Supporting Information for

Quantitative prediction of position and orientation of an octahedral nanoparticle at liquid/liquid interfaces

Wenxiong Shi,[1] Yih Hong Lee,[2] Xing Yi Ling[2] Shuzhou Li[1]**

1 Center for Programmable Materials, School of Materials Science and Engineering, Nanyang Technological University, Singapore 639798.

2 Division of Chemistry and Biological Chemistry, School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore 637371.

* To whom correspondence should be addressed. Email: lisz@ntu.edu.sg and xyling@ntu.edu.sg.

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S1. Thermodynamic model for sphere system

A simple treatment of the energetics of particles at fluid/fluid interfaces was proposed by Pieranski.[1] According to this theory, for a spherical particle the free energy is a function of the surface tension and surface area, which can be given as:

$$F = \gamma_{wo} \times A_{wo} + \gamma_{pw} \times A_{pw} + \gamma_{po} \times A_{po} + \tau \times L \quad \text{(S1)}$$

where F is the free energy relative to the particle being absorbed in oil/water interface, γ_{pw}, γ_{po}, and γ_{wo} are the particle/water, particle/oil, and water/oil surface tensions, respectively, and A_{pw}, A_{po}, and A_{wo} are the particle/water, particle/oil, and water/oil contact surface area, respectively. Based on the surface tension and the area in water and oil, the free energy is obtained. Therefore, the most stable configuration is fixed.

The free energy change of a nanoparticle at an interface with height h, F_{int}, can be rewritten with the free energy ($F(h)$) reference to the free energy of the nanoparticle immersed in oil phases (F_0) for a spherical particle:

$$F_{int}(h) = F(h) - F_0 = (\gamma_{pw} - \gamma_{po})A_{pw} - \gamma_{wo}A_{st} + \tau L \quad \text{(S2)}$$

where A_{st} is the interface area removed by the nanoparticle. Equation (S2) is very general and it can be used to investigate nanoparticles of different shapes.

As shown in Nielsen's work, with the adsorbing number of surfactant increase, the nanoparticle equilibrium position changing from immersed into oil to immerse into water.[2] The free energy curve show the lowest point. The line tension is low order magnitude, and can be ignored. The free energy of the spherical nanoparticle at the interface, F_{int}, is normally expressed with reference to the free energy change of the particle immersed in oil phases, F_0:

$$F_{int}(h) = F(h) - F_0 = 2\pi H^2 \times \left(1 + \frac{h}{H}\right)(\gamma_{pw} - \gamma_{po}) - \gamma_{wo}\pi(H^2 - h^2) \quad \text{(S3)}$$

Where H is the radius of sphere, and $-H < h < H$.

Equation (S3) suggests that the driving force for adsorption of the particle at an oil/water interface is the removal of unfavorable contact between the two liquids. The equilibrium position of the particle, h, can be extracted from the minimum value of Equation (S3). Equation (S3) after differential as shown below:

$$d(F_{int}(h))/d(h) = 0 = (2\pi H)(\gamma_{pw} - \gamma_{po}) - \gamma_{wo} 2\pi h \quad \text{(S4)}$$

For spherical particle, if the surface tensions γ_{pw}, γ_{po}, and γ_{wo} were fixed, the height position is determined by Young's equation.

$$\frac{h}{H} = (\gamma_{pw} - \gamma_{po})/\gamma_{wo} \quad \text{(S5)}$$

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S2. The mathematical method of calculation of the contact surface area with facet up orientation.

Equation (S2) is very general and it can be used to investigate nanoparticles with different shapes. In the case while the Ag octahedron enters the water phase with facet up orientation, the particle/water contact surface area A_{pw} and water/oil cross contact surface area A_{st} can be calculated using mathematical method.

For facet up orientation, the height is defined as the distance between the two opposite surfaces along the z direction. Therefore, the half of the total height $H_F = \sqrt{6}a/6$. Since $H_V = \sqrt{2}a/2$, the height ratio $v = h_F/H_V = 2h/\sqrt{2}a$, where h_F is the height in facet up orientation.

$$f = \frac{h_F}{H_F} = \frac{h_F}{\sqrt{6}a/6} = \frac{h_F}{\sqrt{3}/3 \times \sqrt{2}a/2} = \frac{h_F}{\sqrt{3}/3 \times H_V} = \frac{\sqrt{3}h_F}{H_V} = \sqrt{3}v$$

.

For the particle/water contact surface area A_{pw}

$$A_{wp} = \frac{1}{8}A + \frac{3}{4}A \times \frac{1+f}{2} \tag{S6}$$

As shown in Figure S1, all facets of an octahedron are triangle shape with the length of *a* and the area *S*, which equals $\sqrt{3}a^2/4$. If the total surface area of an octahedron is *A*, $S = A/8$. There are two kinds orientation of the six side facets, three facets are vertex up, and three facets are vertex down. The ratio of octahedron entered into water is defined as *x*, therefore, the edge with length of *ax* immerses into water, the edge with length of *a-ax* stays in oil. For the height, the height with length of $2H_F \cdot x$ immerses into water. The surface area for side facets while the octahedron enters water *ax* can be wrote as below:

$$A_{wp} = 3 \times \left(x^2 S + \left(1 - (1-x)^2\right)S\right) = 3S\left(x^2 + \left(1 - (1-x)^2\right)\right) = 6Sx = \frac{3Ax}{4} \tag{S7}$$

Base on the f definition, $f = -\frac{H_F - 2xH_F}{H_F}$, $x = \frac{1+f}{2}$,

Therefore, $A_{wp} = \frac{1}{8}A + \frac{3}{4}A \times \frac{1+f}{2}$ (S8)

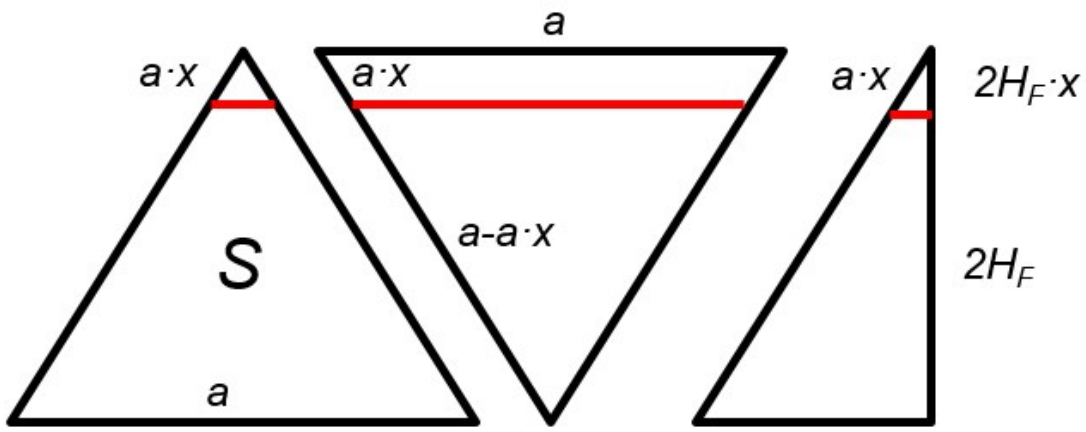


Figure S1. Sketch of the particle/water contact surface area calculation of an octahedron with facet up orientation. The length of one triangle octahedral facet is *a*, the area is *S*, which is *A*/8, and equals $\frac{1}{4}\sqrt{3}a^2$. The ratio of octahedral enter water is defined as *x*, therefore, the edge with length of *ax* immerses into water, the edge with length of *a-ax* stays in oil. For the height, the height with length of $2H_F \cdot x$ immerses into water.

For oil/water cross contact surface area A_{st}

$$A_{st} = \frac{\sqrt{3}}{4} \times a^2 \times ((\frac{3+f}{2})^2 - 3(\frac{1+f}{2})^2) \quad \text{(S9)}$$

As shown in Figure S2, the equation of an octahedron with facet up orientation water/oil cross contact surface area were described. The length of one triangle octahedral facet is *a*. The ratio of octahedral entered water is defined as *x*, therefore, the edge with length of *ax* immerses into water,

the edge with length of *a*-*ax* stays in oil. Left figure is for the *x*=0.5, the nanoparticle stays in water/oil interface. For the height, the height with length of $2H_F \cdot x$ immerses into water.

$$A_{st} = \frac{\sqrt{3}}{4} \times a^2 \times \left((1+x)^2 - 3(x)^2\right) \text{ ,where } x = \frac{1+f}{2}, \quad \text{(S10)}$$

$$= \frac{1}{8}A \times \left(\left(\frac{3+f}{2}\right)^2 - 3\left(\frac{1+f}{2}\right)^2\right) \quad \text{(S11)}$$

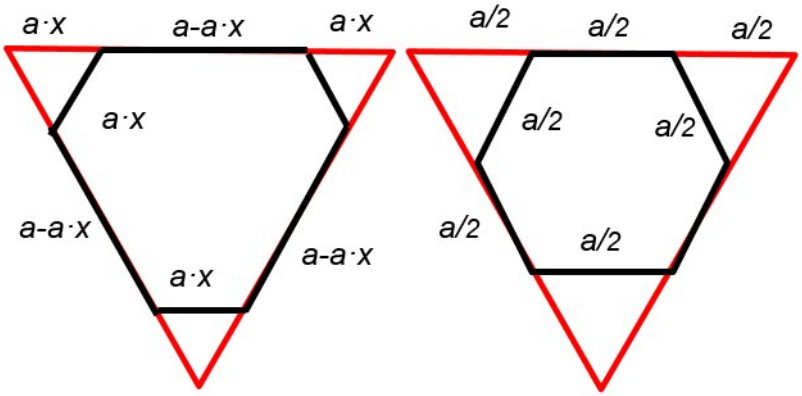


Figure S2. Sketch of the water/oil cross contact surface area calculation of an octahedron with facet up orientation. The length of one triangle octahedral facet is *a*. The ratio of octahedral entered water is defined as *x*, therefore, the edge with length of *ax* immerses into water, the edge with length of *a*-*ax* stays in oil. Left figure is for the *x*=0.5, the nanoparticle stays in water/oil interface. For the height, the height with length of $2H_F \cdot x$ immerses into water.

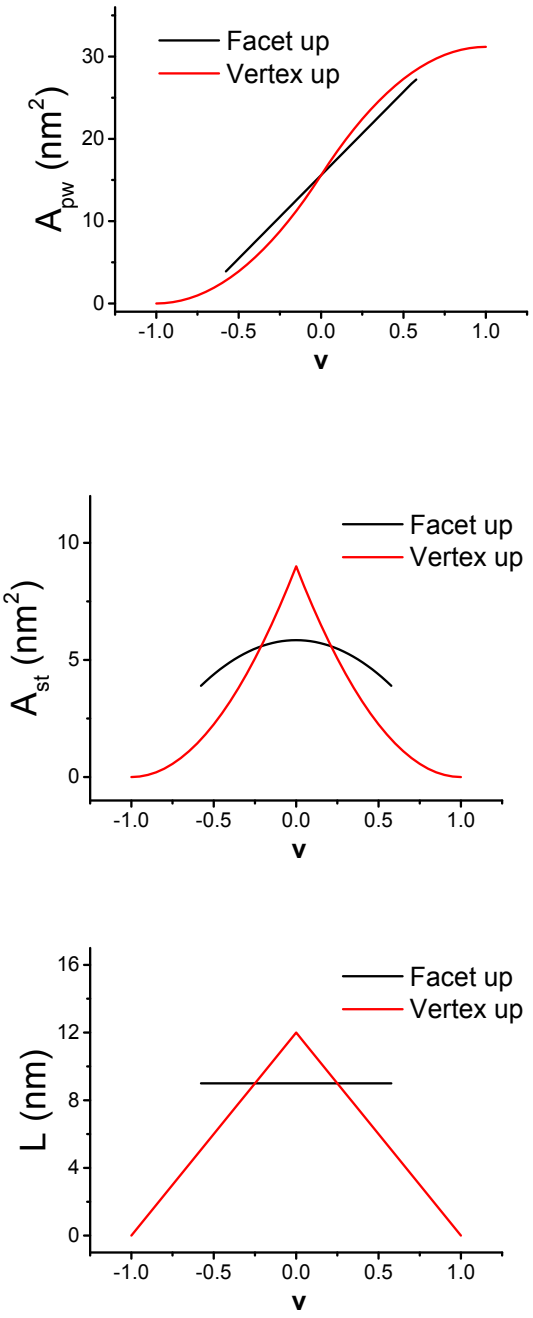


Figure S3. The particle surface area in water A_{pw}, cross surface area A_{st}, and the length of three-phase line, for vertex up and facet up orientations, the edge length a=3 nm.

S3. The relationship of contact angle and height ratio.

Equation (S2) is very general and it can be used to investigate nanoparticles with different shapes.

(a). Vertex up orientation:

$$A_{pw} = A \times \frac{(1-|v|)^2}{2} \quad -1 \leq v \leq 0$$

$$A_{pw} = A - A \times \frac{(1-|v|)^2}{2} \quad 0 < v \leq 1 \tag{S12}$$

$$\frac{d(A_{pw})}{d(v)} = \mp A(1-|v|) = \mp 2\sqrt{3}a^2 \times (1-|v|) \tag{S13}$$

$$A_{st} = a^2 \times (1-|v|)^2 \tag{S14}$$

$$\frac{d(A_{st})}{d(v)} = -2a^2 \times (1-|v|) \tag{S15}$$

$$\frac{d(F_{int}(v))}{d(v)} = 0 = \mp 2\sqrt{3}a^2 \times (1-|v|) \times (\gamma_{pw} - \gamma_{po}) + \gamma_{wo} 2a^2 \times (1-|v|) \tag{S16}$$

For octahedral particle in vertex up orientation, if the surface tensions γ_{pw}, γ_{po}, and γ_{wo} were fixed, the height position has relationship with contact angle. The relationship of contact angle and height ratio can be obtained as below:

$$(\gamma_{po} - \gamma_{pw})/\gamma_{wo} = R = \mp \frac{1}{\sqrt{3}} \tag{S17}$$

The cosine contact angle is $cos\theta$, which is:

$$cos\theta = -R = (\gamma_{po} - \gamma_{pw})/\gamma_{wo} \tag{S18}$$

The relationship between R and h_V^N is that R is a constant with $(\gamma_{pw} - \gamma_{po})/\gamma_{wo} = R = \mp 1/\sqrt{3}$. The v is canceled in the analysis and the R does not depend on v. This is caused by the planar surface of the octahedron. Based on the contact angle definition and mathematical calculation, the four facets

of an octahedron in water have same contact angles in the region of $0 < v \leq 1$, which is $\sqrt{3}/3$, or in the region of $-1 < v \leq 0$, which is $-\sqrt{3}/3$. Therefore, the cases of $(\gamma_{po} - \gamma_{pw})/\gamma_{wo} = R = \pm\sqrt{3}/3$ are two special points, where the octahedron can stay in water or oil phase with vertex up orientation at any positions and does not cause free energy change. This is easy to understand, such as sphere, while the $(\gamma_{po} - \gamma_{pw})/\gamma_{wo} = R = 0$, where the sphere has same interaction with water and oil, the sphere can stay in oil or water at any positions. However, surface tension γ_{pw} and γ_{po} should have a specific value compared to γ_{wo}, which is difficult to achieve in experiment, so that the two special points would not be discussed further.

(b). Facet up orientation:

$$A_{pw} = \frac{1}{8}A + \frac{3}{4}A \times \frac{1+f}{2} \tag{S19}$$

$$\frac{d(A_{pw})}{d(f)} = \frac{3}{8} \times A = 3\frac{\sqrt{3}}{4} \tag{S20}$$

$$A_{st} = \frac{\sqrt{3}}{4} \times a^2 \times ((\frac{3+f}{2})^2 - 3(\frac{1+f}{2})^2) \tag{S21}$$

$$\frac{d(A_{st})}{d(f)} = -\frac{\sqrt{3}}{4}a^2 f \tag{S22}$$

$$\frac{d(F_{int}(f))}{d(f)} = 0 = 3\frac{\sqrt{3}}{4}(\gamma_{pw} - \gamma_{po}) + \frac{\sqrt{3}}{4}f \times \gamma_{wo} \tag{S23}$$

$$(\gamma_{pw} - \gamma_{po})/\gamma_{wo} = R = -\frac{f}{3} = -\frac{\sqrt{3}v}{3} \tag{S24}$$

where $f = \sqrt{3}v$.

The cosine contact angle is $cos\theta$, which is:

$$cos\theta = -R = (\gamma_{po} - \gamma_{pw})/\gamma_{wo} \tag{S25}$$

(c) The Analyses of Free Energy Change Parabola for Vertex up orientation:

As defined before, the half-height in vertex up orientation $H_V = \sqrt{2}a/2$, where a is the edge length of an octahedron. With the total surface area $A = 2\sqrt{3}a^2$ and the height ratio $v = h_V/H_V$, the particle/water interface area A_{pw} can be calculated from equation (S26) for an octahedron with vertex up orientation.

$$A_{pw} = \begin{cases} A \times \dfrac{(1-|v|)^2}{2} & -1 \le v \le 0 \\ A - A \times \dfrac{(1-|v|)^2}{2} & 0 < v \le 1 \end{cases} \tag{S26}$$

The oil/water interface area occupied by the octahedron A_{st} can be calculated from equation (S27)

$$A_{st} = a^2 \times (1-|v|)^2 \tag{S27}$$

Since the express of A_{pw} depends on the sign of v, we discuss the equation (S3) in two regions: $-1 \le v \le 0$ and $0 < v \le 1$, which means the nanoparticle were immersed into water phase and oil phase, respectively.

$$F = \frac{F_{int}}{A\gamma_{wo}} = \begin{cases} \left(\dfrac{R}{2} - \dfrac{1}{2\sqrt{3}}\right)v^2 + 2\left(\dfrac{R}{2} - \dfrac{1}{2\sqrt{3}}\right)v + \left(\dfrac{R}{2} - \dfrac{1}{2\sqrt{3}}\right) & -1 \le v \le 0, \ a \\ -\left(\dfrac{1}{2\sqrt{3}} + \dfrac{R}{2}\right)v^2 + 2\left(\dfrac{1}{2\sqrt{3}} + \dfrac{R}{2}\right)v - \left(\dfrac{R}{2} + \dfrac{1}{2\sqrt{3}}\right) & 0 < v \le 1, \ b \end{cases} \tag{S28}$$

Case 1: $-1 \le v \le 0$,

$$F = \left(\frac{R}{2} - \frac{1}{2\sqrt{3}}\right)v^2 + 2\left(\frac{R}{2} - \frac{1}{2\sqrt{3}}\right)v + \left(\frac{R}{2} - \frac{1}{2\sqrt{3}}\right) \tag{S29}$$

F is a quadratic function of v, which has the general form: $f_{(x)} = a_1x^2 + b_1x + c$. We can get the two coefficients a_1 and b_1 for the normalized free energy change in equation (S29) to check the monotonic of the parabola.

$$a_1 = \left(\frac{R}{2} - \frac{1}{2\sqrt{3}}\right), \quad b_1 = 2\left(\frac{R}{2} - \frac{1}{2\sqrt{3}}\right),$$

The coefficients a_1 and b_1 together control the location of the axis of symmetry of the parabola, which is at $p = -b_1/2a_1 = -1$. The sign of a_1 depends on the value of R, as depicted below:

In the case of $-1 \le R < \sqrt{3}/3$, $a_1 < 0$.

In the case of $R = \sqrt{3}/3$, $a_1 = 0$.

In the case of $\sqrt{3}/3 < R \le 1$, $a_1 > 0$.

Case 2: $0 < v \le 1$

$$F = -\left(\frac{1}{2\sqrt{3}} + \frac{R}{2}\right)v^2 + 2\left(\frac{1}{2\sqrt{3}} + \frac{R}{2}\right)v - \left(\frac{R}{2} + \frac{1}{2\sqrt{3}}\right) \tag{S30}$$

which has the general form: $f_{(x)} = a_2x^2 + b_2x + c$.The two coefficients a_2 and b_2 are given by $a_2 = -\left(\frac{1}{2\sqrt{3}} + \frac{R}{2}\right)$, $b_2 = 2\left(\frac{1}{2\sqrt{3}} + \frac{R}{2}\right)$ for the normalized free energy change in equation (S30) to check the monotonic of the parabola.

The location of the axis of symmetry of the parabola is at $p = -b_2/2a_2 = 1$. The sign of a_2 depends on the value of R, as depicted below:

In the case of $-1 \le R < -\sqrt{3}/3$, $a_2 > 0$.

In the case of $R = -\sqrt{3}/3$, $a_2 = 0$.

In the case of $-\sqrt{3}/3 < R \le 1$, $a_2 < 0$.

Therefore, based on the location of the axis of symmetry and the open direction of the parabola, we can divide the region $-1\sim1$ to five regions, which are $-1 \le R < -\sqrt{3}/3$, $R = -\sqrt{3}/3$, $-\sqrt{3}/3 < R < \sqrt{3}/3$, $R = -\sqrt{3}/3$, and $\sqrt{3}/3 < R \le 1$, as shown in Figure 2a and Table 1.

The minimum value of F depends on the location of the axis of symmetry p and the orientation of the parabola. a_1, b_1 and a_2, b_2 are the coefficients for the equation (6) a and b, respectively, as shown in Section S3. Based on the location of p and the orientation of the parabola, we can divide the region $-1\sim1$ to five regions, which are (1) $-1 \le R < -\sqrt{3}/3$, (2) $R = -\sqrt{3}/3$, (3) $-\sqrt{3}/3 < R < \sqrt{3}/3$, (4) $R = \sqrt{3}/3$, and (5) $\sqrt{3}/3 < R \le 1$, as shown in Figure 2a and Table 1.

In the case of $-1 \le R < -\sqrt{3}/3$.

When $-1 \le v \le 0$, F follows equation (6) a, and is monotonic decreasing because the axis of symmetry is $p = -1$ and the parabola opens downward. When $0 < v \le 1$, F follows equation (6) b and is monotonic decreasing because the axis of symmetry is $p = 1$ and the parabola opens upward. Therefore, when $v = 1$, F reaches its minimum value of R, the octahedron is more hydrophilic and prefers to stay in water. F is plotted as the function of v in Figure 2b curve 1, where $R = -0.7$.

(2) In the case of $R = -\sqrt{3}/3$.

Similarly, when $-1 \le v \le 0$, F follows equation (6) a, and is monotonic decreasing because the axis of symmetry is $p = -1$ and the parabola opens downward. When $0 < v \le 1$, the F follows equation (6) b, and $F = 0$. Therefore, F reaches its minimum value of R in the region of $0 < v \le 1$, which means that the octahedron prefers to stay in water with any position. F is plotted as a function of v in Figure 2b curve 2, where $R = -\sqrt{3}/3$. As discussed in Section S3, the relationship between R and v is that R is a constant with $R = \sqrt{3}/3 = (\gamma_{pw} - \gamma_{po})/\gamma_{wo}$. v is canceled in the analysis and the R does not depend on v, arising from the planar surface of the octahedron. Based on the contact angle definition and mathematical calculation, the four facets of an octahedron in water have

identical contact angles in the region of $0 < v \leq 1$, which is $\sqrt{3}/3$. Therefore, the octahedron prefers to stay in water with any position when $R = -\sqrt{3}/3$.

(3) In the case of $-\sqrt{3}/3 < R < \sqrt{3}/3$.

When $-1 \leq v \leq 0$, F is monotonic decreasing because the axis of symmetry is $p = -1$ and the parabola opens downward. When $0 < v \leq 1$, it is monotonic increasing because the axis of symmetry is $p = 1$ and the parabola opens downward. Therefore, when $v = 0$, F reaches its minimum value of $(3R - \sqrt{3})/6$, half octahedron stays in water and half octahedron stays in oil. The F has its maximum value of 0 at $v = -1$, when R is negative, while it has its maximum value of R at $v = 1$ when R is positive. F is plotted as a function of v in Figure 2b curve 3, where R = − 0.2.

(4) In the case of $R = \sqrt{3}/3$.

When $-1 \leq v \leq 0$, $F = 0$. When $0 < v \leq 1$, the F is monotonic increasing because the axis of symmetry is $p = 1$ and the parabola opens downward. Therefore, in the region of $-1 \leq v \leq 0$, F reaches its minimum value of 0, which means that octahedron prefers to stay in oil with any position. F is plotted as the function of v in Figure 2b curve 4, where R = $\sqrt{3}/3$.

(5) In the case of $\sqrt{3}/3 < R \leq 1$.

When $-1 \leq v \leq 0$, F is monotonic increasing because the axis of symmetry is $p = -1$ and the parabola opens upward. When $0 < v \leq 1$, it is also monotonic increasing because the axis of symmetry is $p = 1$ and the parabola opens downward. Therefore, when $v = -1$, F reaches its minimum value of 0, which means that octahedron is more hydrophobic and prefers to stay in oil. F is plotted as the function of v in Figure 2b curve 5, where R = 0.7.

Molecular Dynamics (MD) Simulations. MD simulations were conducted on single Ag Octahedron placed at the water/oil interface using the GROMACS 4.07 simulation package[3] and GROMOS96 force fields[4]. See Section S4 for detailed discussion.

S4. Molecular Dynamics Simulation Model

The aim of utilizing molecular dynamics simulations is to understand the mechanism of Ag octahedron stabilized at the water/oil interface. Molecular dynamics simulation enables us to trace the nanoscale events occurring over the interfacial behaviors and at the same time provides molecular information at nanoscale interfaces. For this purpose, we utilize all-atomic models for our simulations.

Computational details. The GROMACS 4.07 simulation package and GROMOS96 force field were used for all our MD simulations. Two neighboring atoms interact with each other through van der Waals interactions, which is treated using a 12-6 Lennard - Jones (LJ) potential summed over all pairs of atoms i and j. The LJ potential may also be written in the following form:

$$V_{LJ}(\mathrm{r_{ij}}) = 4\varepsilon_{ij}\left(\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6}\right) \tag{S31}$$

where r_{ij} is the distance between the interacting pairs of atoms, σ_{ij} and ε_{ij} are the LJ parameters between atoms. The GROMACS LJ potential parameters $C_i^{(6)}$ and $C_i^{(12)}$ can be defined using the combination rules:

$$C_i^{(6)} = 4\varepsilon_i\sigma_i^6 \tag{S32}$$

$$C_i^{(12)} = 4\varepsilon_i\sigma_i^{12} \tag{S33}$$

The combinations for different atom-types can be computed according to the combination rule:

$$C_{ij}^{(6)} = (C_i^{(6)}C_j^{(6)})^{\frac{1}{2}} \tag{S34}$$

$$C_{ij}^{(12)} = (C_i^{(12)}C_j^{(12)})^{\frac{1}{2}} \tag{S35}$$

The LJ parameters σ_0 = 0.2955 nm and ε_0 = 19.0790 kJ/mol for Ag atoms were used.[5] Ag Octahedron with about 3 nm edge length were constructed using an all-atomic model, made up by 670 Ag atoms, with 344 Ag atoms inside as the core and 326 surface Ag atoms outside as the surface layer. The surface wettability of Ag octahedron is adjusted by changing the charge amount (***q***) on outlayer Ag atoms, where the unit is elementary charge (*e*) as depicted in Section S4 and shown in Figure S4. To preserve the octahedron shape of Ag nanoparticle after the introduction of charge, the interactions between Ag atoms were strengthen. Solvent molecule 1-hexane molecular model employed in this study was generated from the small-molecule topology generator PRODRG.[6] Water was modeled using the single point charge (SPC) model, with the bond lengths and angles held constant through the use of the SETTLE algorithm. Bond lengths of molecules were constrained using the LINCS algorithm. The cutoff distance for short-range non-bonded interactions was chosen to be 12 Å and long-range electrostatic forces were computed using the PME approach.

Simulations for Ag octahedron on water/hexane interface.

To study the roles of interfacial properties of Ag octahedron, the Ag octahedron was put into the vicinity of water/hexane interface. The edge length of the Ag octahedron core was approximately 3 nm. One Ag octahedron was placed in an 8× 8 × 16 nm^3 simulation box. The cutoff distance for short-range non-bonded interactions was chosen to be 12 Å.

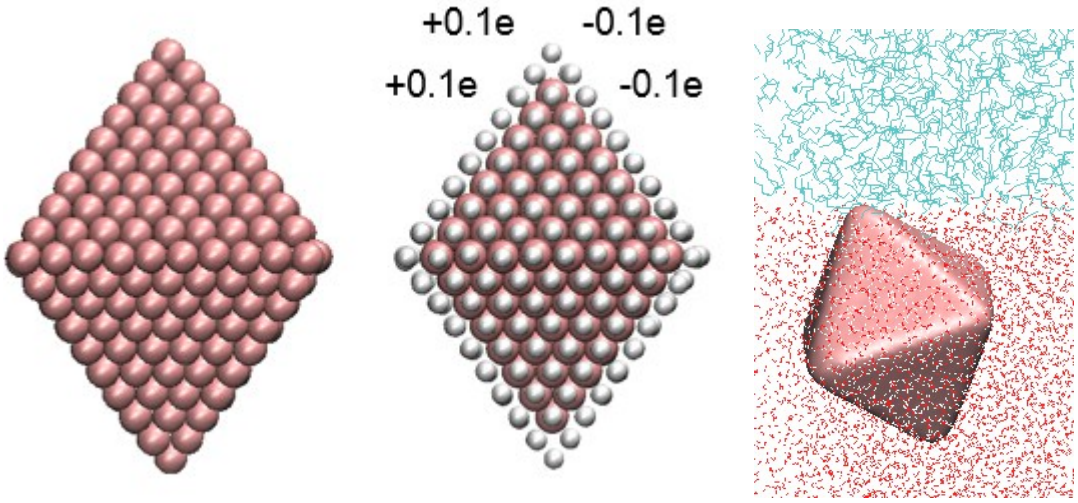
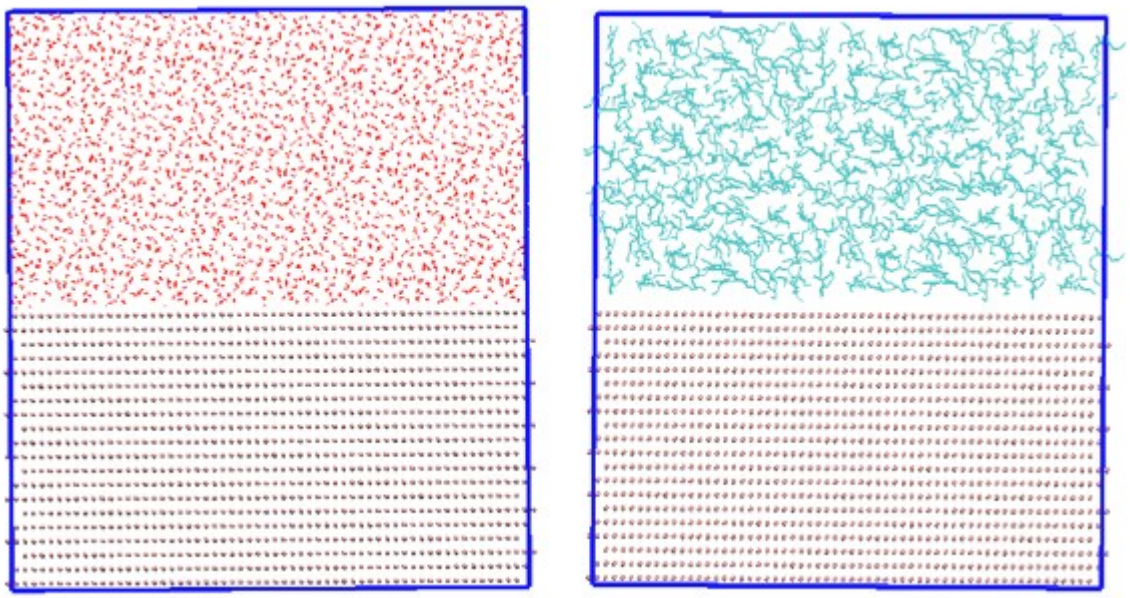


Figure S4. Octahedron models constructed for simulations. (a) Ag octahedron built using 344 Ag atoms inside and 326 surface Ag atoms; (b) surface Ag atoms shown by silver color, the surface Ag atoms with positive or negative charge randomly, and the total net charge is zero; (c) initial state for Ag nanoparticle at the vicinity of water/hexane interface.

Simulations were performed using the NPT ensemble, the temperature was maintained at 300 K using the Berendsen temperature coupling method[7] and Berendsen bath coupling scheme[8] were used to keep a constant pressure 1 bar. Simulations were run over 5 ns in steps of 2 fs.

S5. Simulations for surface tension of Ag slab with different *q* in water and in hexane.



(a) **(b)**

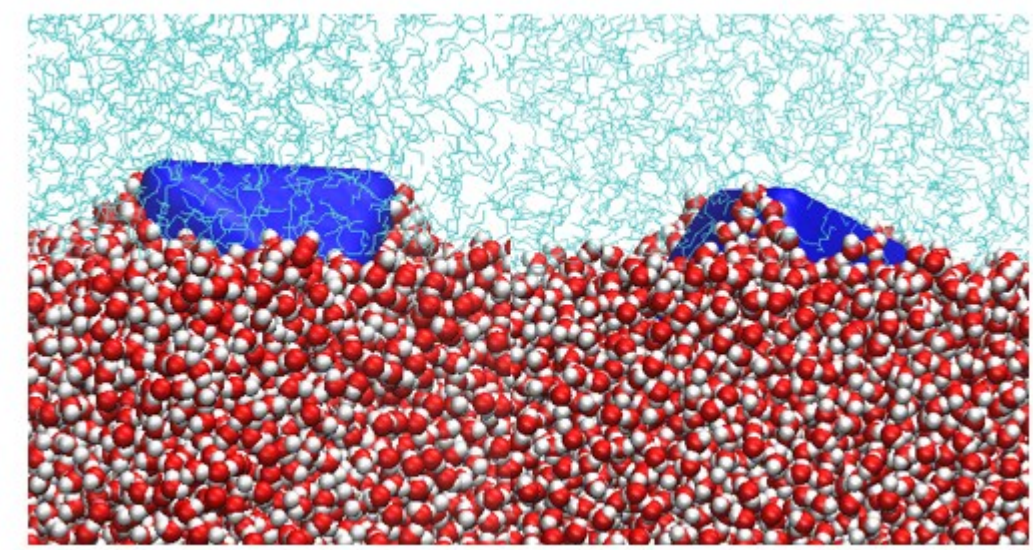
Figure S5. Illustration of the calculation of the (a) Ag-water and (b) Ag-hexane surface tension, the surface Ag atoms charged with various *q*, using the same charged method for octahedron.

Simulations were performed using the NVT ensemble, the temperature was maintained at 300 K using the Berendsen temperature coupling method and Berendsen bath coupling scheme was

used to keep a constant volume. Simulations were performed over 1 ns in steps of 2 fs. The interfacial tensions γ is defined as the difference of the normal, P_N, and lateral, P_L, pressures in the box:

$$\gamma=< (P_N-P_L)L_Z >/2 \quad \text{(S36)}$$

where Lz is the box normal size and $P_L=(P_{xx}+P_{yy})/2$. The factor (1/2) outside the bracket takes into account the fact that there are two interfaces in the system. The water/oil surface tension is calculated using same method.



(a) **(b)**

Figure S6. Snapshots of the water molecules covers on the Ag octahedron surface, the Ag octahedron with q (a) 0.34 e, and (b) 0.36 e.

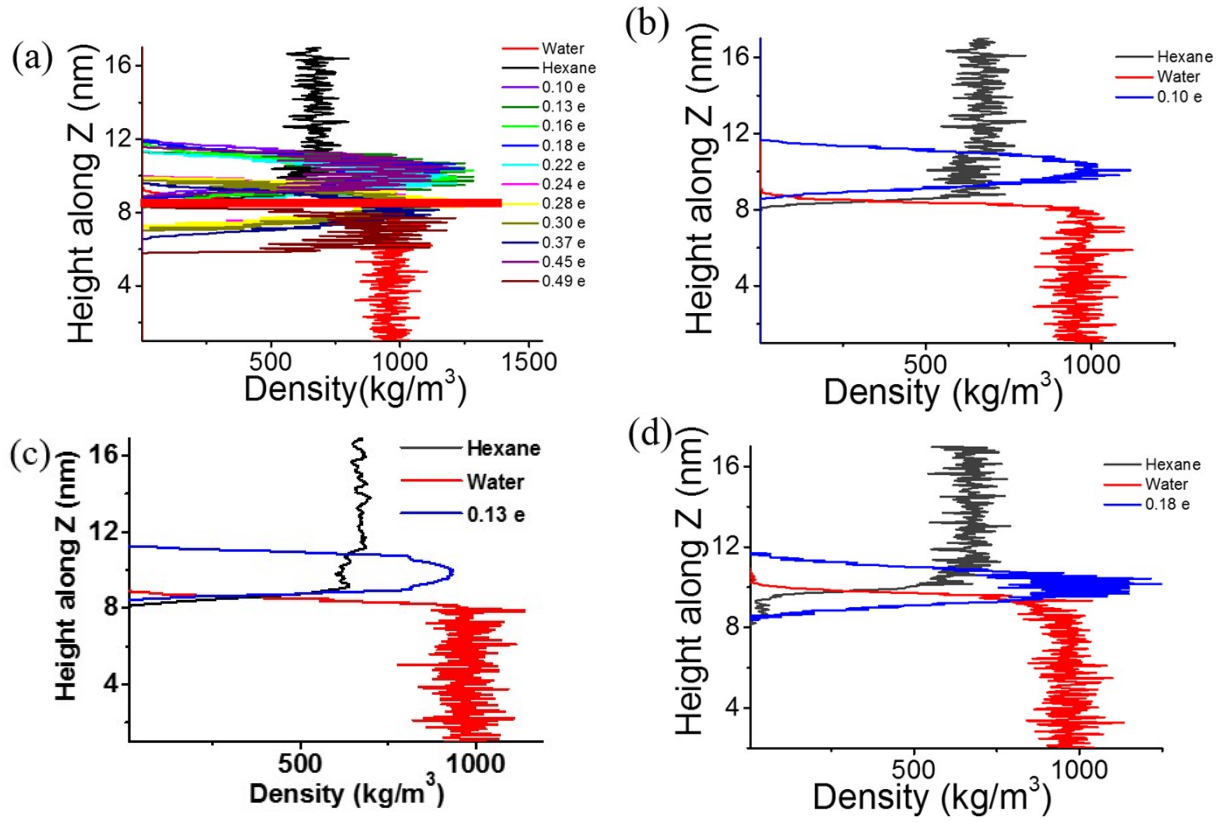


Figure S7. a) The density distribution of one Ag octahedron with different q. The water/hexane interface position is highlighted by the red straight line. b) The density distribution of one Ag octahedron with q = 0.10 e. c) The density distribution of one Ag octahedron with q = 0.13 e. d) The density distribution of one Ag octahedron with q = 0.18 e.

S6. Supporting Information References

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