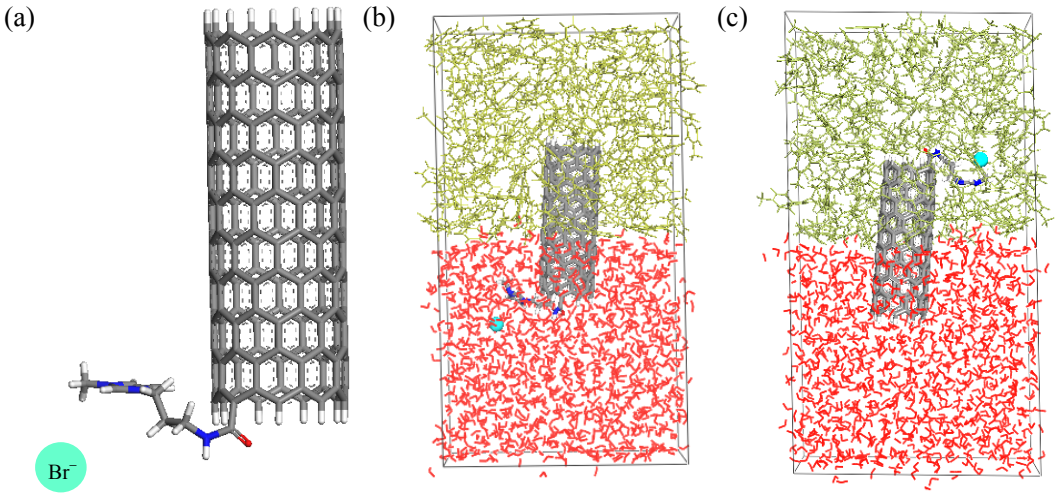

Figure S2. (9, 0) SWNT-Im (a); Initial 3D structure of system 1, i.e. Im part of SWNTs-Im in water phase (b) and system 2, i.e. Im part of SWNTs-Im in toluene phase (c) for MD simulation

To investigate the orientation of SWNT-Im (Fig. S2a) with the toluene and water interface, the stability of the following two possible orientations, i.e. Im part of SWNTs-Im in water phase (system 1) or in toluene phase (system 2), respectively, was evaluated *via* Materials Studio software[2]. The density of toluene phase and water phase was set to 0.866 and 1.00 g/mL, respectively. The initial models of the interfacial systems were constructed using the Amorphous Cell module[3] and the Build module. The final cell-box size was a = b = 32.8 Å, c = 62.8 Å, α = ß = γ = 90°. Considering the cost of simulations, the size of the introduced SWNT (9, 0) was ca. 20 Å, and the SWNT-Im was optimized by employing density functional theory (B3LYP/3-21G*) before introduced onto the interfaces. Fig. S2b shows the initial 3D structure of system 1 for molecular dynamics (MD), in which Im part of SWNTs-Im was in the water phase. Similarly, in system 2 Im part of SWNTs-Im was in the toluene phase (Fig. S2c). After primarily energy minimization, the constructed models were equilibrated under 298 K for 20 ps using the Discover module[4], with the NVT ensemble adopted. The COMPASS force field, employed here, is considered to be compatible to reproduce the properties of organic and inorganic materials especially in their gas and condensed phases[5]. The final equilibrated conformations were energy minimized and the energy components were listed in Table 1. It was found that $E_{potential}$ of system 1 was much smaller than that of system 2 ($E_{potential}$= -8884.32 kcal/mol) , i.e. Im part of SWNTs-Im on SWNTs-Im was more preferred in the water phase. The main contributions to the stability of system 1 was from the electrostatic interaction.

Reference

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