Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Stabilization of Aqueous Graphene Dispersions Utilizing A Biocompatible Dispersant: A Molecular Dynamics Study

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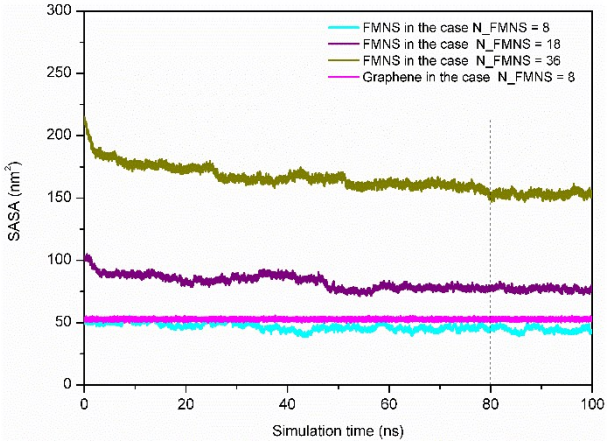

Fig. S1 SASA of FMNS as a function of simulation time in three different cases and the representative result for graphene

Table S1. Simulation parameters used in this work

Simulation system	Morphology simulation part			PMF simulation part	
	Morphology (8 FMNS case)	Morphology (18 FMNS case)	Morphology (36 FMNS case)	PMF (High surface coverage)	PMF (Low surface coverage)
Number of graphene flakes	1	1	1	2	2
Number of FMNS molecules	8	18	36	22	12
Number of water molecules	23486	23284	53964	54978	54988
Total number of atoms	71554	71468	164444	167438	166948
Simulation box size (nm^3)	9*9*9	9*9*9	12*12*12	12*12*12	12*12*12
Simulation time (ns)	100	100	100	5	5
Concentration ration of graphene and FMNS	2.13:1	0.95:1	0.47:1	/	/

Note:

The graphene flake size in all simulations is 4 nm * 4 nm, containing 680 carbon atoms;

Table S2. The maximum density value of both high surface coverage case and low surface coverage case at different critical positions

Position	I	II	III	IV	V	VI
High surface coverage (11 FMNS/flake)	15.7	12.9	17.7	14.5	13.6	13.1
Low surface coverage (6 FMNS/flake)	7.07	/	7.76	9.38	/	7.85

Table S3. Comparison results of different surfactants for the stabilization of aqueous graphene dispersions from both simulation and experimental works

Surfactant	Simulation results			Obtained graphene concentration reported experimentally in other's work (μg/ml)
	Relative amount of surfactant [a]	Surface coverage of graphene by surfactant [b] (molecules/nm^2)	PMF energy barrier (kJ/mol/nm^2) [c]	
SDS	0.048	1.00	15.00 [1]	12 [2]
SDBS	0.029	0.58	11.40 [3]	20 [2]
SC	0.026	0.49	10.00 [4]	27 [2]
FMNS	0.026 this work	0.34 this work	10.25 this work	200 [5]

a. relative amount of surfactant is calculated as follows, number of surfactants/numbers of carbon atoms in graphene flake.

b. surface coverage of graphene by surfactant is calculated as follows; number of surfactants adsorbed on each graphene flake/both sides area of each graphene flake.

c. PMF barrier is the barrier of the first local maximum energy barrier on the PMF profile.

Reference:

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