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Supporting Information

An intensive dispersion and synchronous assembly of single-walled carbon nanotubes in surfactant-oil-water association system

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The details of dissipative particle dynamics simulation

Dissipative particle dynamics (DPD) as a mesoscopic simulation technique has been described in detail elsewhere[1,2] and will be covered here only briefly. In the simulation, molecules are represented by beads. The motions of beads follow Newton's equations:

$$\frac{\mathrm{d}r_i}{\mathrm{dt}} = v_i \qquad m_i \frac{\mathrm{d}v_i}{\mathrm{dt}} = F_i \tag{1}$$

Where r_i, v_i, F_i, are the position, velocity and total force of the i beads, respectively. The total force exerted on a given bead i is

$$F_i = \sum_{i \neq j} (F_{ij}^C + F_{ij}^D + F_{ij}^R) \tag{2}$$

F_{ij}^C is the conservative force, F_{ij}^D and F_{ij}^R are the dissipative and random forces, respectively.[1,3] The conservative force F^C is a soft repulsive central force between beads i and j.

$$F_{ij}^C = \begin{cases} a_{ij}(1 - r_{ij})\widehat{r_{ij}} & r_{ij} < 1 \\ 0 & r_{ij} > 1 \end{cases} \tag{3}$$

Where a_{ij} is a maximum repulsive parameter between beads i and j; $r_{ij} = |r_i - r_j|$. All three forces tend to 0 when the distance between two particles is larger than the cutoff radius.[1,4,5]

The head group and tail group of DDA are represented as two beads, which are connected by a harmonic spring with the spring constant C = 4 (in kT units); oil is represented as single bead. Oil beads, head groups, and tail

groups are denoted by o, h, and t, respectively. The size of the box with periodic boundary conditions is 30×30×30 DPD units in the simulation system containing 81000 beads (ρ=3). DPD units are adopted in simulation for length, energy, and time. The mass of all of the beads is 1, and k_BT (the temperature of the thermostat) is the units of energy, we set the temperature of the system as k_BT=1.0. As the DPD technique is based on soft sphere interactions, the repulsion parameter a_{ij} needs to be chosen while taking into account the compressibility of the system. A linear relationship for the repulsion parameters a_{ij} and the Flory–Huggins interaction parameters $\chi_{ij}(T)$ is given[6] in k_BT units:

$$\mathrm{a}_{ij} = a_{ii} + \frac{\chi_{ij}(T)}{0.306} = 25 + 3.27\chi_{ij}(T) \qquad (4)$$

Between beads of the same type, the repulsion parameters are taken as

$$\mathrm{a_{ij}} = 75\mathrm{k_B\,T}/\rho = 25\mathrm{k_BT}\ (\rho = 3) \qquad (5)$$

Simulations were run for 20000 time steps with a time step of 0.05. And the simulation was performed through the Gibbs canonical ensemble. The DPD simulation a_{ij} parameters calculated by the above theories and methods are given in Table S1 which is determined according to the liner relationship with Flory-Huggins parameters χ_{ij}. The χ_{ij} between pairs of particles can be obtained from the calculation of the mixing energy with Blend module.

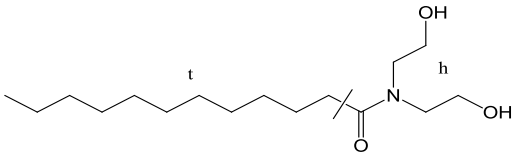
All simulations were carried out by Materials Studio 4.3 from Accelrys in this paper.

The details of the method of determination of the yield of dispersed SW-CNTs

In the paper, the raw SWNT material was used without any other purification or centrifugation steps prior to dispersion. A set of parallel samples were used to determine the yield of the dispersed SWNTs in the supernatant. Precipitates could be found in the bottom of centrifuge tube after 12333 g centrifugation at the end of the SWNT dispersing process, which contains mainly the residual SWNT bundles, the entrained amorphous carbon, and the Co-Mo catalyst, the adsorbed DDA and oil. After the upper homogeneous phase was removed, the precipitate was kept in an oven for 24 h at 80 ℃ to get dried. Then the precipitate was mixed with benzinum, sonicated for 1 h, and centrifuged at 5000 RPM for 1h, the upper supernatant was removed, the residual was stoved at 80 ℃ for 24 h, repeated the process for three times to completely remove the DDA and oil. The residual precipitate (W_r) was weighed. The yield of the dispersed SWNTs in the supernatant was determined by the following formula:

$$\mathrm{Y}\% = \frac{W_t - W_r}{W_t} \times 100\%$$

W_t is the total weight of the added SWNTs; W_r is the weight of the residual precipitate (SWNTs bundles, amorphous carbon, and the Co-Mo catalyst).



Scheme S1. The chemical structure of N,N-bis(2-hydroxyethyl)dodecanamide (DDA).

Table S1. The interaction parameters a_{ij} of DDA-water systems (in kT units).

a_{ij}	o	h	t
o	25.0		
h	117.0	25.0	
t	27.5	117.0	25.0

Note: h represents head groups, t the tail chain, o dodecane.

Table S2. The information of the SWNT product purchased from SIGMA-ALDRICH.

Property	Tube diameter / nm	Tube length range / nm	Carbon content	SWNT content	Aspect ratio
SWNT	1.0±0.3	400-800	>90%	≥70%	1000

Note: the average length of the SWNT product was 800nm.

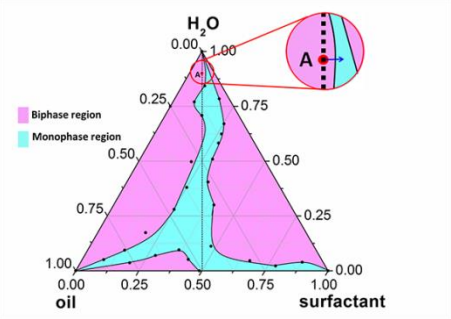


Figure S1. The ternary phase diagram of DDA-dodecane-H_2O system, T=298 K.

Figure S2. The images of the solution of the first step in the SOW-SWNTs dispersing process with or without DDA: the DDA (1 g) - oil (1 g) - SWNTs (1 mg) mixture (left); and the oil (1 g) –SWNTs (1 mg) mixture (right).

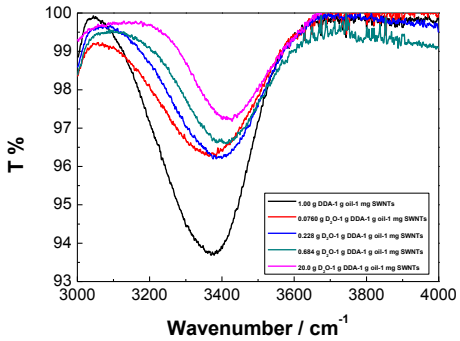


Figure S3. FTIR spectroscopy of the stretching peaks of O-H of DDA in the ternary mixture of DDA-dodecane-SWNTs containing 1 g dodecane, 1 g DDA and 1 mg SWNTs (the dark line) and the SOW-SWNTs dispersing system with increasing water content (0.0760, 0.228, 0.684, 20.0 g D_2O).

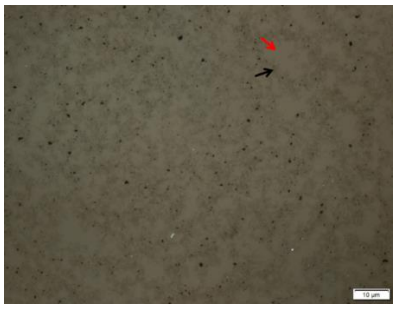


Figure S4. The microscopic image of the oil-water bicontinuous phase of the SOW-SWNTs dispersion after 18 g water was dropwise addition under magnetic stirring. The gray region marked by black arrow represented the network architecture of SWNT bundles. The blank region indicated by red arrow represented the water phase.

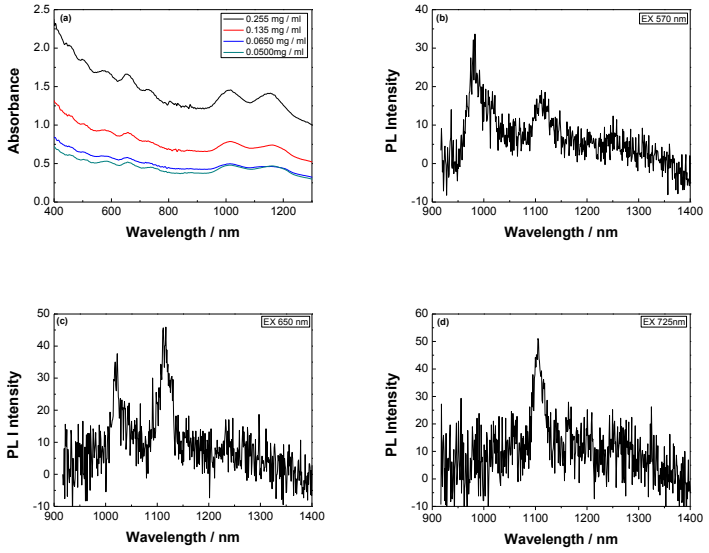


Figure S5. (a) The Visible to near infrared absorption spectra of the different concentrations of SWNT suspensions (0.0500, 0.0650, 0.135, 0.255 mg/ml) dispersed by the SOW association system. PL spectra of the 0.255 mg / ml SWNT suspension under excitation (b) at 570nm; (c) at 650 nm; (d) at 725 nm.

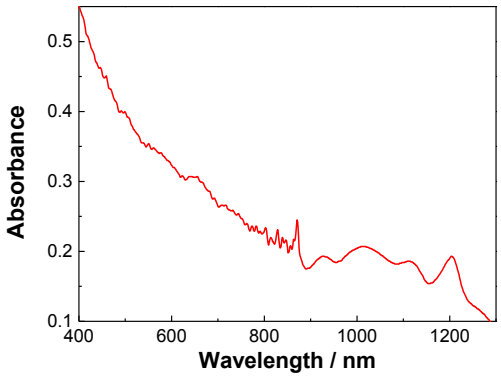


Figure S6. Visible to near infrared absorption spectrum of the SWNTs dispersion in which 18 g of water was added into the system all at once.

References

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