Supplementary Information

Passive Fractionating Mechanism for Oil Spill Using Shear-Wettability Modulation

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SI. Force field equations and parameters

The force field equations are mathematically expressed using the set of equations S1-S5 which are as follows:

$$U(r)=U_{non-bonded}(r)+U_{bond}(r)+U_{angle}(r)+U_{dihedral}(r) \tag{S1}$$

where,

$$U_{non-bonded}(r)=f_{ij}\left(\frac{q_i q_j}{r_{ij}^2}+4\varepsilon_{ij}\left[\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{12}-\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6}\right]\right) \tag{S2}$$

$$U_{bond}=k_b\left(r-r_0\right)^2 \tag{S3}$$

$$U_{angle}=k_\theta\left(\theta-\theta_0\right)^2 \tag{S4}$$

$$U_{dihedral}=0.5k_1\left(1+\cos\left(\phi\right)\right)+0.5k_2\left(1+\cos\left(2\phi\right)\right)+0.5k_3\left(1+\cos\left(3\phi\right)\right)+0.5k_4\left(1+\cos\left(4\phi\right)\right) \tag{S5}$$

Moreover, Table S1 indicates the parameters used for the simulations performed.

Table S1. Interaction parameters in the simulations[1]

Non-bonded interaction parameters (used in Equation 2)			
	$\varepsilon\ (eV)$	$\sigma(nm)$	Charge

Graphene C	0.07	0.355	0
Terminal alkane C	0.002862	0.35	-0.18
Other carbons in alkanes	0.002862	0.35	-0.12
Hydrogen atoms	0.001301	0.25	0.06

Bond interaction parameters (used in Equation 3)

Bonds	$k_b\,(eV)$	$r_0(nm)$
C-C	11.6216	0.1529
C-H	14.7438	0.1090

Angle Interaction parameters (used in Equation 4)

Angles	$k_\theta\,(eV)$	$\theta_0\,(^\circ)$
C-C-C	2.5303	112.7
H-C-C	1.6262	110.7
H-C-H	1.4310	107.8

Dihedral Interaction parameters (used in Equation 5)

Dihedrals	$k_1\,(eV)$	$k_2\,(eV)$	$k_3\,(eV)$
C-C-C-C	0.07545	-0.00681	0.01210
H-C-C-C	0	0	0.01587
H-C-C-H	0	0	0.01379

SII. Results from $NPzT$ simulations

Table S2. Number of water (N_{water}) and *n*-dodecane (N_{D12}) molecules for different *n*-dodecane mass percentages (DMP) and wall wettability (ε) values obtained from $NPzT$ simulations

	Number of Molecules		
DMP	$\varepsilon = 0.2\ kJ/mol$	$\varepsilon = 0.5\ kJ/mol$	$\varepsilon = 1\ kJ/mol$
Pure water	N_{water}: 12869	N_{water}: 13090	N_{water}: 13253
5%	N_{D12}: 67 N_{water}: 12019	N_{D12}: 68 N_{water}: 12248	N_{D12}: 69 N_{water}: 12425
10%	N_{D12}: 132 N_{water}: 11222	N_{D12}: 135 N_{water}: 11441	N_{D12}: 136 N_{water} :11585
15%	N_{D12}: 195 N_{water}: 10456	N_{D12}: 198 N_{water}: 10630	N_{D12}: 201 N_{water} :10776
20%	N_{D12}: 256 N_{water}: 9683	N_{D12}: 261 N_{water}: 9860	N_{D12}: 264 N_{water} :9994
40%	N_{D12}: 487 N_{water}: 6912	N_{D12}: 496 N_{water}: 7029	N_{D12}: 499 N_{water} :7071
60%	N_{D12}: 696 N_{water}: 4384	N_{D12}: 703 N_{water}: 4427	N_{D12}: 711 N_{water}: 4480
80%	N_{D12}: 886 N_{water}: 2092	N_{D12}: 899 N_{water}: 2122	N_{D12}: 904 N_{water}: 2135
Pure *n*-dodecane	N_{D12}: 1066	N_{D12}: 1085	N_{D12}: 1092

References

[1] S. Schmitt, F. Fleckenstein, H. Hasse, and S. Stephan, “Comparison of Force Fields for the Prediction of Thermophysical Properties of Long Linear and Branched Alkanes,” J. Phys. Chem. B **127**(8), 1789–1802 (2023).