

Supporting information

Transportation of Janus Nanoparticles in Confined Nanochannels: A Molecular Dynamics Simulations

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S1. The selection of suitable characteristic energy

To construct Janus nanoparticles (JNPs), half hydrophilic and half hydrophobic surface should be formed on particles. The interaction energies for NP with water or oil were tuned by characteristic energy ε . The hydrophilic surface should have strong interaction with water and weak interaction with oil, while the hydrophobic part should be opposite. In light of our previous simulations, ¹ the detailed value of ε for JNPs were listed in Table S1. The characteristic interaction energy ε_{nn} between JNPs was set relatively small as 0.01 kcal/mol, and ε_{ns} between JNP and solid capillary was chosen 0.7 kcal/mol, designating the stronger interaction between JNPs and solid capillary. It was proven that the assigned characteristic energy enabled JNPs to stay stably at fluids interface. The CHARMM force field was used for decane molecules,² listed in Table S2.

Table S1 Force fields parameters for JNPs

Characteristic energy, kcal/mol	Water	Oil	JNP	Solid
Hydrophilic	0.4	0.01	0.01	0.7
Hydrophobic	0.01	0.2	0.01	0.7

Table S2 Force field parameters for oil molecules and silica

Atoms	ε (Kcal/mol)	σ (Å)
C(CH3)	0.0779	3.6349
C(CH2)	0.0560	3.5814
H (C-H)	0.0240	2.3876

S2. Displacement curves for nanofluids

The displacement curves for nanofluids with different characteristic energy were shown in Figure S1.

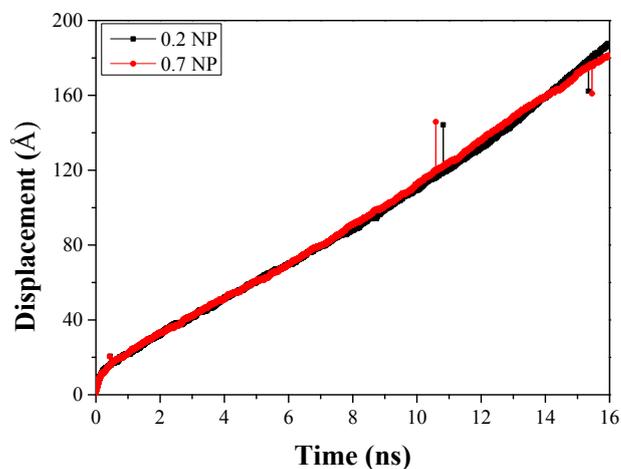


Figure S1 The displacement of nanofluids with different characteristic energy ϵ_{ns}

S3. Density of water molecules around Janus NPs

The density of water molecules on Janus NP was calculated in Figure S2.

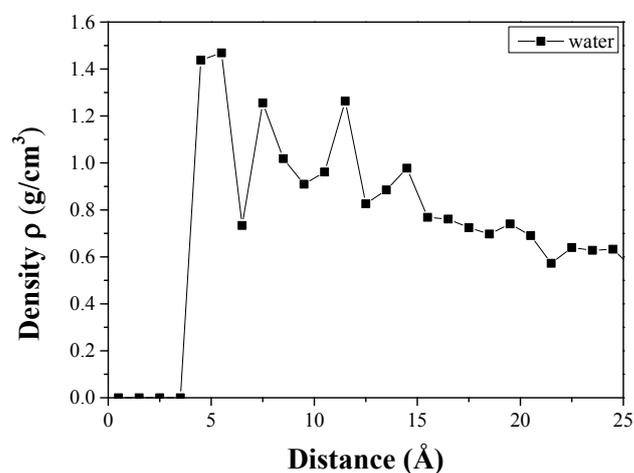


Figure S2 Density profile of water molecules around surface of Janus NP in water phase.

S4. The histograms of configurations

The histograms of the configurations within umbrella sampling window were plotted in Figure S3.

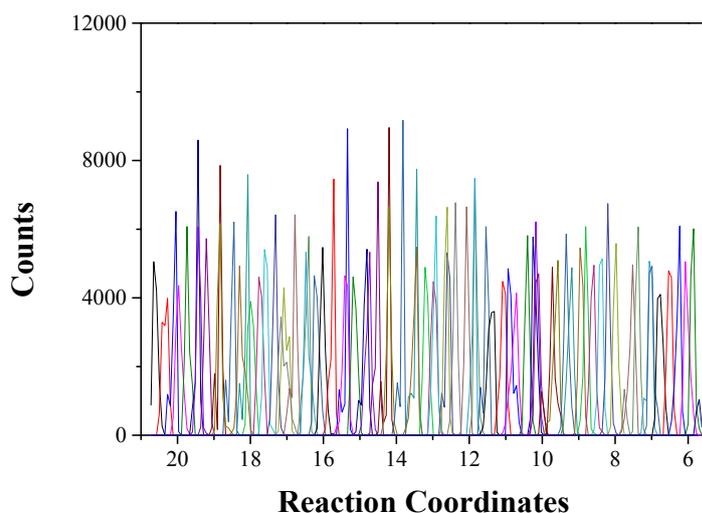


Figure S3 The histograms of configurations along reaction coordinate.

The histograms showed reasonable overlap between windows of the COM spacing, indicating the properly sampled reaction coordinate.

S5. Local pressure distribution along capillary

The local pressure distribution for fluids along the capillary was characterized to clarify the influence of Janus NPs on displacement process. The system at 8.0 ns displacement process was chosen, and the results are shown in Figure S4. The local pressure distribution along capillary can be divided into four regions, bulk fluid outside capillary (Region I: distance less than zero), nanofluids in confined capillary (Region II: distance from zero to fluids interface), oil phase in confined capillary (Region III: distance from fluids interface to capillary length of 194.15 Å), and oil phase outside the capillary (Region IV: distance greater than 194.15 Å). In the Region I, water phase containing Janus NPs tended to enter into the capillary and local pressure distribution along the capillary decreased to negative value. Due to confinement of the capillary, large fluctuation on the local pressure distribution was observed for fluids in Region II, while small fluctuation for oil phase confined in the capillary in Region IV, and reached almost stable after the oil phase out of the capillary in Region IV.

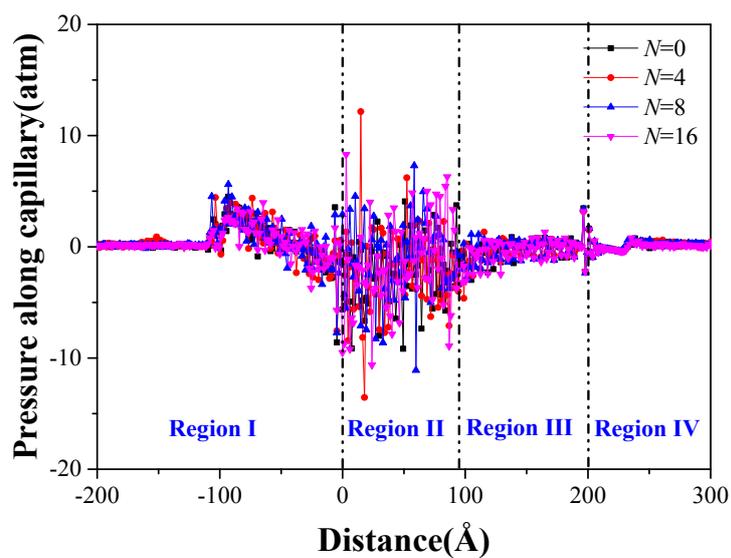


Figure S4 Local pressure distribution for nanofluids along the axial direction of the capillary.

References:

1. X. Wang, Z. Zhang, O. Torsaeter and J. He, Atomistic insights into the nanofluid transport through an ultra-confined capillary, *Phys. Chem. Chem. Phys.*, 2018, **20**, 4831-4839.
2. X. Wang, S. Xiao, Z. Zhang and J. He, Displacement of nanofluids in silica nanopores: influenced by wettability of nanoparticles and oil components, *Environ. Sci.: Nano*, 2018, **5**, 2641-2650.