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

Supporting Information

Stability, deformation and rupture of Janus oligomer enabled self-emulsifying water-in-oil microemulsion droplet

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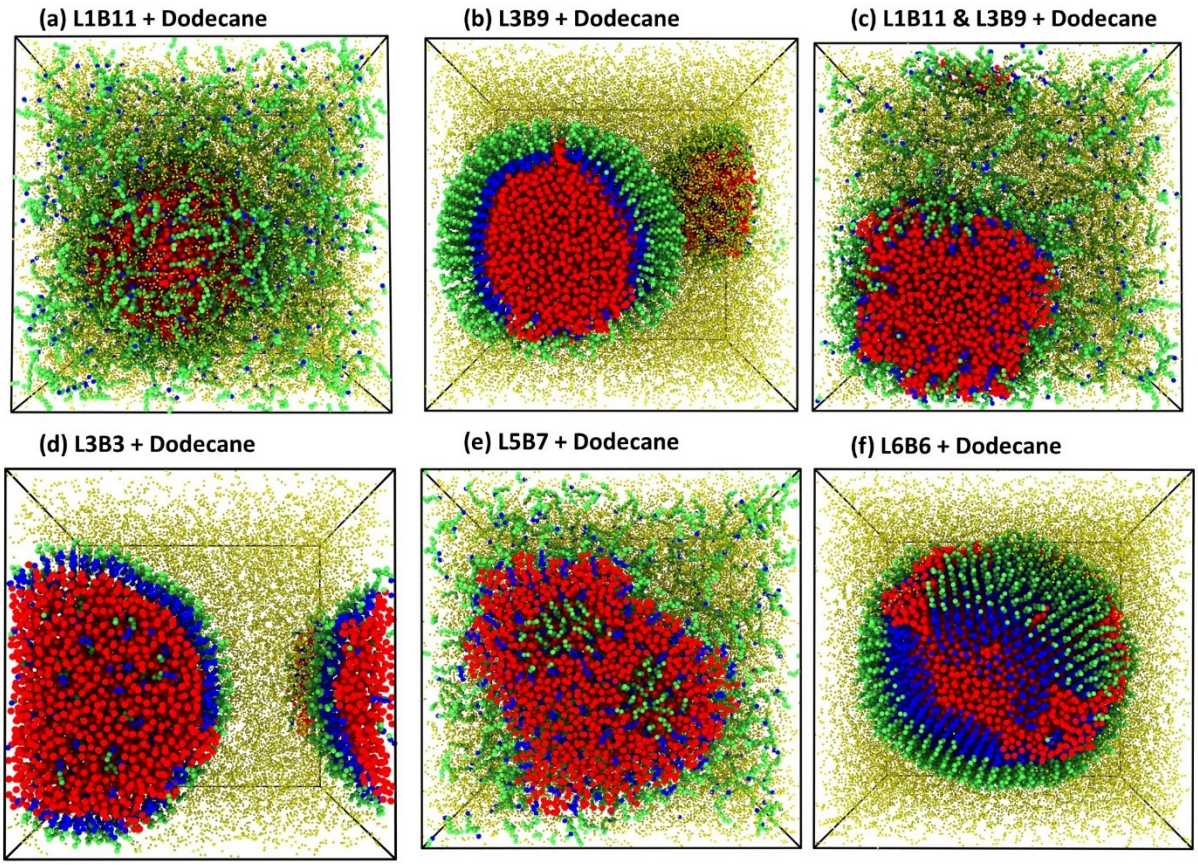

Figure S1 Atoms with red color are water molecules; atoms with blue and green color are janus oligomer molecules; the yellow atoms are oil molecules. With same mole ratio of water:surfactant:oil (6144:1024:3072), three microemulsion droplet were built up. (a) water, surfactant L1B11 (512)+ L3B9 (512), and dodecane oil; (b) water, surfactant L3B9 and dodecane oil; (c) water, surfactant L1B11 (512)+ L3B9 (512), and dodecane oil; (d) water, surfactant L3B3 and dodecane oil; (e) water, surfactant L5B7 and dodecane oil; (f) water, surfactant L6B6 and dodecane oil.

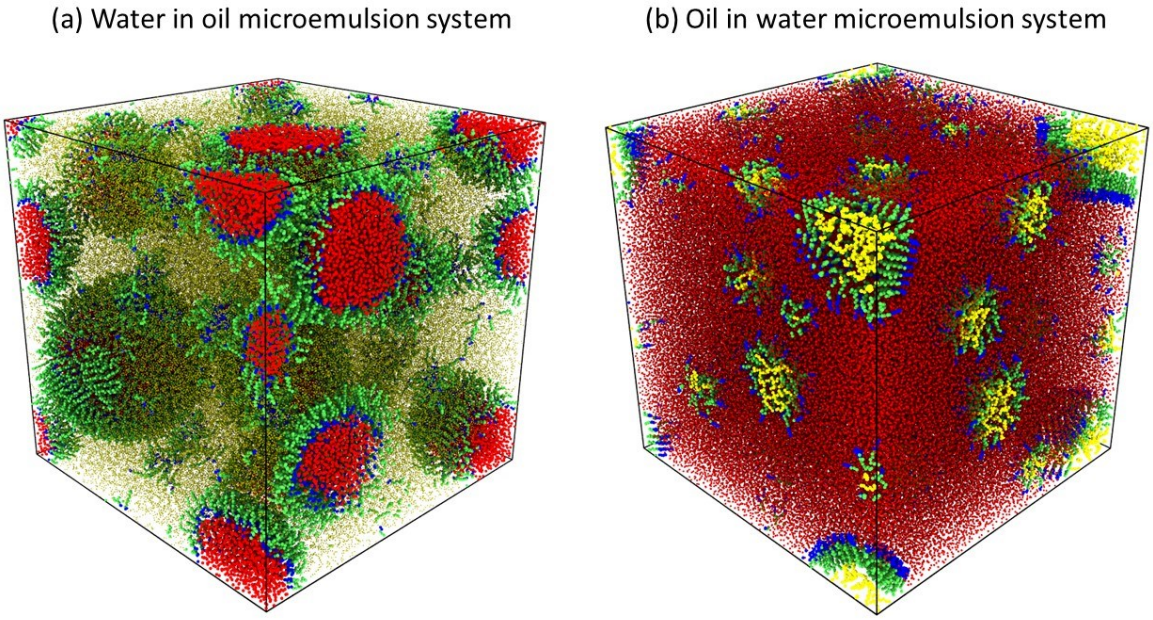

Figure S2 With same forcefield parameter, two microemulsion systems were simulated. (a) water in oil microemulsion system consisting of water molecules (32928), L2B10 surfactant molecules (5488) and dodecane oil molecules (16464); (b) oil in water microemulsion system consisting of water molecules (47928), L2B10 surfactant molecules (5488) and dodecane oil molecules (16464).

In order to get a statistical significance, we calculated the thickness of interface of each system from X-, Y-, and Z- axis direction.

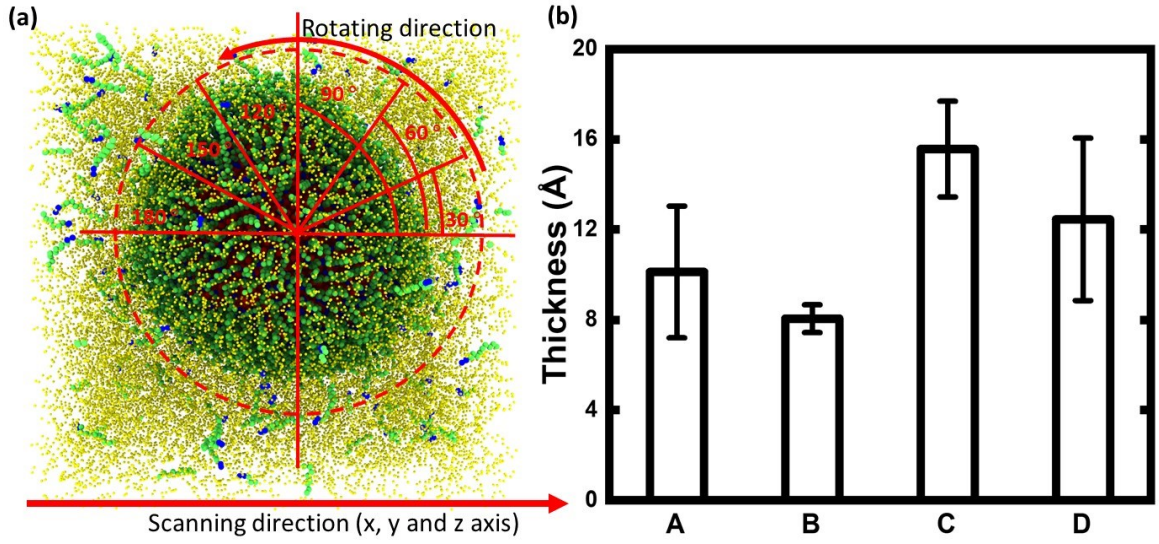

Figure S3 The method to scan the density of the system. (a) When the scanning direction is fixed, the rotating angle is set to 30°, 60°, 90°, 120°, 150° and 180°, that is to say, in every axis direction six density values are calculated. All density values of four systems are collected into (b).

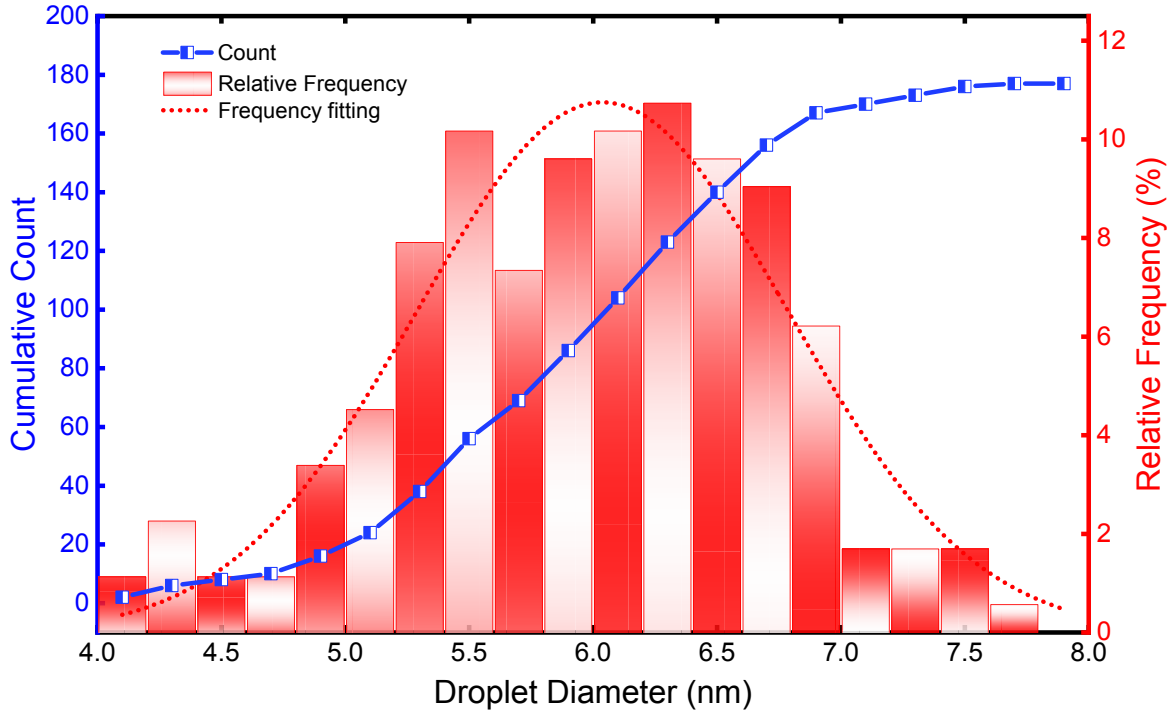

Figure S4 The microemulsion droplets diameter distribution in a large system.

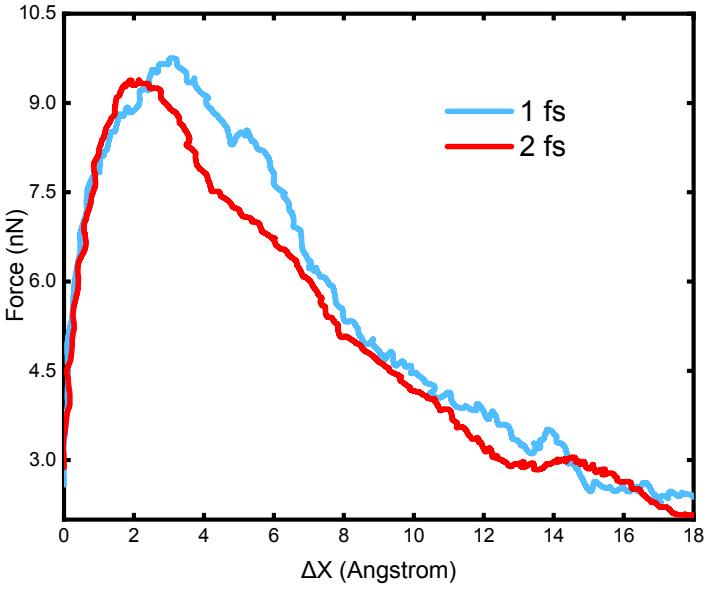

Figure S5 Rupturing force profiles of the same microemulsion droplet using timesteps of 1 and 2 fs.