

## Supplementary Materials

# Demulsification of Heavy Oil-In-Water Emulsion by a Novel Janus Graphene Oxide Nanosheet: Experiments and Molecular Dynamic Simulations

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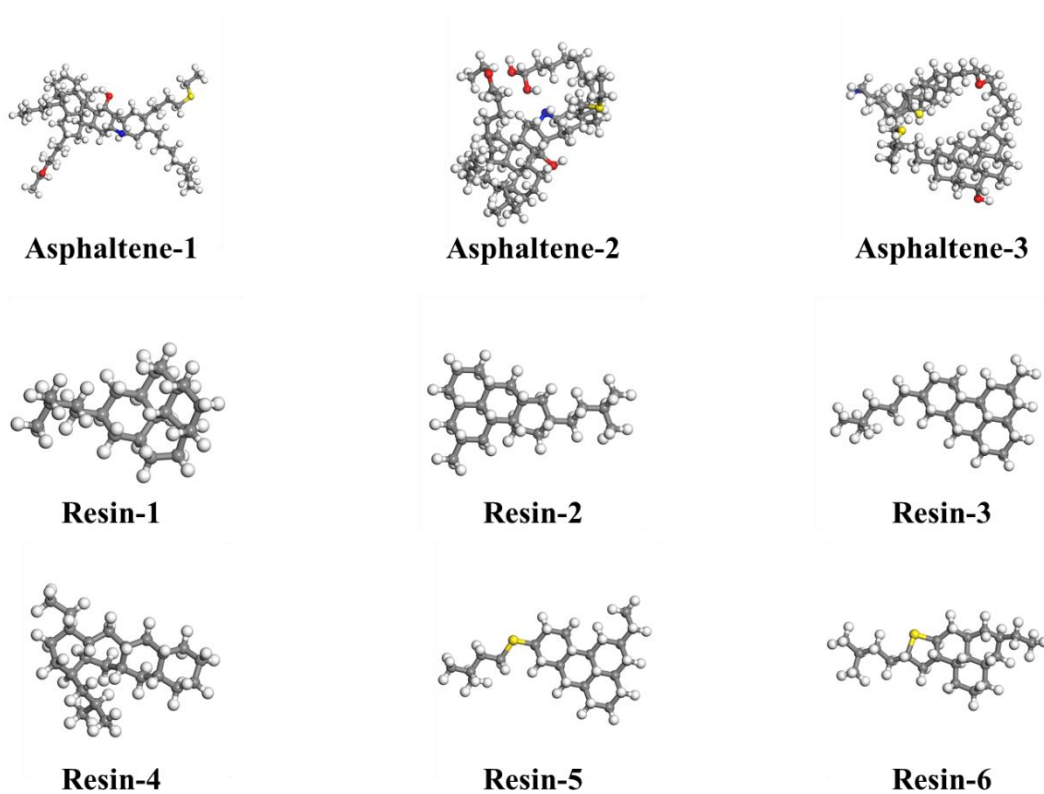
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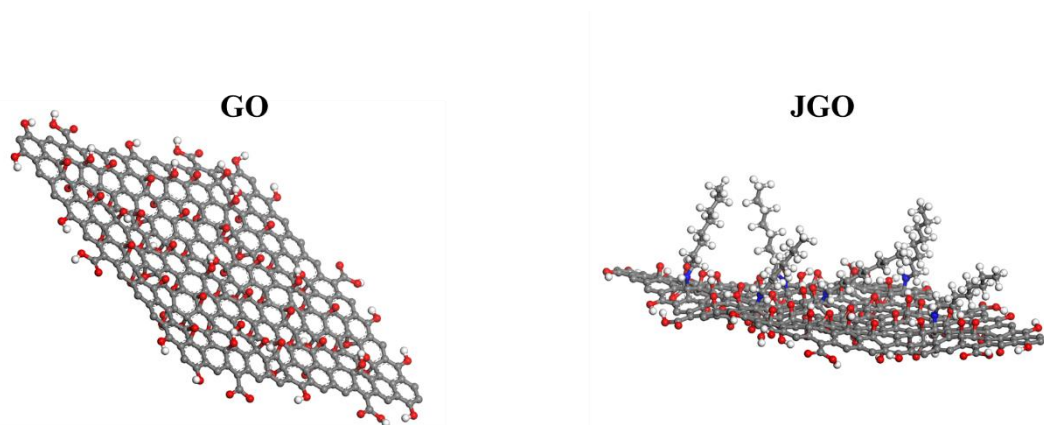
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**Table S1.** Compositions of the crude oil model.

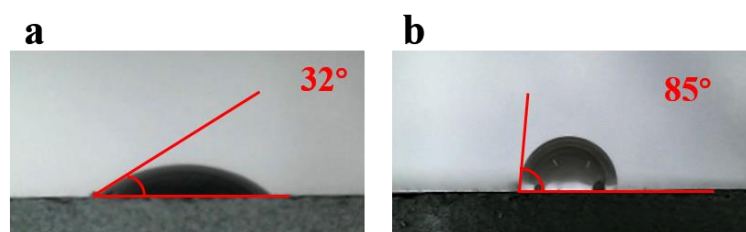
Component	Number	Component	Number
Asphaltene-1	23	Toluene	359
Asphaltene-2	23	Benzene	138
Asphaltene-3	23	Cycloheptane	359
Resin-1	53	Cyclohexane	221
Resin-2	53	Nonane	414
Resin-3	53	Octane	359
Resin-4	53	Heptane	304
Resin-5	53	Hextane	331
Resin-6	53		



**Scheme S1.** Molecular structures of different asphaltenes and resins.



**Scheme S2.** Molecular structures of GO and JGO.



**Figure S1.** The water contact angle of the unmodified side of JGO (a) and n-octylamine grafted side of JGO (b).

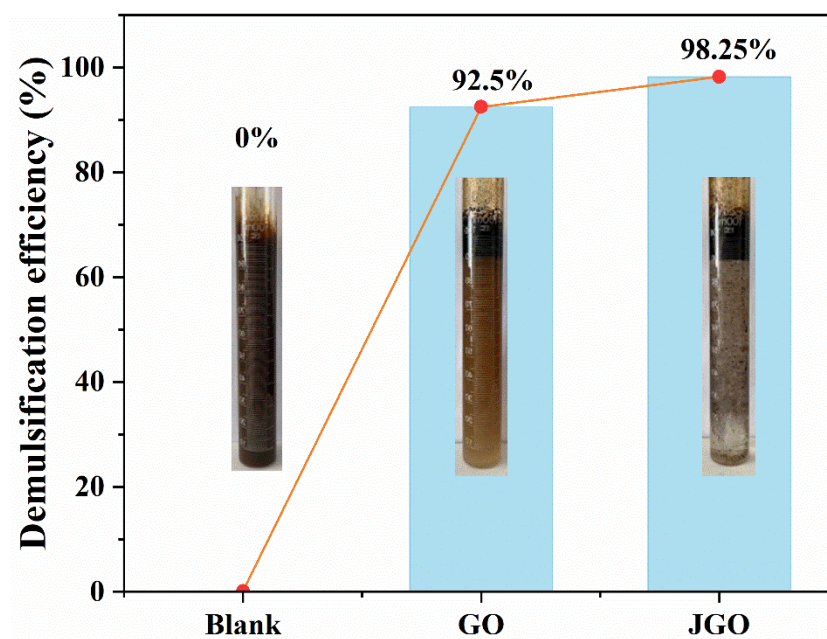


Figure S2. Demulsification performance of GO and JGO.

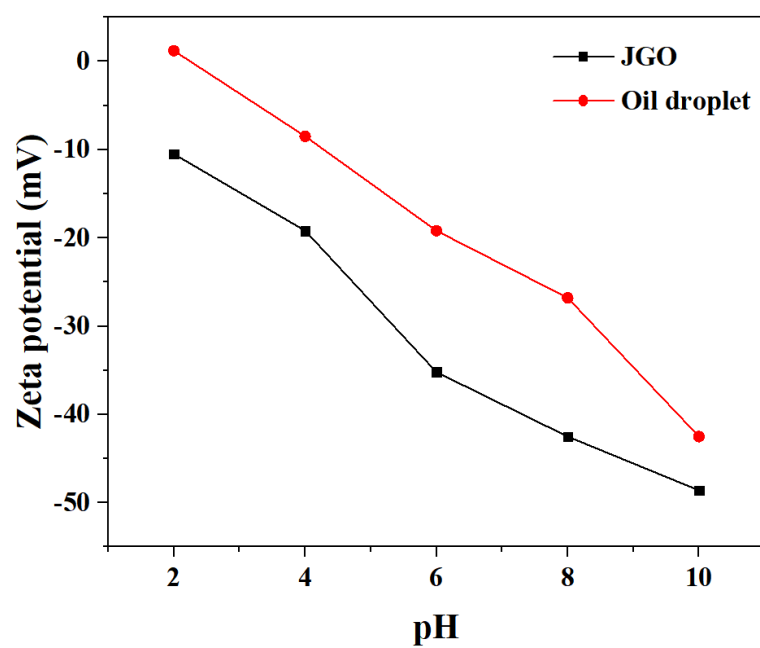
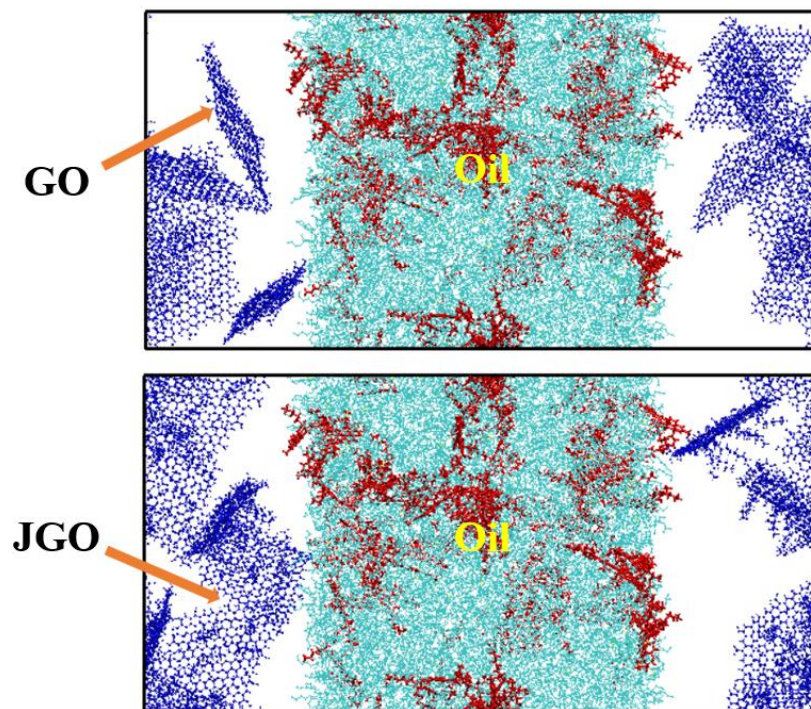
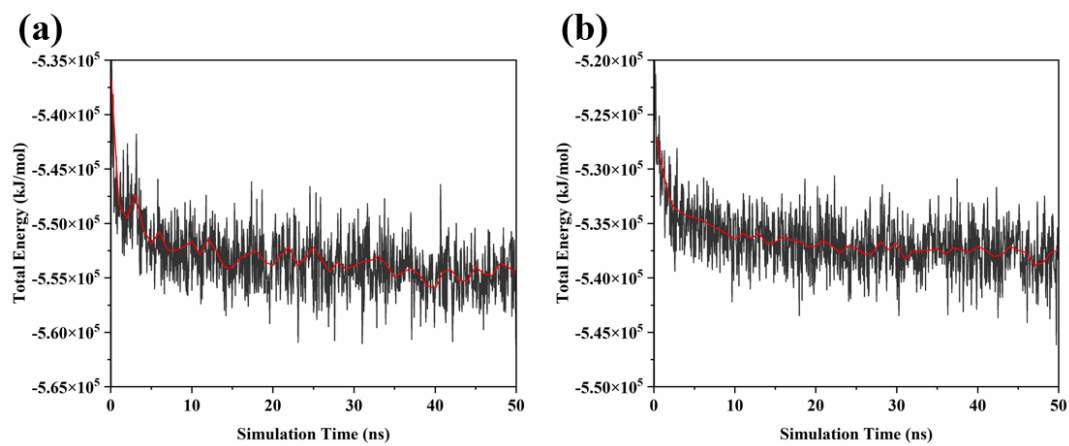


Figure S3. Zeta potential of JGO and oil droplets with increasing pH values.



**Figure S4.** The initial configuration of GO and JGO in the crude oil/water system, oil components are colored in cyan excepting asphaltenes which are colored in red, and GO and JGO are colored in blue. Water molecules are not shown for clarity.



**Figure S5.** Total energy curves in the simulation process with 10 GO (a) and JGO (b) randomly inserted into oil/water systems.