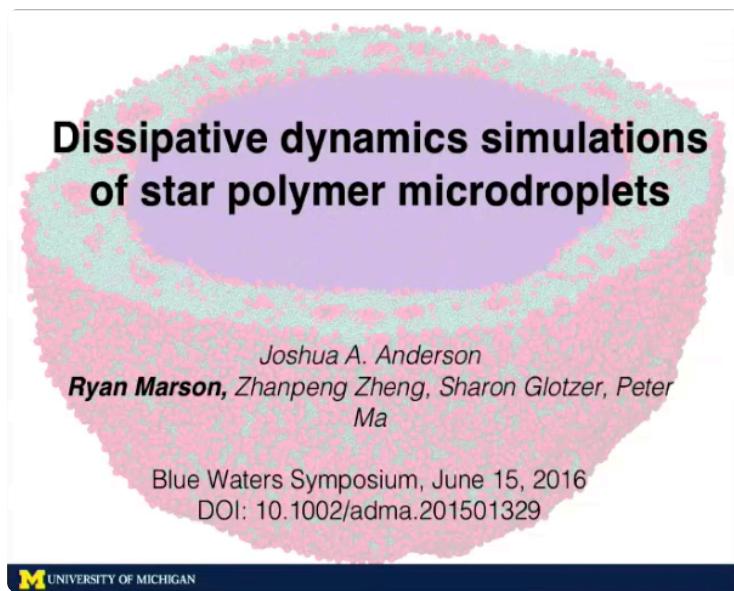


## An Example of Dissipative Particle Dynamics (DPD)

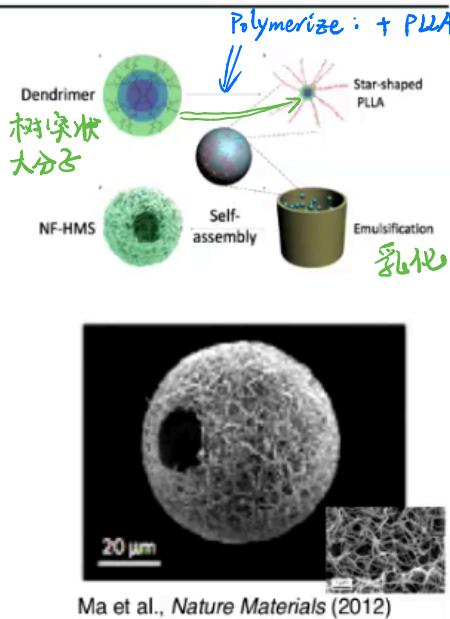
Title: Dissipative Particle Dynamics Simulations of Star Polymer Microdroplets -- Ryan Marson  
Link: <https://www.youtube.com/watch?v=Vm5aQw1osSg>

Description for the Video in the beginning: "Star polymer droplets can be used as scaffolds for tissue regeneration. Experiments of these systems demonstrate a variety of hollow, non-hollow, and porous structures. We perform dissipative particle dynamics simulations (DPD) of 10 million particles using HOOMD-blue on Blue Waters XK7 GPU nodes. Our simulations map the phase diagram of droplet morphologies as a function of hydroxyl density and star polymer architecture (arm length and number) and offers predictive power to direct future experiments. This system demonstrates the possibility of functional droplets composed of complex networks, with a hierarchy of scales that can be tuned for specific applications."



## Intro – Hollow microspheres for tissue regeneration

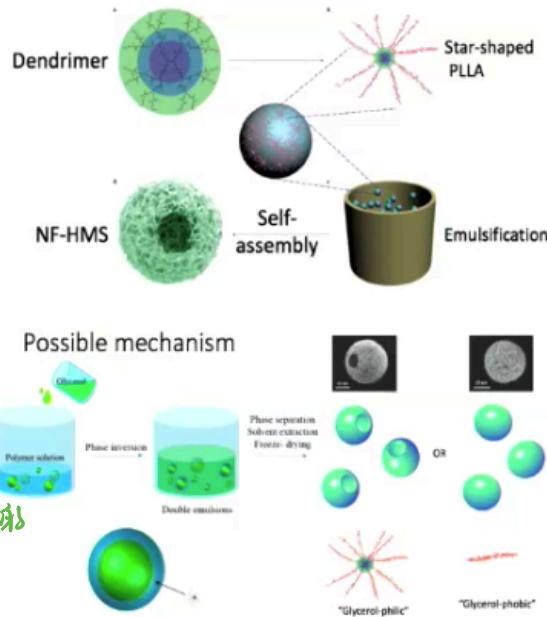
- Droplet morphology convenient for implanting in tissue.
- Initial structure formation was poorly understood. Mechanism for pore formation.
- Combined experimental/computational study to elucidate formation mechanisms.



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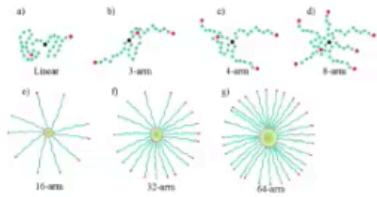
## Experiments - Star polymer double emulsion

- PLLA star polymer
- Double emulsion leads to a confined assembly at droplet surface
- Immiscible 不混溶物 components



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## Droplet morphologies - Affect of building blok



2-Arm  
PLLA-200

3-Arm  
PLLA-100

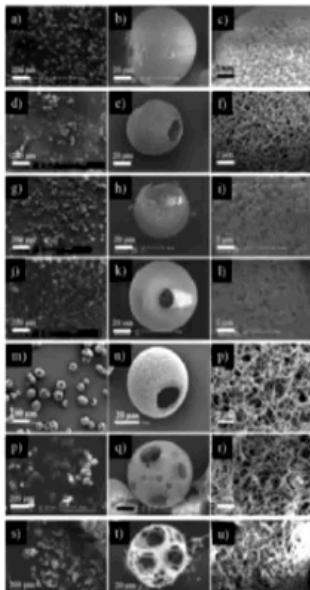
4-Arm  
PLLA-100

8-Arm  
PLLA-100

16-Arm  
PLLA-100

32-Arm  
PLLA-100

64-Arm  
PLLA-100

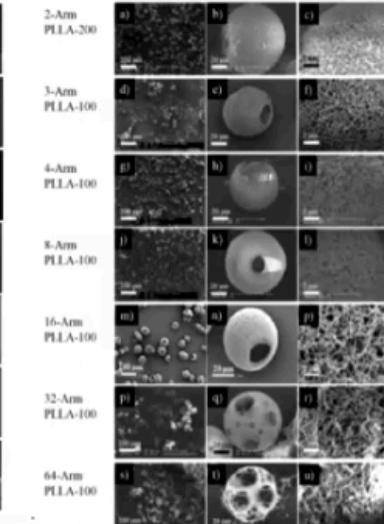
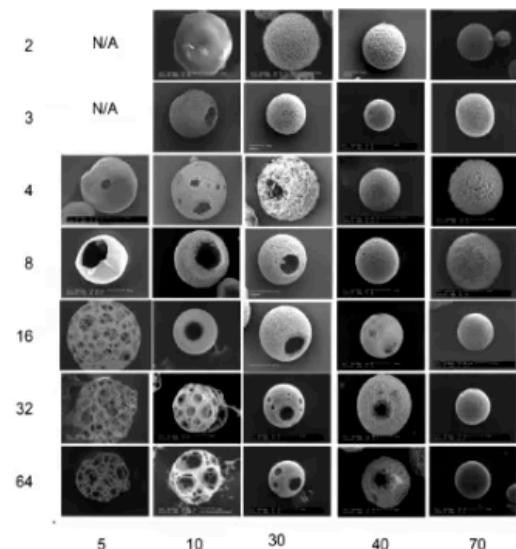


- Varying arm number and length affect the assemblies
- Short arms favor the formation of hollow, porous structures.
- Hydroxyl density plays a very important role

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## Parameter space

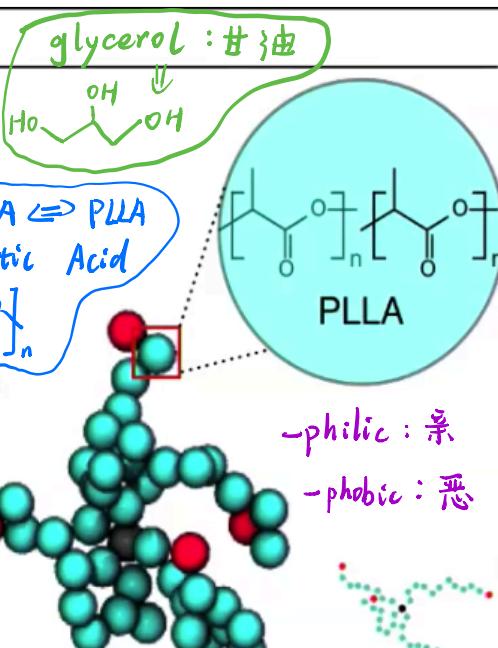
Arm Number



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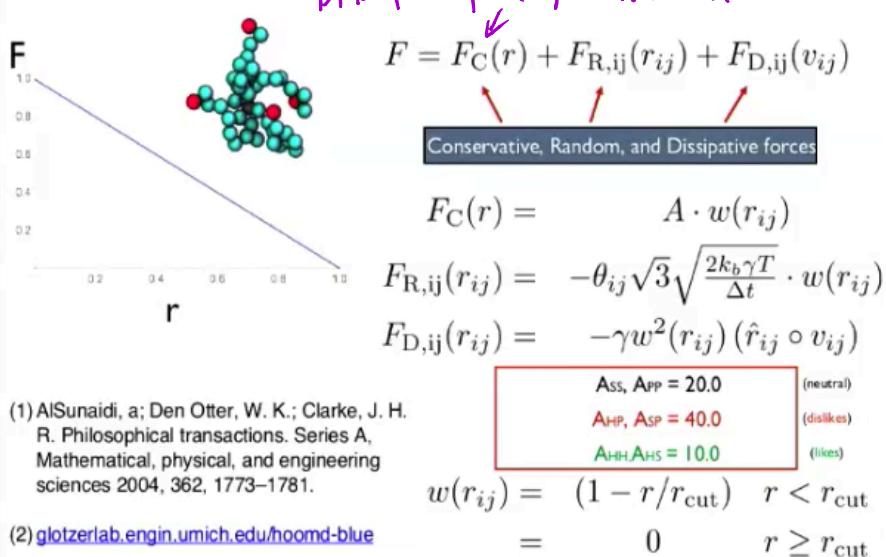
## Model - Coarse graining

- Hydroxyl groups are **glycerophilic** - want to contact glycerol solution.
- Polymer is **glycerophobic** - wants to avoid glycerol.
- Central core with unreacted and/or exposed hydroxyl groups



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## Model - Dissipative Particle Dynamics - HOOMD



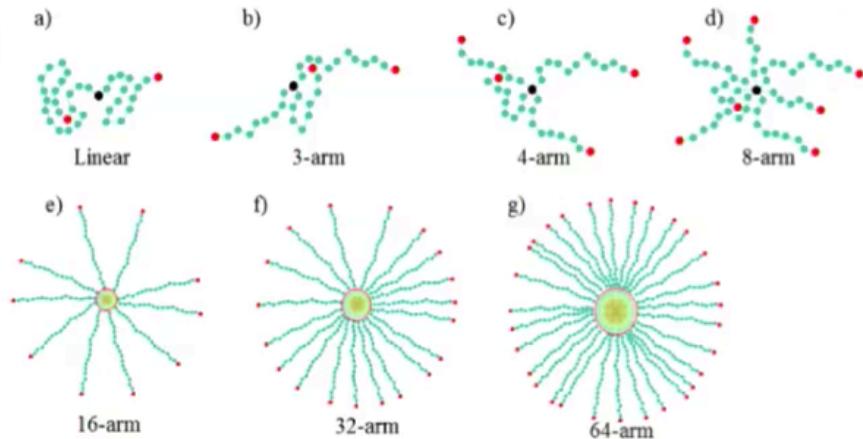
This is implemented in HOOMD, which is a simulation code, developed by the presenter.

It is a GPU-accelerated, micro dynamics, Monte Carlo simulation code, driven by Python.

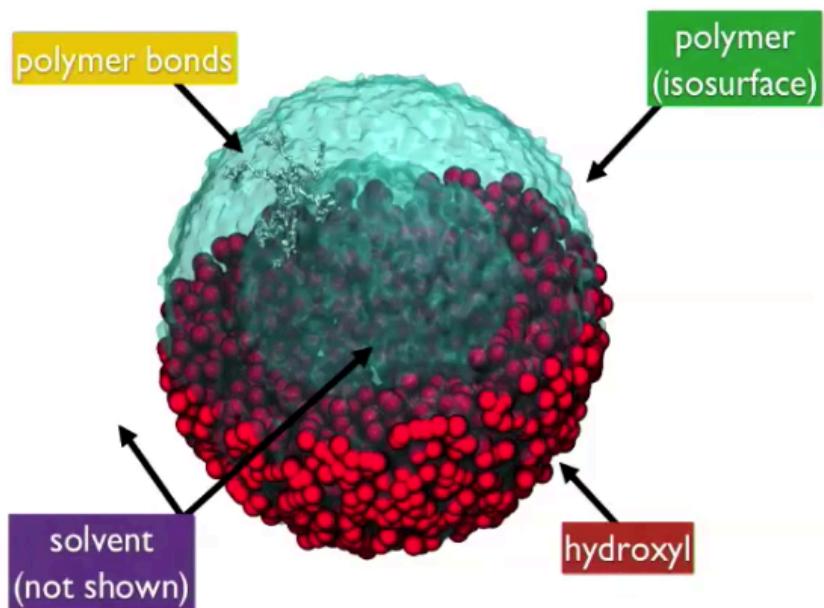
Random force: in a timestep, you are looking at a pair of particles and you are actually applying random forces. Pseudo-number generators generate these random forces between these 2 particles.

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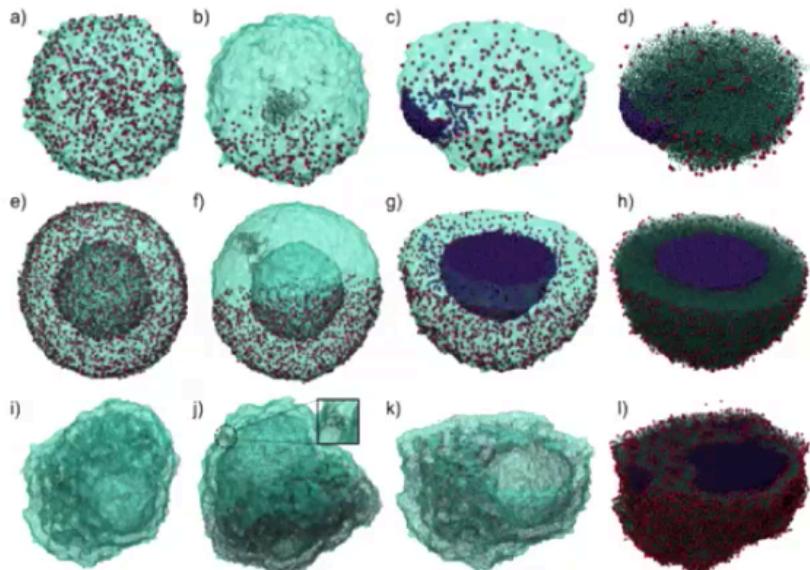
## Model - Experimental arm numbers



## DPD - Constructed droplet assembly

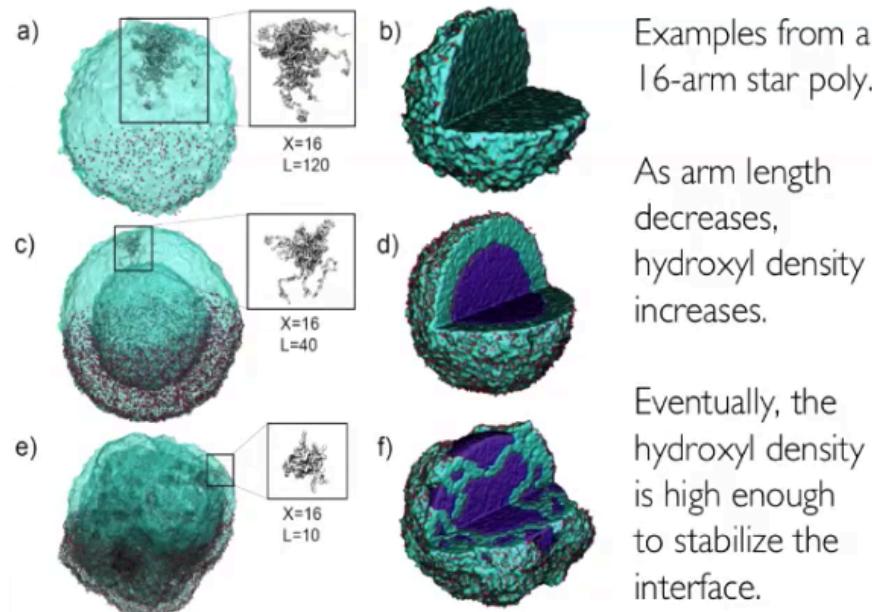


### Droplets - hollow, non-hollow, and porous (4 and 8 arm)



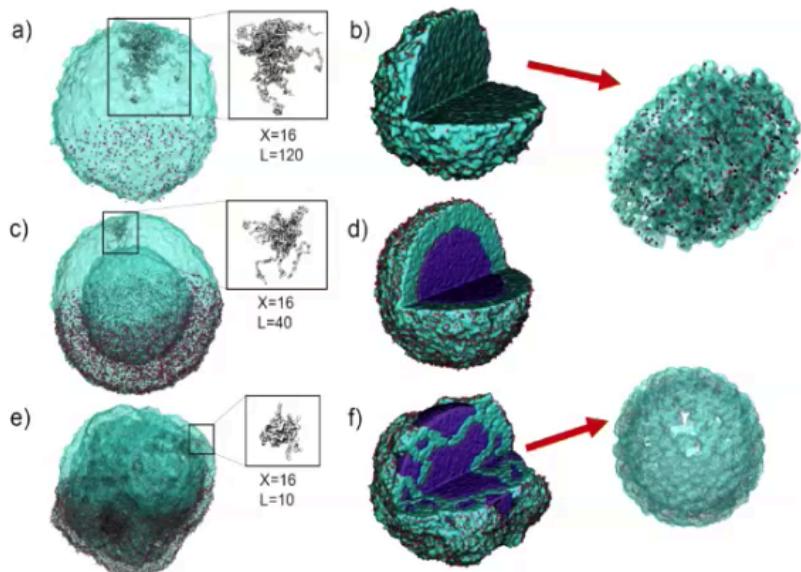
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### Droplets - Transitions based on arm length (16 arm)



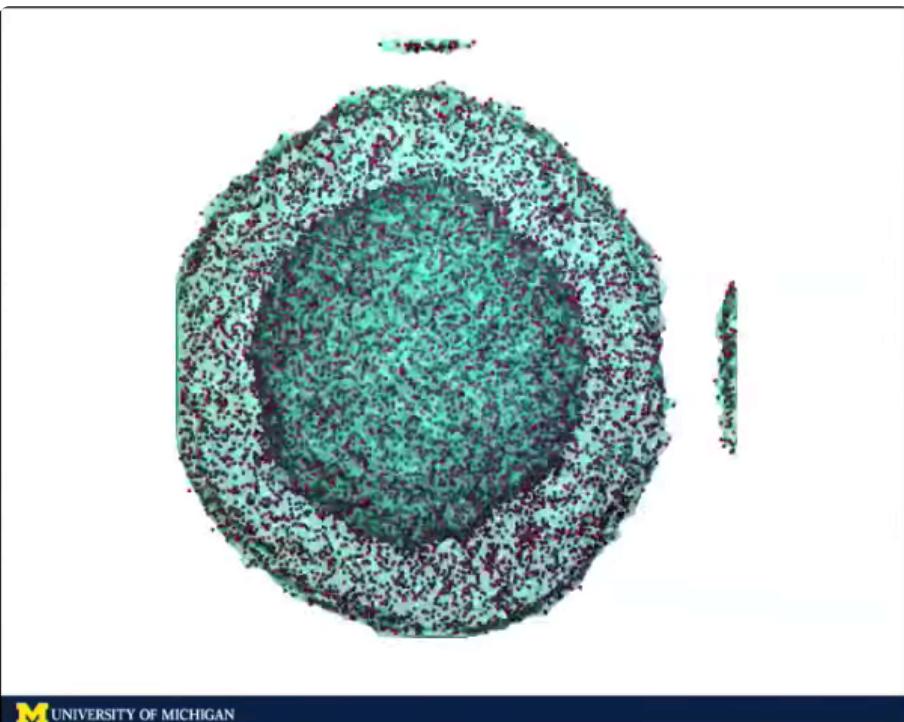
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## Droplets - 50 million DPD timesteps



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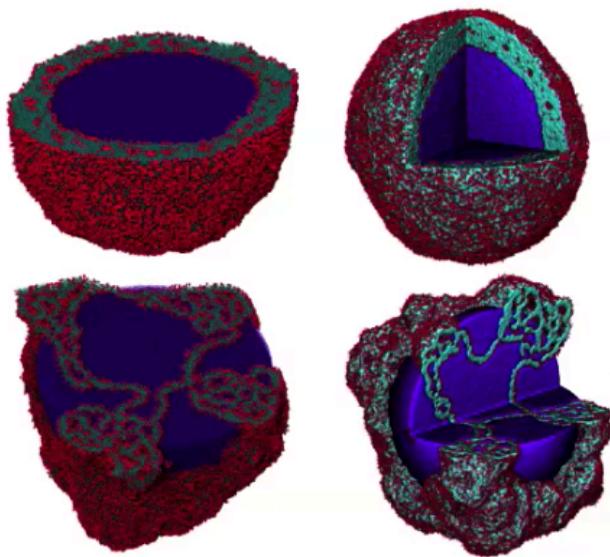
THE GLOTZER GROUP



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## 11 million+ particle simulations

- 128 GPUs



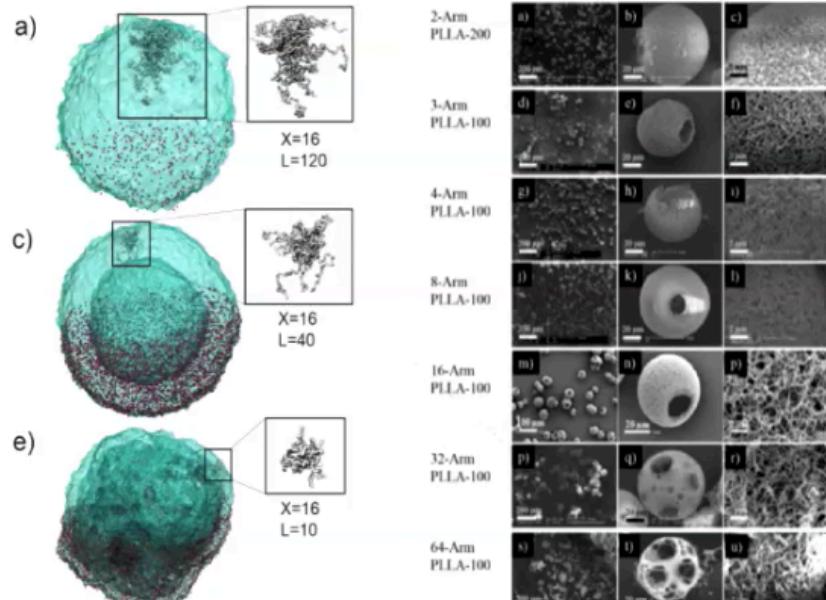
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## Hydroxyl Hypothesis - Final Conformation

- Doubling Hydroxyl repulsion stabilizes hollow structure

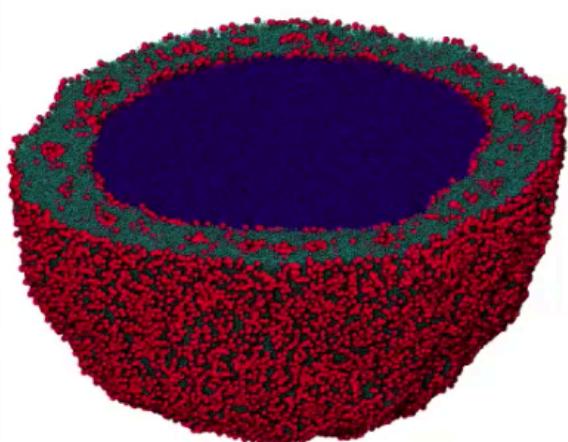
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## Parameter space - trends corroborate experiments



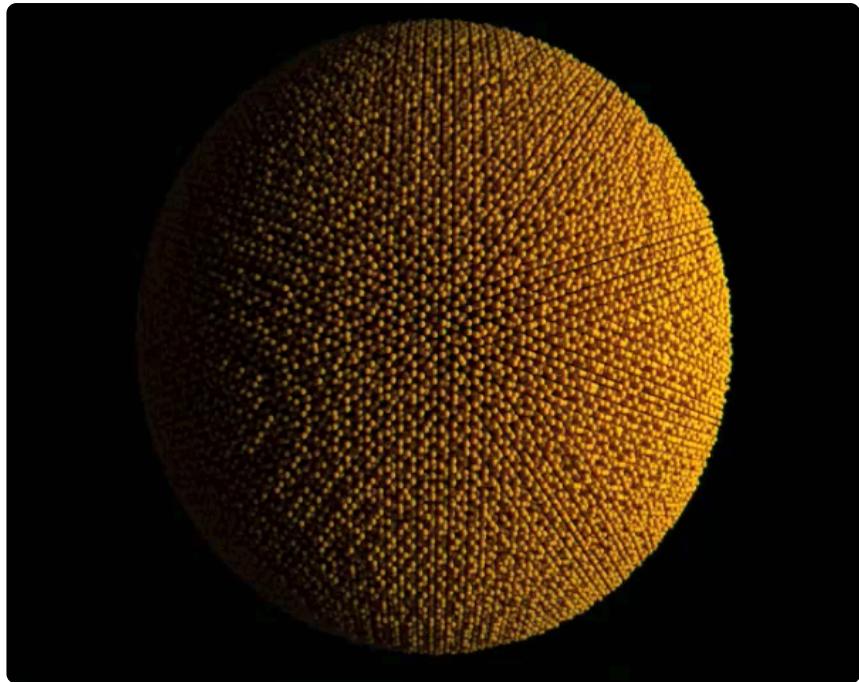
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## Droplet Study - Conclusions



- Versatile assembly platform
- Fine scale control of micro and nano-scale.
- Interesting regions that could lead to more complex structures.

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An another Demo video showing the use of DPD simulation.

Link: <https://www.youtube.com/watch?v=o48whIisE4s>