Multiscale Simulation Study of Polymer Systems Based on Dissipative Particle Dynamics

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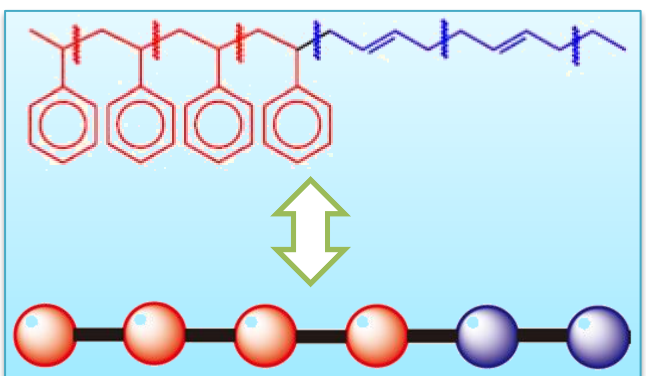
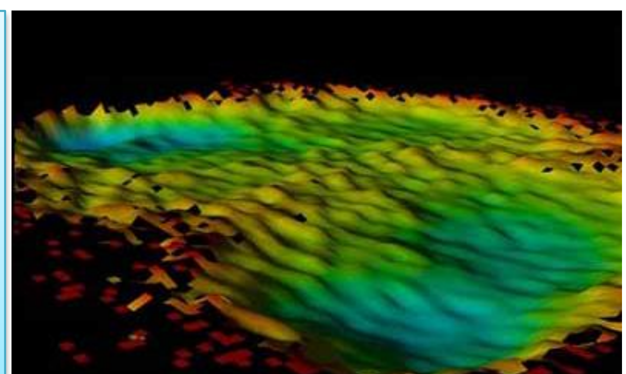
Multiscale simulations

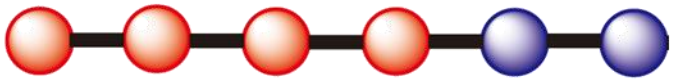
- **Polymer models at coarse-grained (CG) level**
- **Combining different scales in one simulation**
- **Enhanced sampling**
- **Powerful simulation package**





Generic polymer model

Dissipative particle dynamics (DPD) :



$$\vec{F}_i = \sum_{j \neq i} \left(\vec{F}^c_{ij} + \vec{F}^d_{ij} + \vec{F}^r_{ij} \right)$$

$$\vec{F}^c_{ij} = -\nabla V(r_{ij}) = \begin{cases} a_{ij}\left(1 - r_{ij}/r_c\right)\hat{r}_{ij} & (r_{ij} < r_c) \\ 0 & (r_{ij} \geq r_c) \end{cases}$$

$$\vec{F}^d_{ij} = -\gamma \omega^D(r_{ij})\left(\vec{v}_{ij} \cdot \hat{r}_{ij}\right)\hat{r}_{ij}$$

$$\vec{F}^r_{ij} = \sigma \omega^R(r_{ij})\xi_{ij}\hat{r}_{ij}$$

$$a\rho = 75$$

$$\chi = 0.2\rho(a_{AB} - a)$$

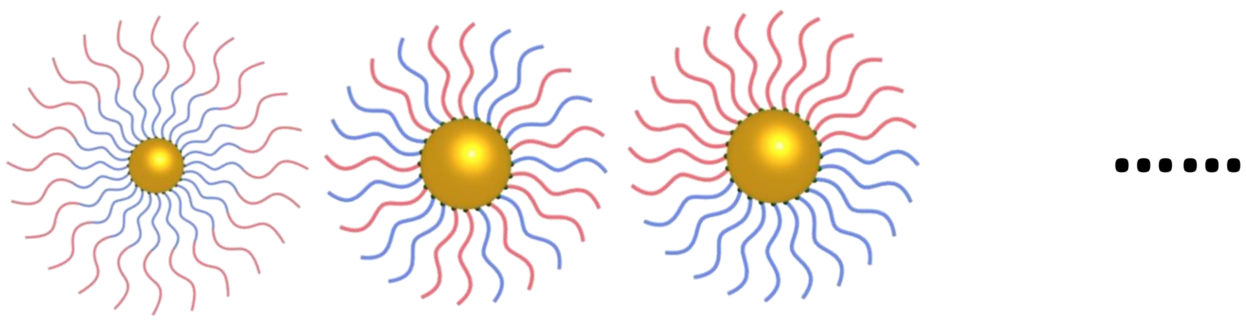
$$\omega^D(r) = {\omega^R}^2(r)$$

$$\sigma = (2k_B T\gamma)^{1/2}$$

Generic polymer model

With DPD:

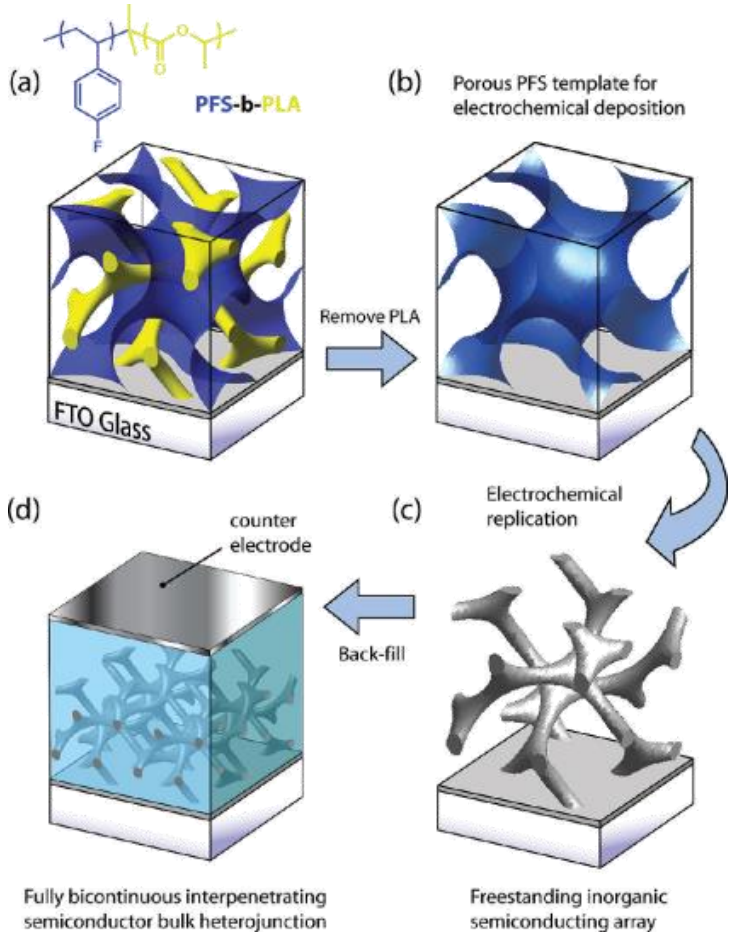
Block copolymers with different sequences, flexibilities, topologies, and so on.

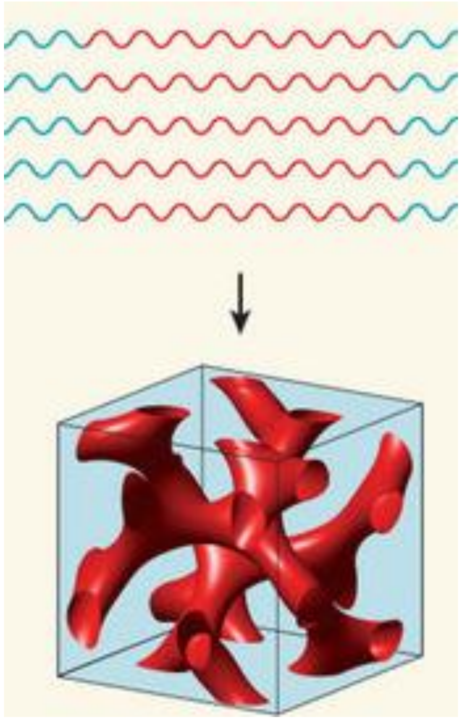


Polymer grafted nanoparticle with different polymer compositions, nanoparticle shapes, and so on.

Network morphology

Solid-state dye-sensitized solar cell





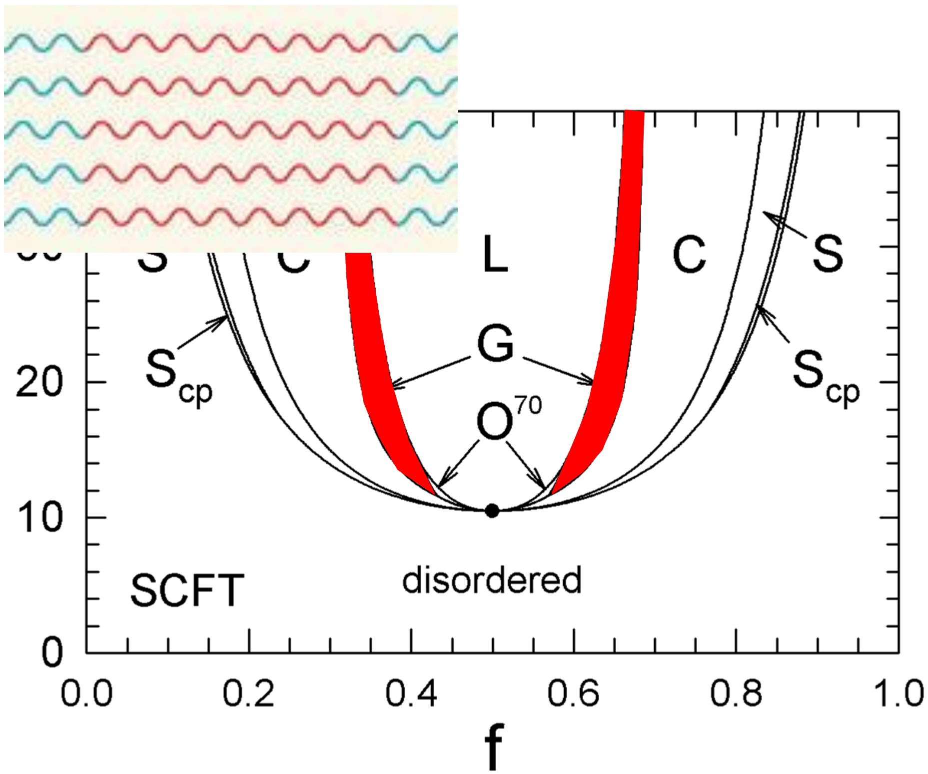
Advantage:

- A large surface/volume ratio of metal oxide
- A short diffusion length for exciton to the interface

Crossland et al., Nano Lett. 9, 2807, 2009.

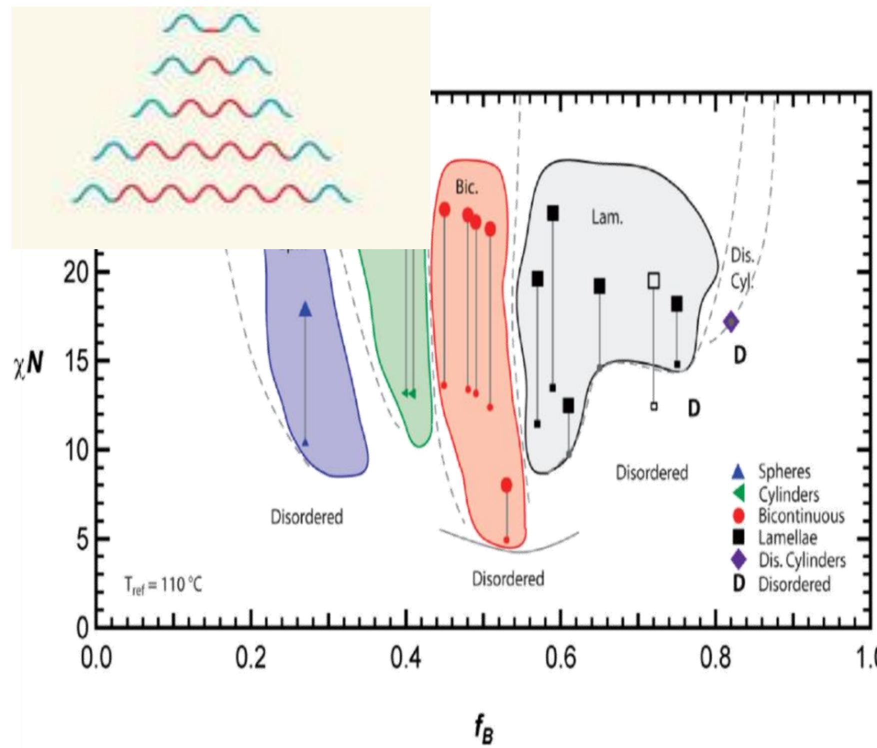
Network morphology

Gyroid structure only forms in a very narrow composition window (~3%).



Hillmyer et al. Prog. in Polym. Sci., 33, 875, 2008.

Irregular bicontinuous network structure forms in composition window (~10%).



Mahanthappa et al. J. Am. Chem. Soc. 134, 3834, 2012.

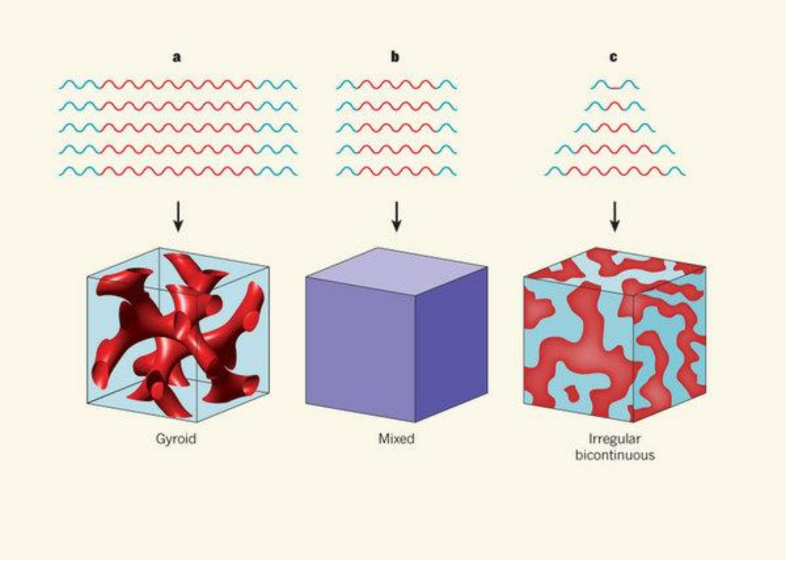
Network morphology

nature International weekly journal of science

Materials science: Continuity through dispersity

Richard A Register

Nature **483**, 167–168 (08 March 2012) | doi:10.1038/483167a
Published online 07 March 2012



- Whether asymmetric polydispersity is required -- that is whether the lengths of A blocks must be narrowly distributed?
- Whether both domains are fully continuous across the entire composition range for which the irregular bicontinuous structure forms?

Network morphology

Schulz-Zimm (SZ) distribution:

$$p(N) = \frac{u^u \delta^{u-1} \exp(-u\delta)}{N_n \Gamma(u)}$$

$$\delta = N/N_n\,,\ \mathrm{PDI} = N_w/N_n = (1+u)/u$$

- $A_x B_{N-2x} A_x$, N_n= 8~18
- V_{box} = 40 × 40 × 40

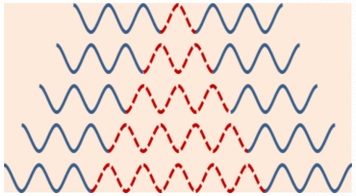
Simulated systems:

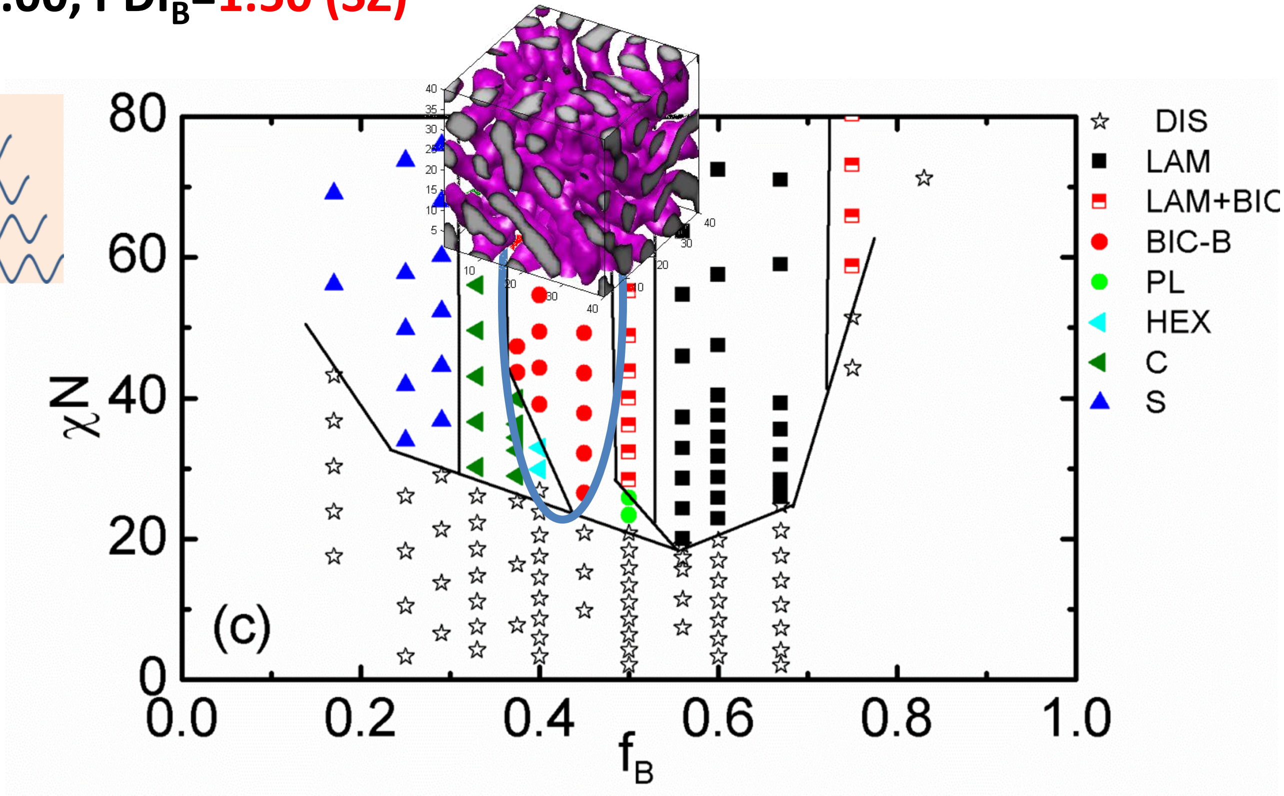
System	PDI_A	PDI_B
Asymmetric PDI	1.0	1.5 (SZ)
Symmetric PDI	1.5 (SZ)	1.5 (SZ)

Network morphology

- **Whether the lengths of A blocks must be narrowly distributed?**

PDI_A=1.00, PDI_B=1.50 (SZ)



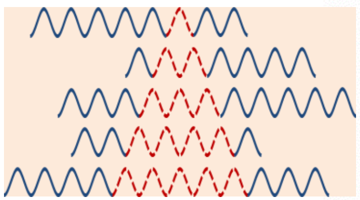


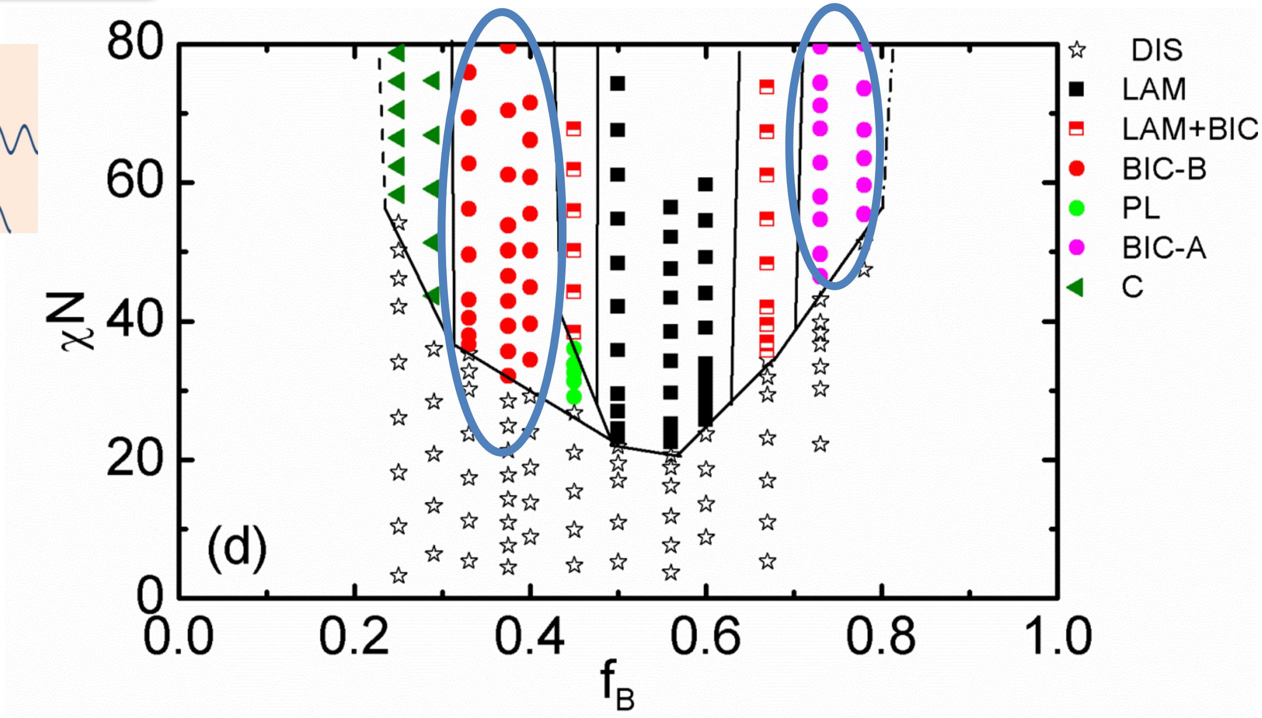
irregular bicontinuous phase (BIC) ~ 10%

Network morphology

➢ **Whether the lengths of A blocks must be narrowly distributed?**

PDI$_A$ = 1.50 (SZ), PDI$_B$ = 1.50 (SZ)

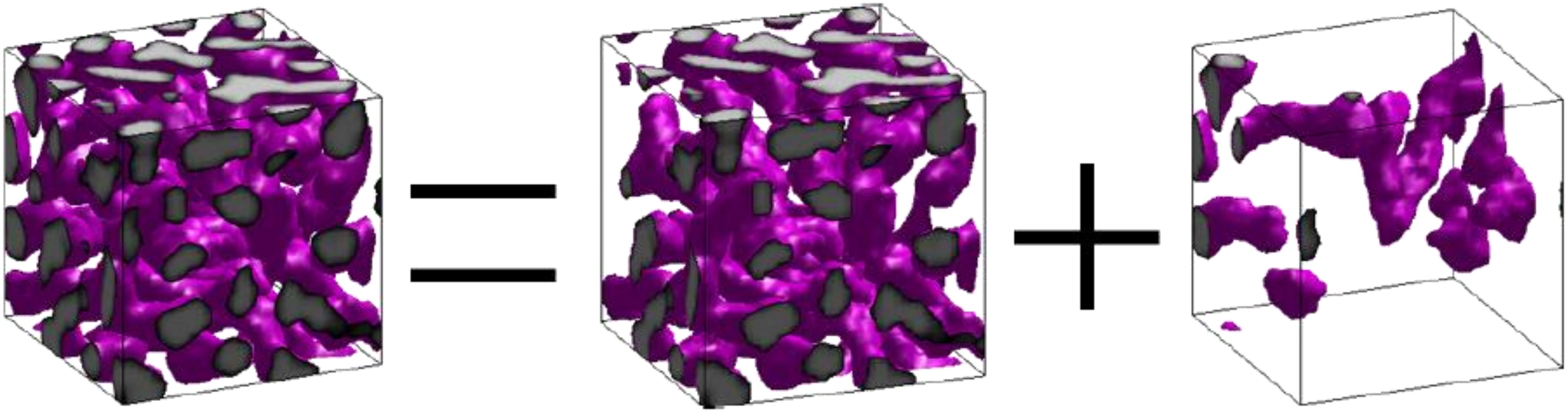




irregular bicontinuous phase (BIC) ~ 20%

Network morphology

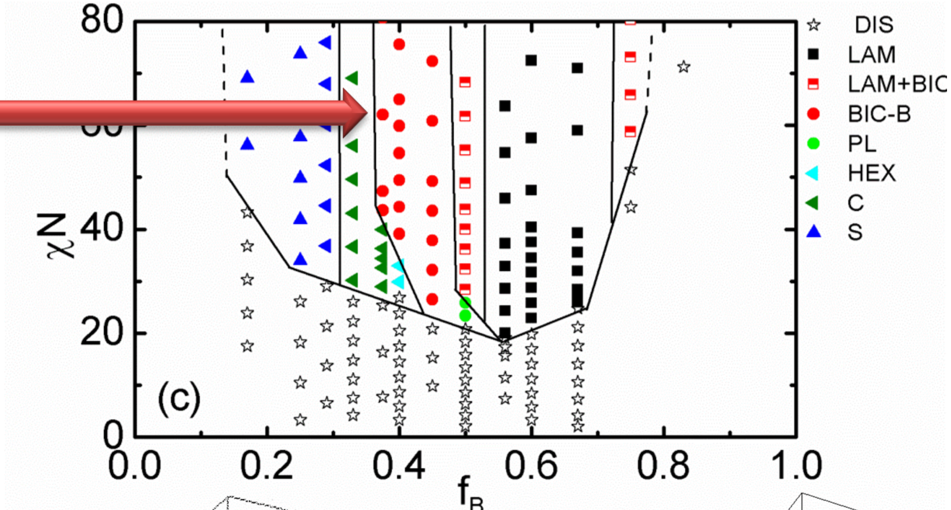
- Whether both domains are fully continuous across the entire composition range for which the irregular bicontinuous structure forms?

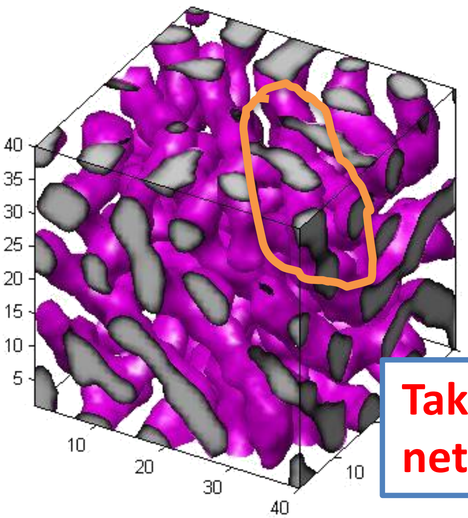


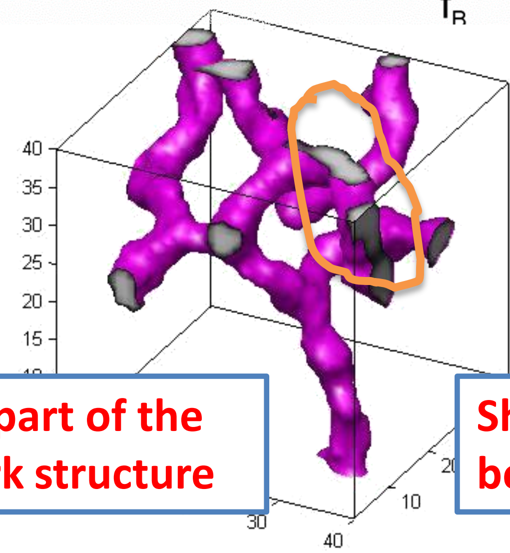
The BIC structures have good continuity.

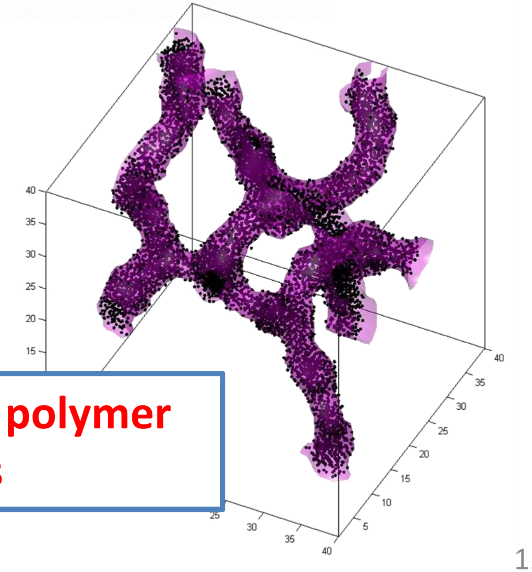
Network morphology

The system of ABA (PDI_A=1.00, PDI_B=1.50): f_B=0.375, χN=62.04





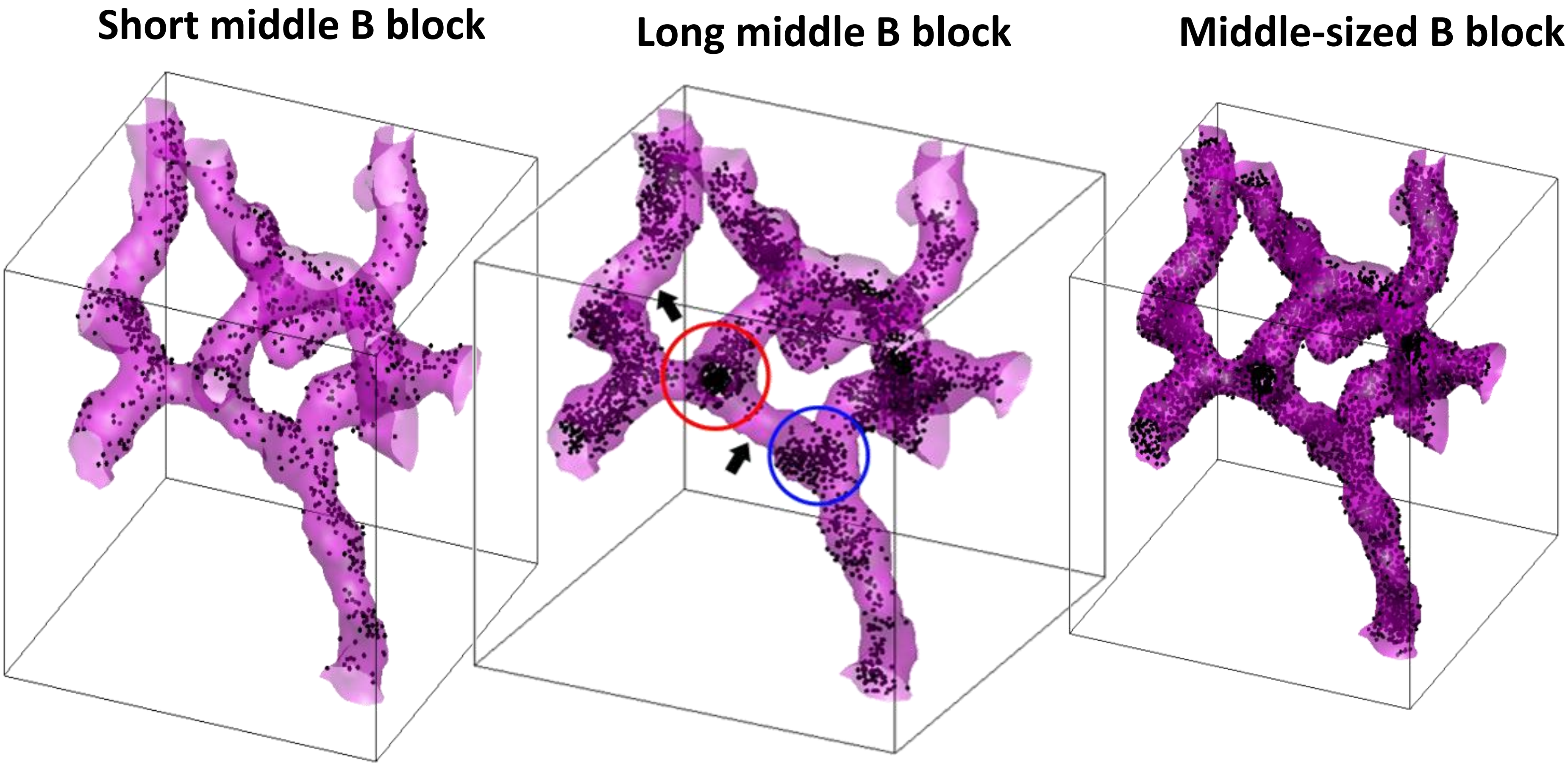




Take a part of the network structure

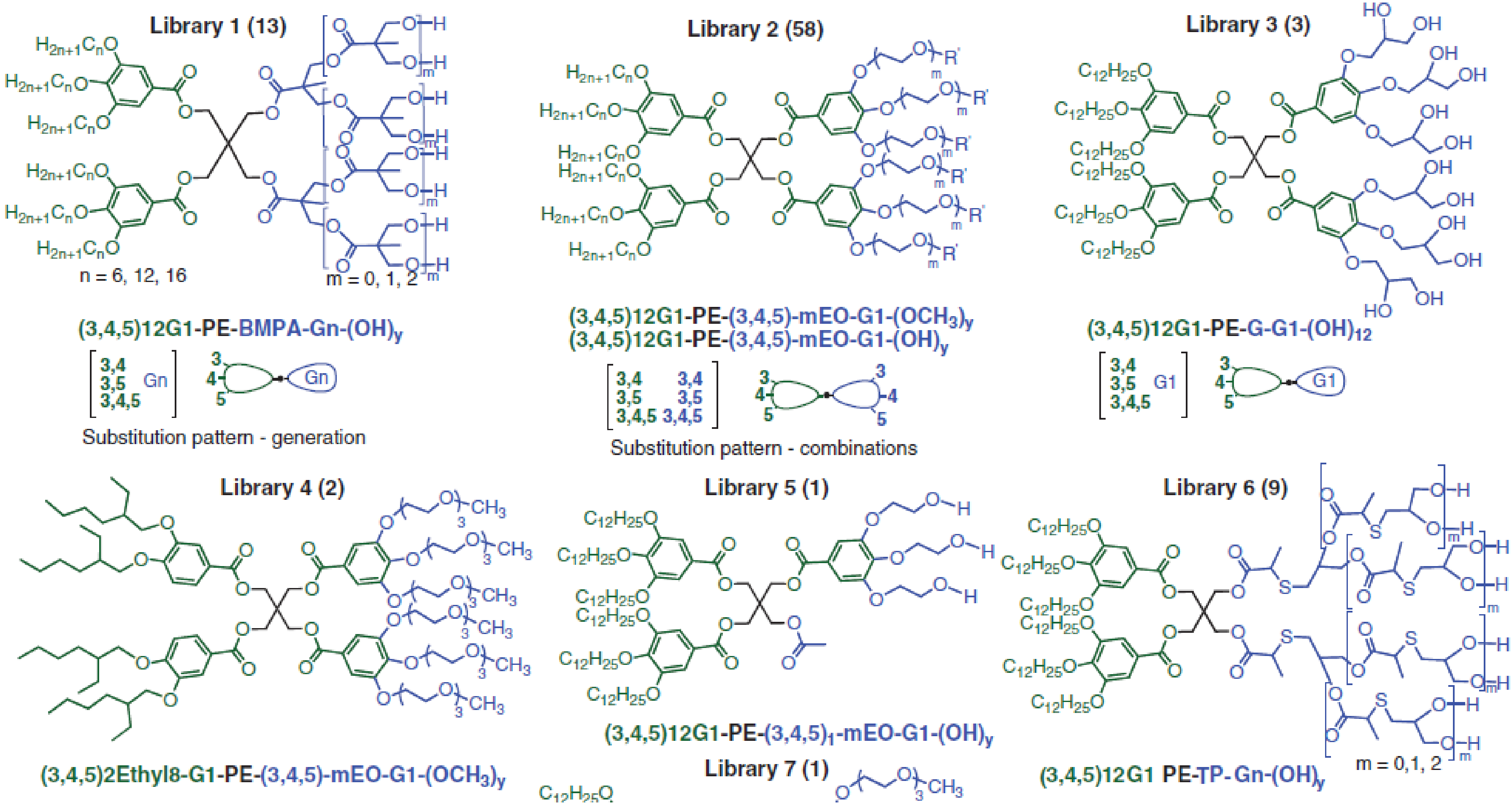
Show polymer beads

Network morphology



Selective distribution of blocks with different chain lengths can stabilize the BIC phase.

Soft Janus particle model

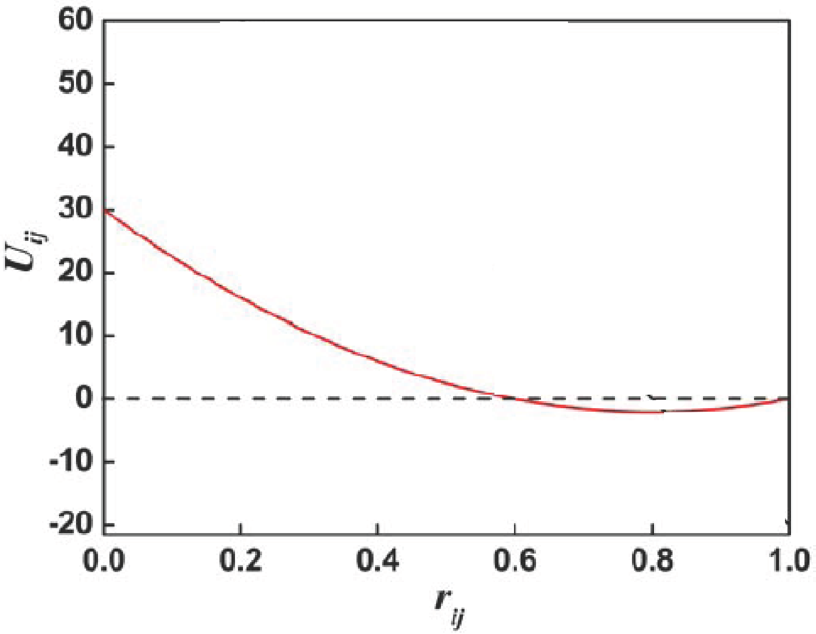


Percec et al. Science, 328, 1009, 2010.

Soft colloidal particle model

We need to describe patchy particles with a simple model. We have proposed a potential to represent the interactions between two colloidal particles:

$$U_{ij} = \frac{\alpha_{ij}^{R}}{2}\left(1 - r_{ij}/r_c\right)^2 - \frac{\alpha_{ij}^{A}}{2}\left(r_{ij}/r_c - \left(r_{ij}/r_c\right)^2\right)$$



$$k_B T = 1.0$$
$$r_c = 1.0$$

as the units.

Soft colloidal particle model

$$U_{ij} = \frac{\alpha_{ij}^R}{2}(1 - r_{ij}/r_c)^2 - \frac{\alpha_{ij}^A}{2}\left(r_{ij}/r_c - (r_{ij}/r_c)^2\right)$$

$$\alpha_{ij}^R = EV/k_B T$$

E: elastic modulus

$$F_{ij} = -\frac{\partial U}{\partial r} = 0$$

$$\Rightarrow d = \frac{\alpha_{ij}^R + \alpha_{ij}^A/2}{\alpha_{ij}^R + \alpha_{ij}^A}$$

d: diameter of colloidal particle

Define $(1+\delta)d = r_c$

δd*:* the range of attraction

Substitute r_{ij} by d in U_{ij}, we have

$$G = \alpha_{ij}^A(1-d)/4$$

G: potential well depth

Soft colloidal particle model

$$U_{ij} = \frac{\alpha_{ij}^R}{2}(1 - r_{ij}/r_c)^2 - \frac{\alpha_{ij}^A}{2}\left(r_{ij}/r_c - (r_{ij}/r_c)^2\right)$$

If we know the modulus of colloid particle (***E***), the size of the colloid particle (***d***), the attraction range (***δd***), and the attraction strength (***G***), we can exclusively define the parameters in our model.

Suppose:

nanoparticle diameter d = 20 nm

Elastic modulus E = 8.3×10^{7} Pa

Attraction range δd = 0.4 nm

Attraction well depth G = 2 $k_B T$

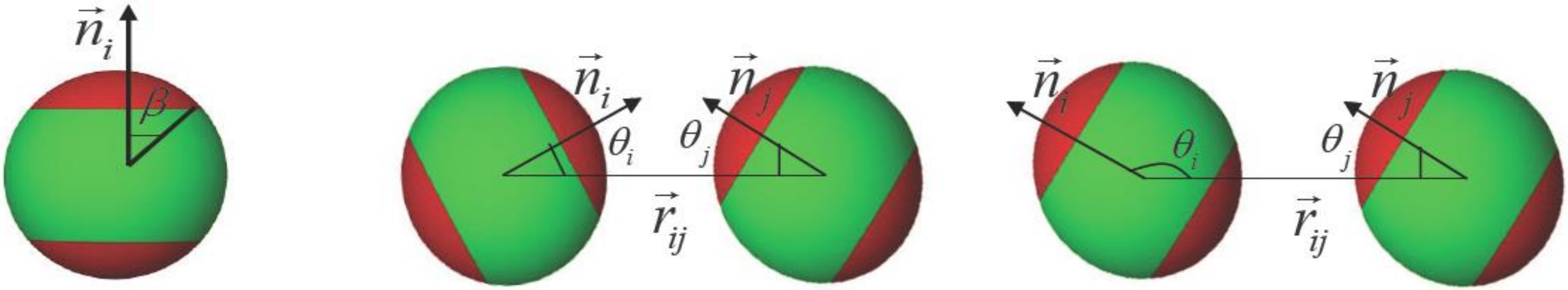
$$\alpha_{ij}^R \approx 10000$$
$$\alpha_{ij}^A \approx 400$$
$$r_c = 1.0(\approx 20.5nm)$$

Describe the patch size

$$U_{ij} = \frac{\alpha_{ij}^R}{2}(1 - r_{ij}/r_c)^2 - f^\nu \frac{\alpha_{ij}^A}{2}\left(r_{ij}/r_c - (r_{ij}/r_c)^2\right)$$

$f = \cos\theta_i' \cos\theta_j'$ for $|\cos\theta_i| \geq \cos\beta$ and $|\cos\theta_j| \geq \cos\beta$

$\theta_i' = \arccos(|\cos\theta_i|)$ $\theta_j' = \arccos(|\cos\theta_j|)$

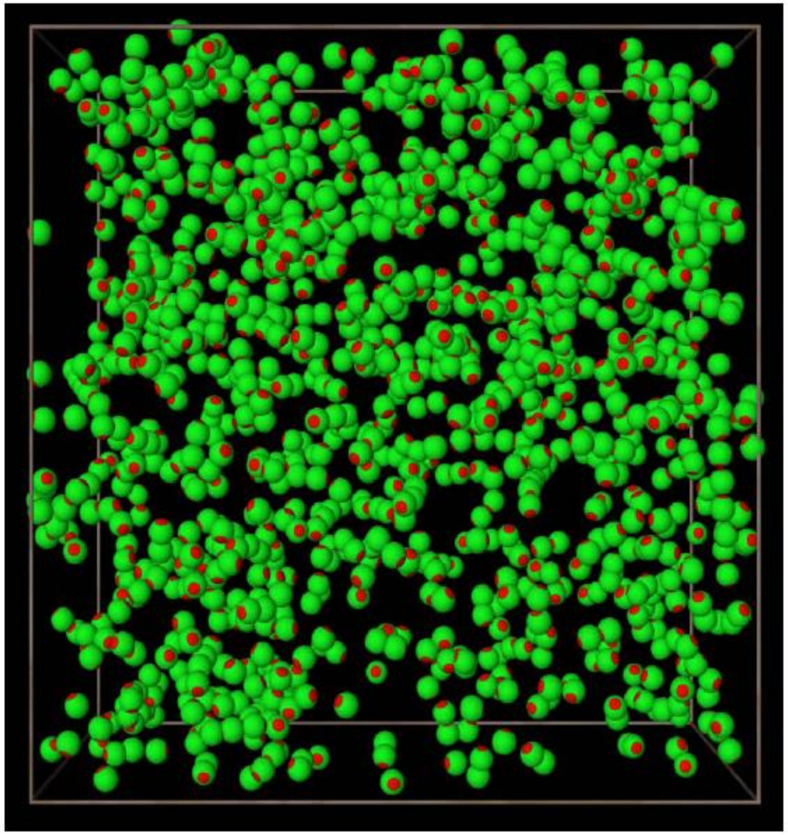


$\beta \in [0, \pi/2]$

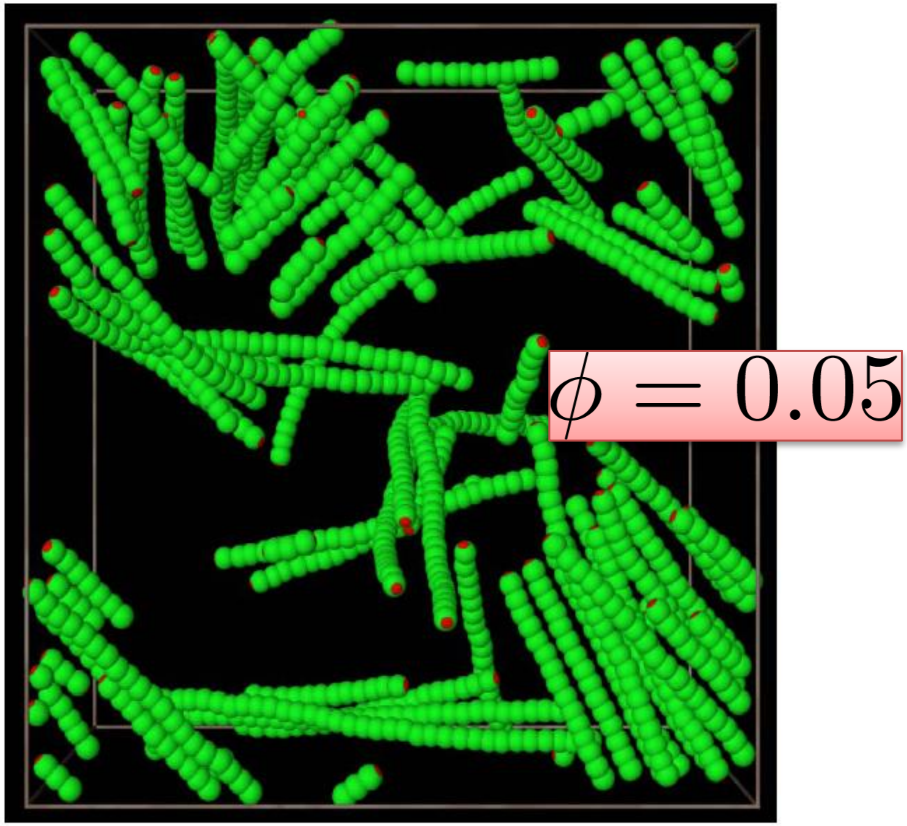
The patch parts are hydrophobic.

Patchy particle self-assembly

We then focus on the soft two-patch particle with diameter *d* ~ 20 nm and modulus *E* ~ 4.1×10^6 Pa:

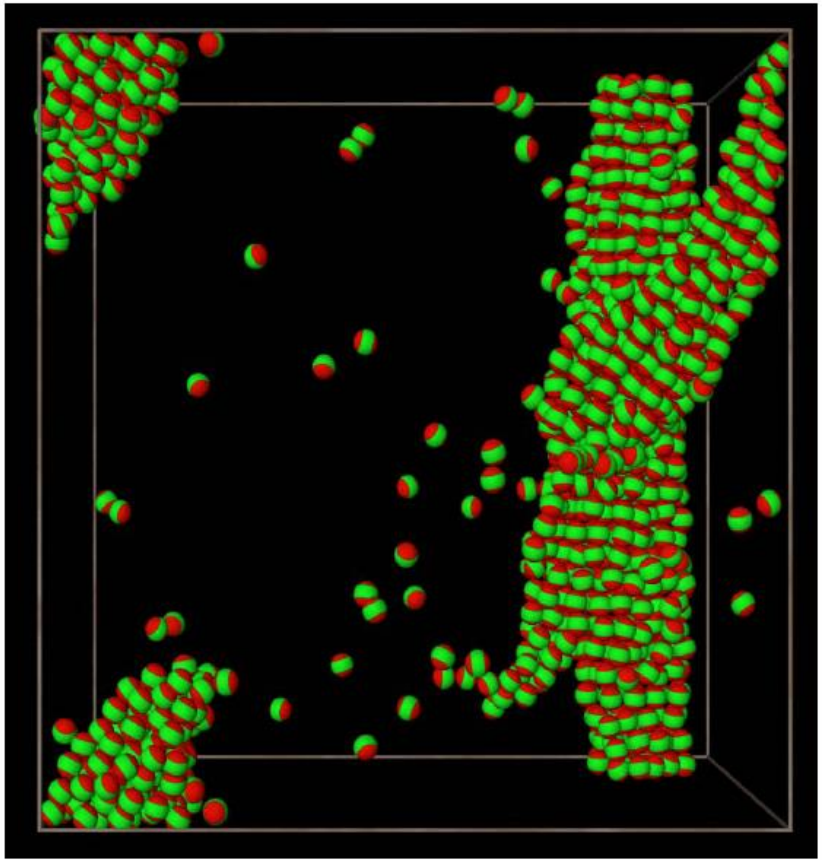


G=2.0 k_BT; β=30^o

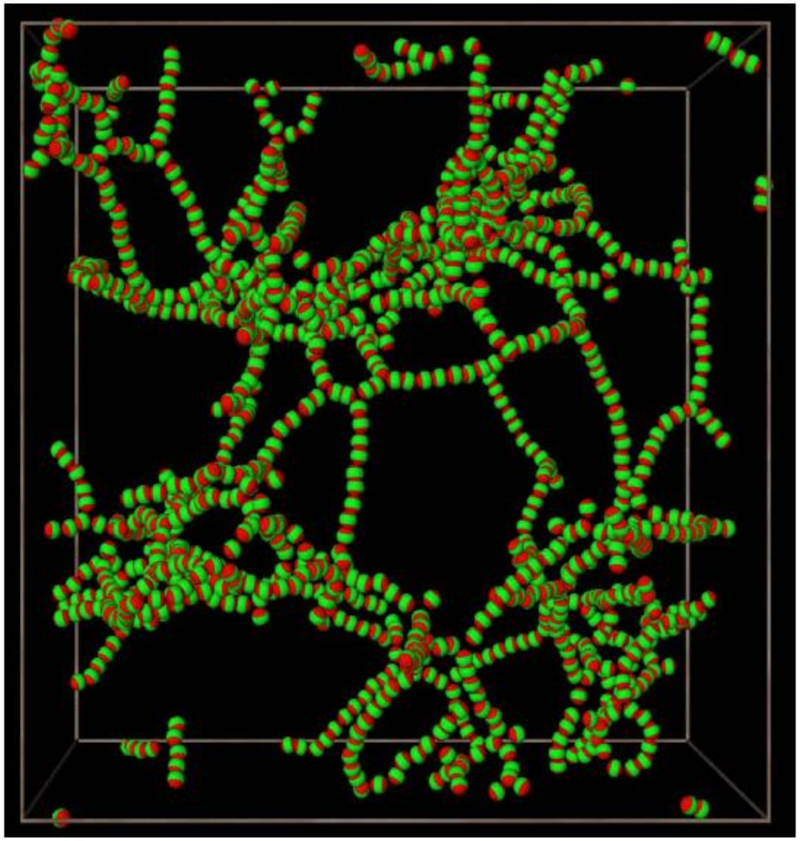


G=9.8 k_BT; β=30^o

Patchy particle self-assembly



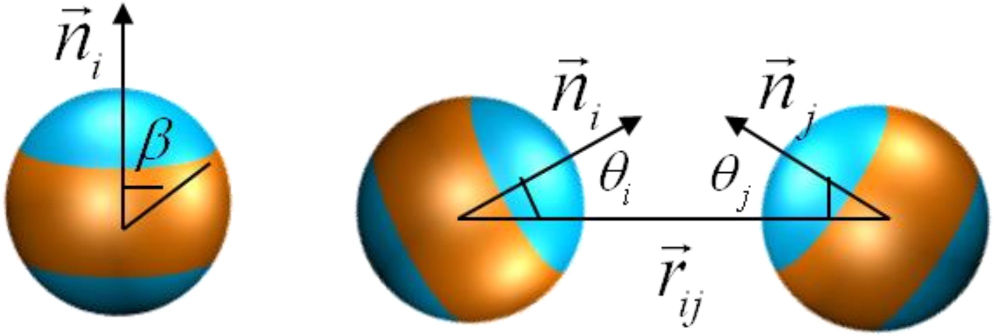
G=2.0 k_BT; β=60^o



G=9.8 k_BT; β=60^o

Describe patchy particle

$$U_{ij} = \frac{\alpha_{ij}^R}{2}(1 - r_{ij}/r_c)^2 - f^{\nu}\frac{\alpha_{ij}^A}{2}\left(r_{ij}/r_c - (r_{ij}/r_c)^2\right)$$



$$f = \begin{cases} \cos\frac{\pi}{2}\left(\frac{\pi/2-\theta_i'}{\pi/2-\beta}\right)\cos\frac{\pi}{2}\left(\frac{\pi/2-\theta_j'}{\pi/2-\beta}\right) & \text{if } |\cos\theta_i| \le \cos\beta \text{ and } |\cos\theta_j| \le \cos\beta \\ 0 & \text{otherwise.} \end{cases}$$

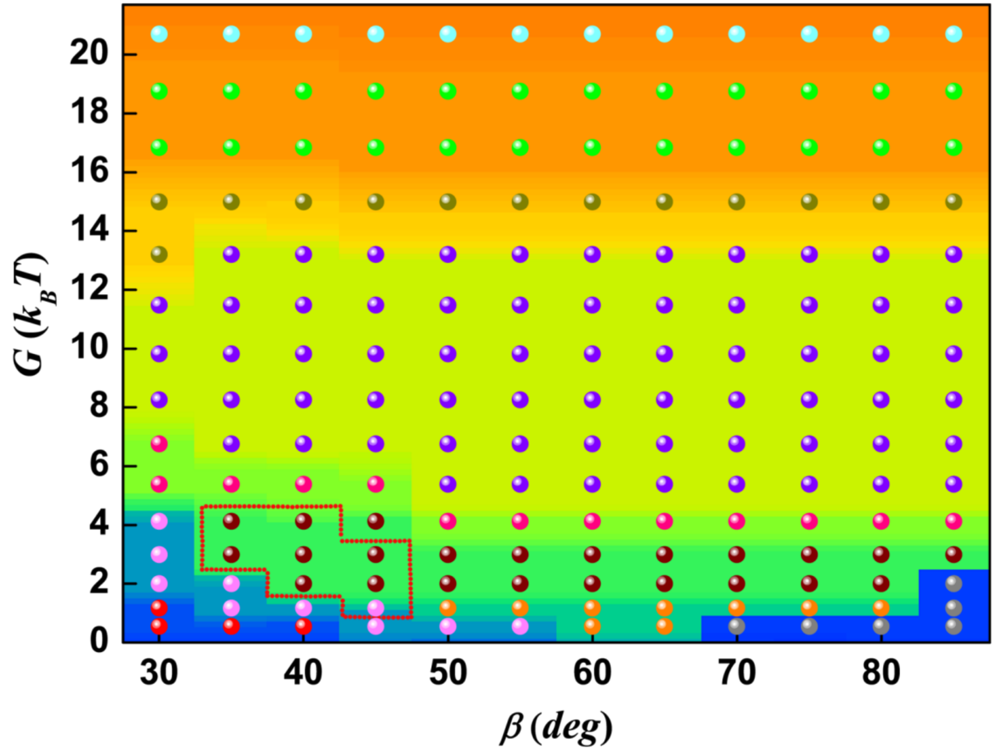
$$\theta_i' = \arccos(|\cos\theta_i|) \qquad \theta_j' = \arccos(|\cos\theta_j|)$$

$\beta \in [0, \pi/2]$

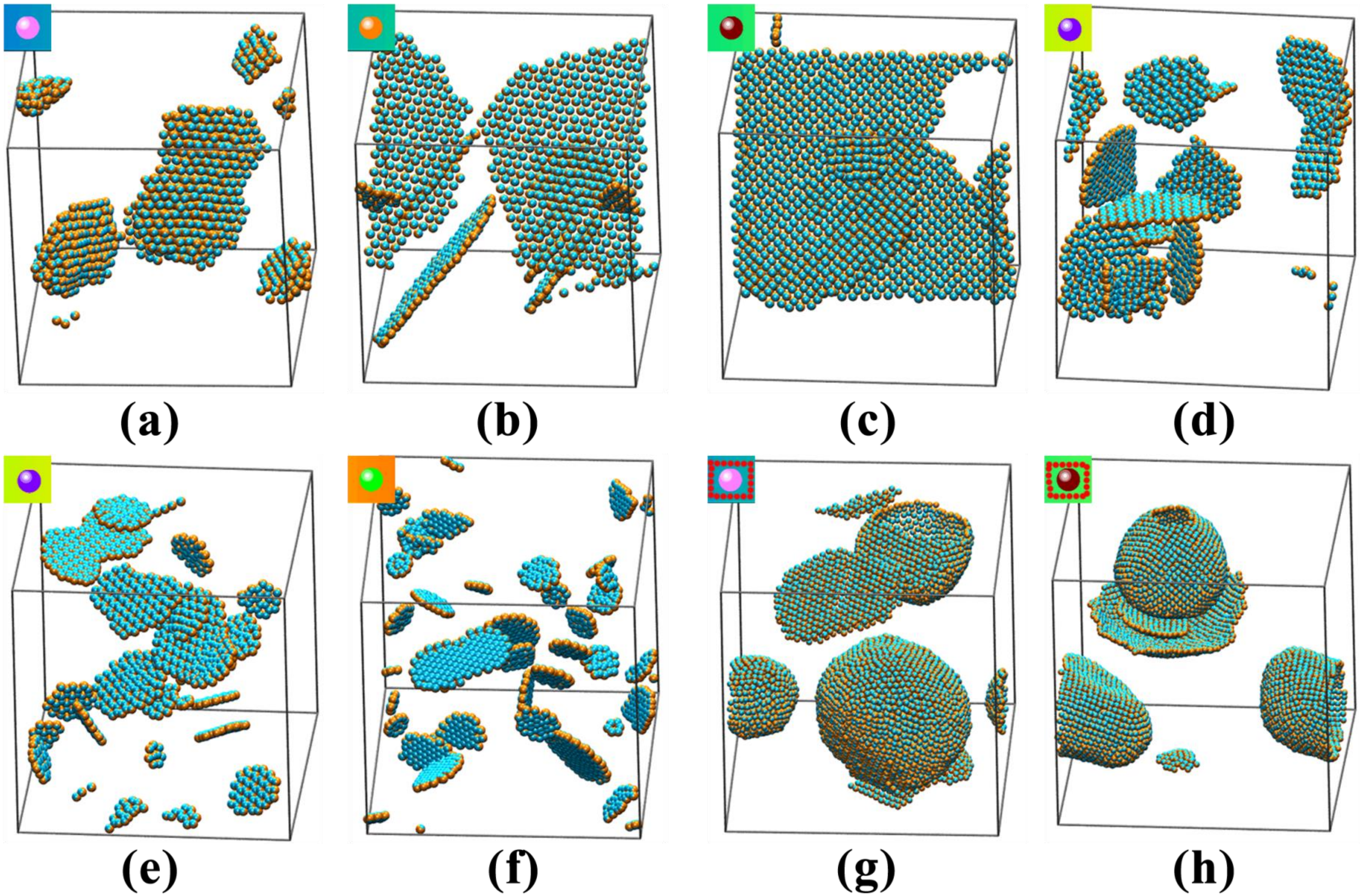
The middle part is hydrophobic.

Patchy particle self-assembly

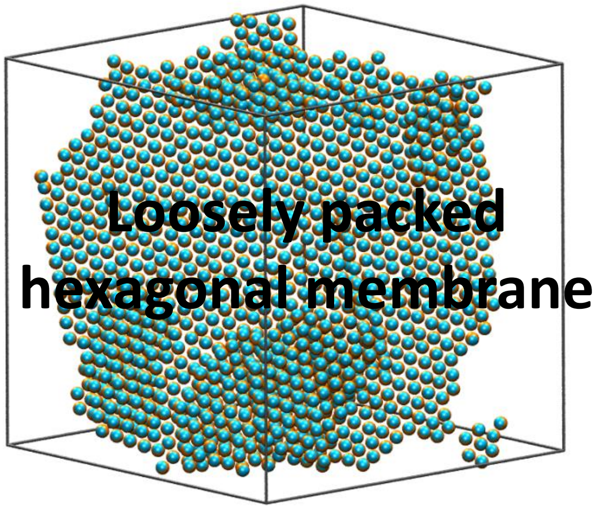
We then focus on the soft two-patch particle with diameter *d* ~ 20 nm and elastic modulus *E* ~ 4.1×10^6 Pa, and build up phase diagram by scanning the attraction well depth G and the surface coverage β. The volume fraction is $\phi = 0.05$ **.**

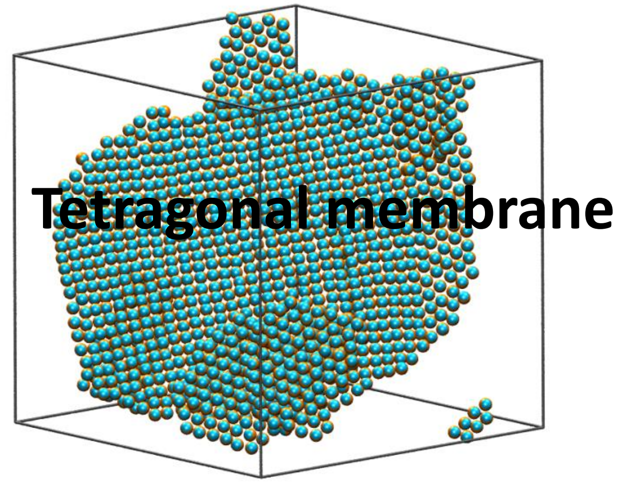


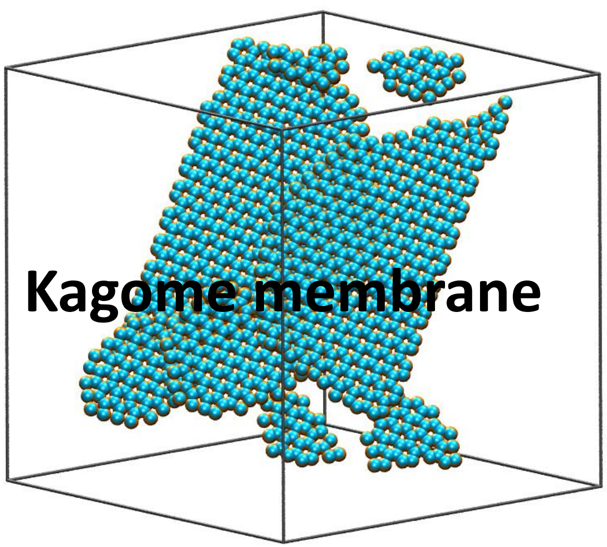
Patchy particle self-assembly

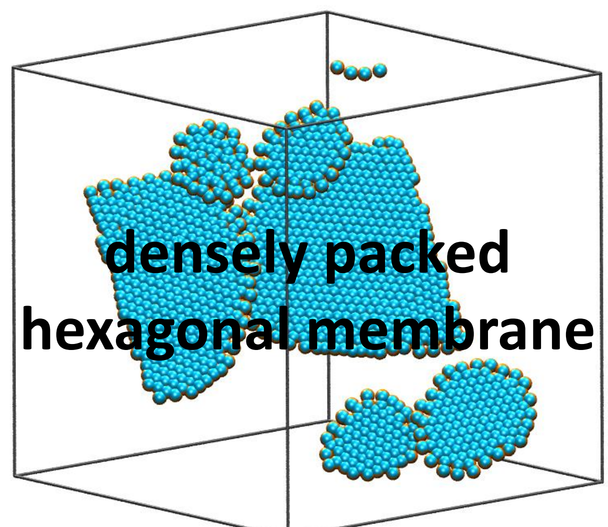


Patchy particle self-assembly

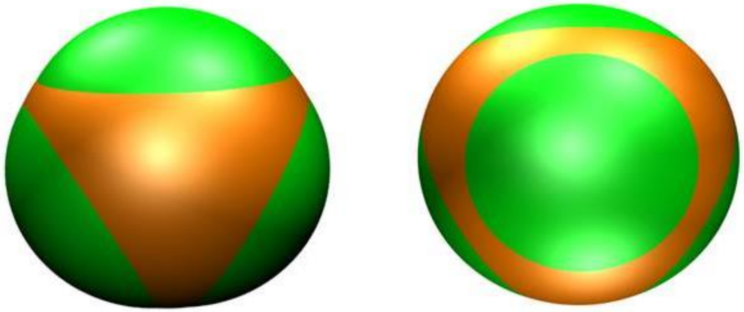








Multi-patch particle model



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$$U_{ij} = \begin{cases} \frac{\alpha_{ij}^R d_{ij}}{2}\left(1 - \frac{r_{ij}}{d_{ij}}\right)^2 - \sum_{\kappa=1}^{M_i}\sum_{\lambda=1}^{M_j} f^{\nu}\left(\mathbf{n}_i^{\kappa}, \mathbf{n}_j^{\lambda}, \mathbf{r}_{ij}\right)\frac{\alpha_{ij}^A d_{ij}}{2}\left[\frac{r_{ij}}{d_{ij}} - \left(\frac{r_{ij}}{d_{ij}}\right)^2\right] & r_{ij} \le d_{ij} \\ 0 & r_{ij} > d_{ij}, \end{cases} \quad (1)$$

$$f\left(\mathbf{n}_i^{\kappa}, \mathbf{n}_j^{\lambda}, \mathbf{r}_{ij}\right) = \begin{cases} \cos\frac{\pi\theta_i^{\kappa}}{2\theta_m^{\kappa}}\cos\frac{\pi\theta_j^{\lambda}}{2\theta_m^{\lambda}} & \text{if } \cos\theta_i^{\kappa} \ge \cos\theta_m^{\kappa} \text{ and } \cos\theta_j^{\lambda} \ge \theta_m^{\lambda} \\ 0 & \text{otherwise.} \end{cases} \quad (2)$$

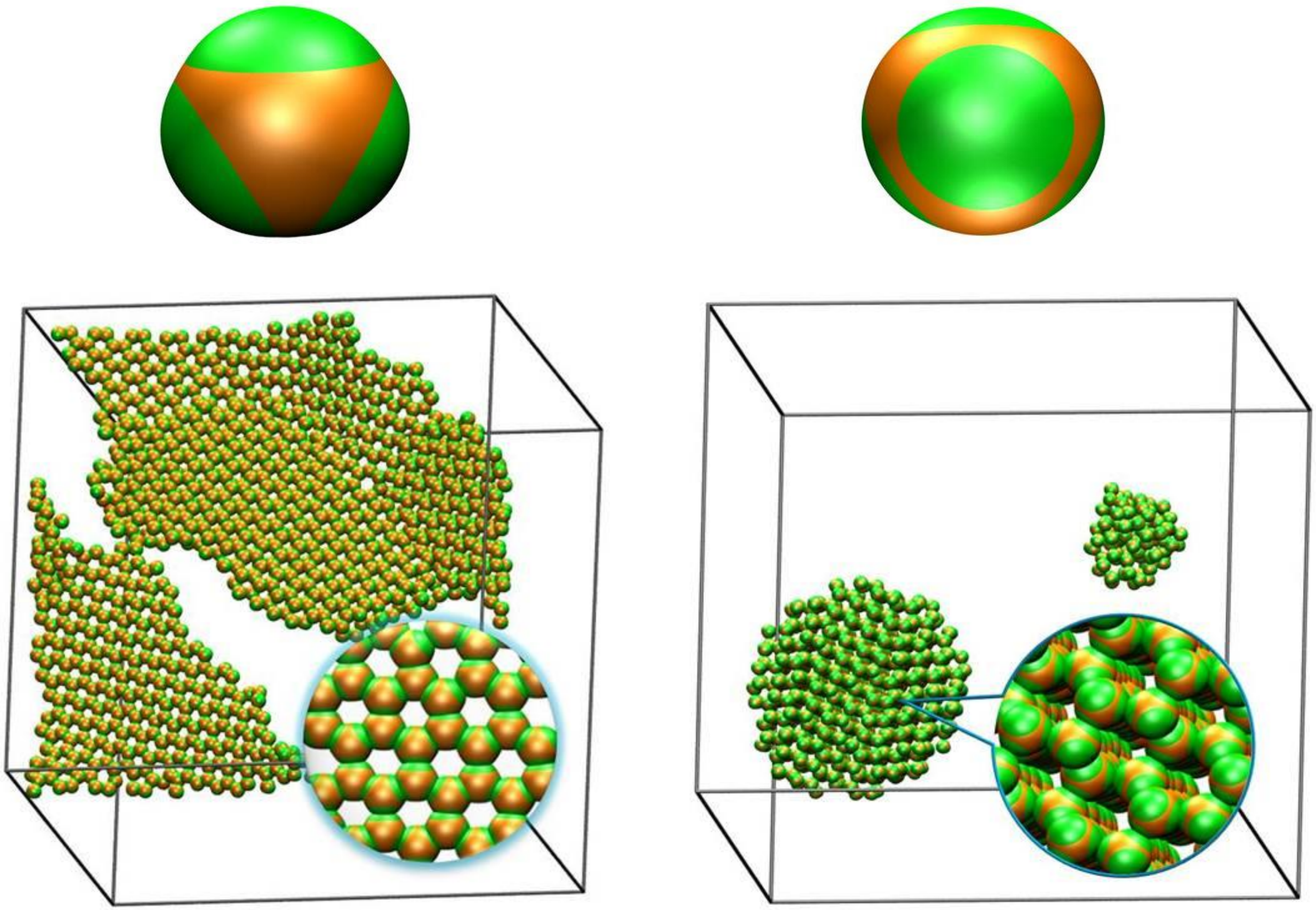
Multi-patch particle model

$$
\begin{aligned}
\mathbf{F}_{ij} &= -\frac{\partial U_{ij}}{\partial \mathbf{r}_{ij}} \\
&= \alpha_{ij}^{R}\left(1-\frac{r_{ij}}{d_{ij}}\right)\frac{\mathbf{r}_{ij}}{r_{ij}} + \sum_{\kappa=1}^{M_i}\sum_{\lambda=1}^{M_j}\left\{\alpha_{ij}^{A} f^{\nu}\left(\mathbf{n}_i^{\kappa},\mathbf{n}_j^{\lambda},\mathbf{r}_{ij}\right)\left(\frac{1}{2}-\frac{r_{ij}}{d_{ij}}\right)\frac{\mathbf{r}_{ij}}{r_{ij}} - \frac{\alpha_{ij}^{A}}{2}\left[\frac{r_{ij}}{d_{ij}}-\left(\frac{r_{ij}}{d_{ij}}\right)^{2}\right]\right. \\
&\quad \nu f^{\nu-1}\left(\mathbf{n}_i^{\kappa},\mathbf{n}_j^{\lambda},\mathbf{r}_{ij}\right)\left(\frac{\pi}{2\theta_m^{\kappa}}\sin\frac{\pi\theta_i^{\kappa}}{2\theta_m^{\kappa}}\frac{\partial\theta_i^{\kappa}}{\partial\cos\theta_i^{\kappa}}\frac{\partial\cos\theta_i^{\kappa}}{\partial\mathbf{r}_{ij}}\cos\frac{\pi\theta_j^{\lambda}}{2\theta_m^{\lambda}} + \frac{\pi}{2\theta_m^{\lambda}}\sin\frac{\pi\theta_j^{\lambda}}{2\theta_m^{\lambda}}\frac{\partial\theta_j^{\lambda}}{\partial\cos\theta_j^{\lambda}}\right. \\
&\quad \left.\left.\frac{\partial\cos\theta_j^{\lambda}}{\partial\mathbf{r}_{ij}}\cos\frac{\pi\theta_i^{\kappa}}{2\theta_m^{\kappa}}\right)\right\}, \qquad (13)
\end{aligned}
$$

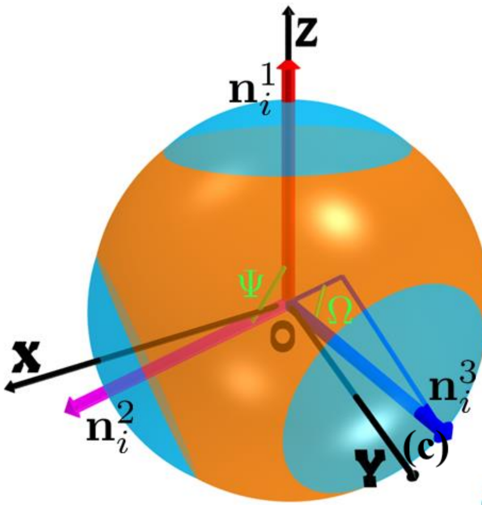
$$
\begin{aligned}
\boldsymbol{\tau}_{ij} &= \sum_{\kappa=1}^{M_i} -\frac{\partial U_{ij}}{\partial \mathbf{n}_i^{\kappa}} \\
&= \sum_{\kappa=1}^{M_i}\sum_{\lambda=1}^{M_j}\frac{\pi\alpha_{ij}^{A} d_{ij}}{4\theta_m^{\kappa}}\left[\frac{r_{ij}}{d_{ij}}-\left(\frac{r_{ij}}{d_{ij}}\right)^{2}\right]\nu f^{\nu-1}\left(\mathbf{n}_i^{\kappa},\mathbf{n}_j^{\lambda},\mathbf{r}_{ij}\right)\sin\frac{\pi\theta_i^{\kappa}}{2\theta_m^{\kappa}}\frac{\partial\theta_i^{\kappa}}{\partial\cos\theta_i^{\kappa}}\cos\frac{\pi\theta_j^{\lambda}}{2\theta_m^{\lambda}}\frac{\mathbf{r}_i}{r_{ij}}. \qquad (18)
\end{aligned}
$$

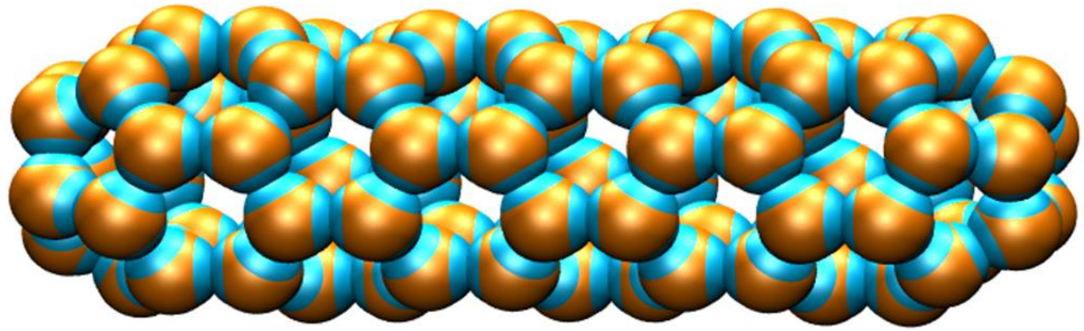
We use quaternion method to integrate equations of motion.

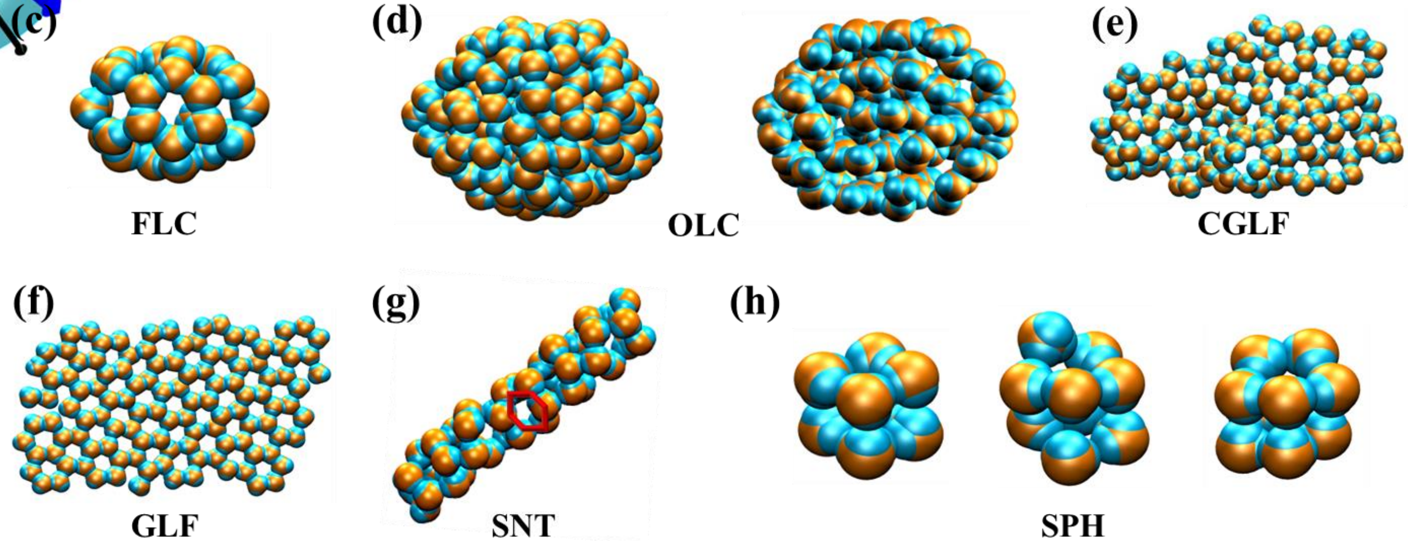
Multi-patch particle model



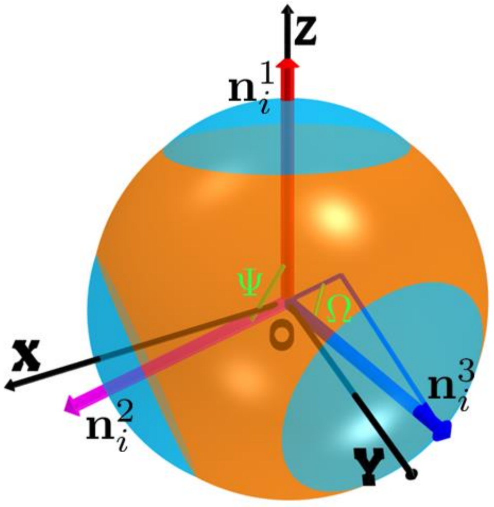
Multi-patch particle model

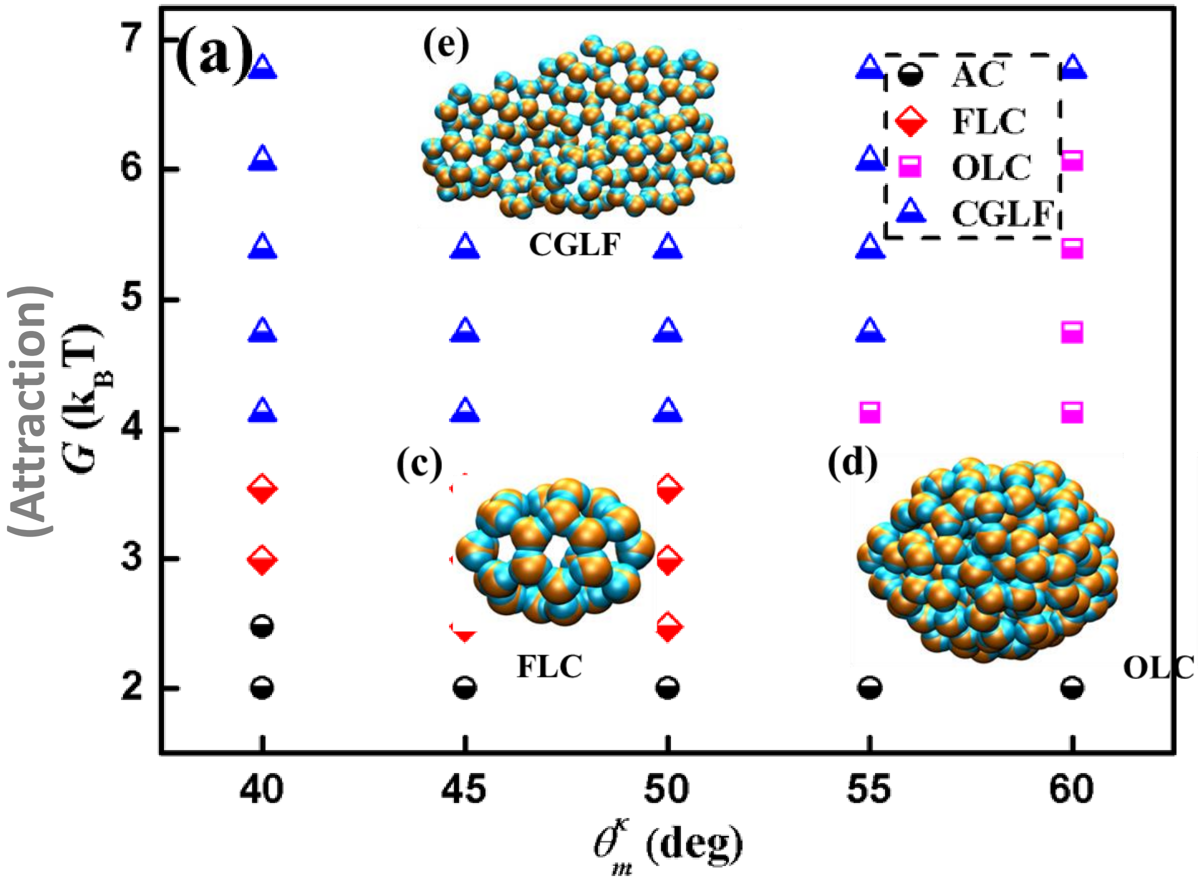






Multi-patch particle model

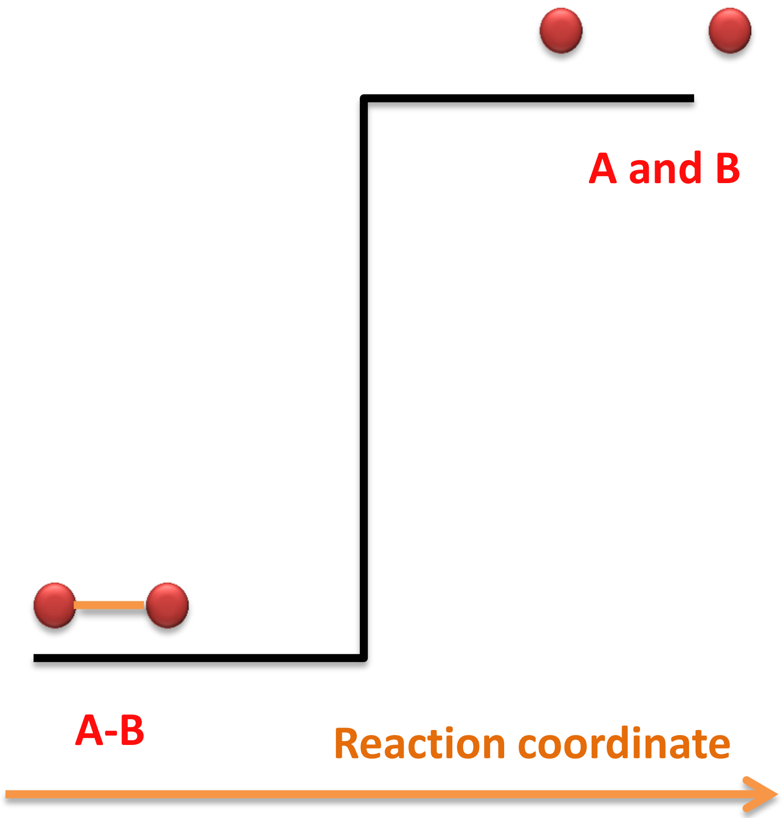




(Patch size)

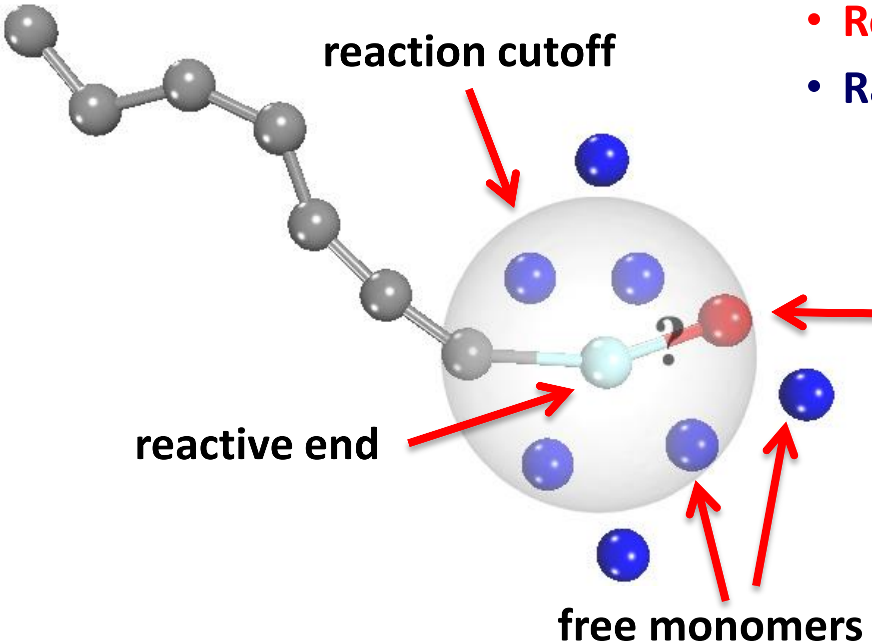
Combining 2 scales in 1 simulation

Reaction models in CG Simulations



Stochastic-reaction-in-a-cutoff method.
Can be used to generate polymerization products.

Stochastic reaction in a cutoff

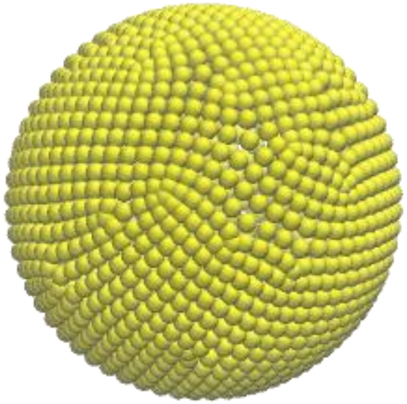


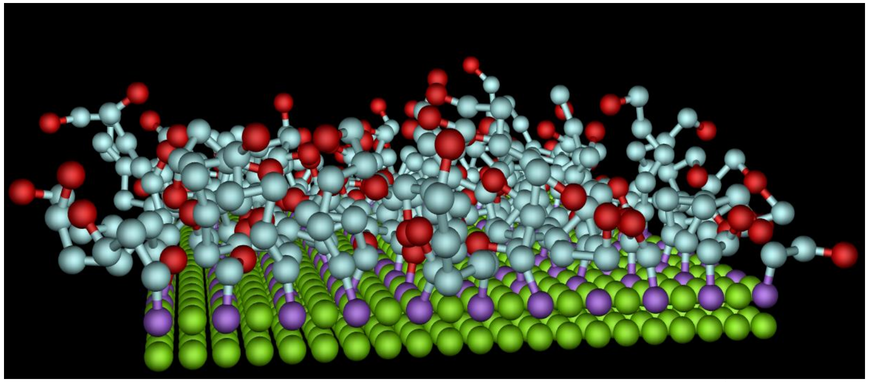
- Reaction probability P_r : predefined, $0 \le P_r \le 1$.
- Random generator (uniform random number P).

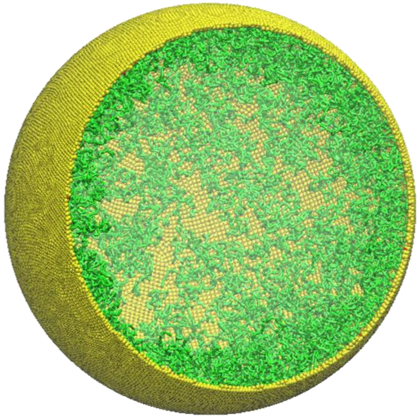
If $P \le P_r$, connect;
Else if $P > P_r$, do not connect.

Advantages:
- Simple
- Ready to be implemented in generic/CG models

Stochastic reaction in a cutoff







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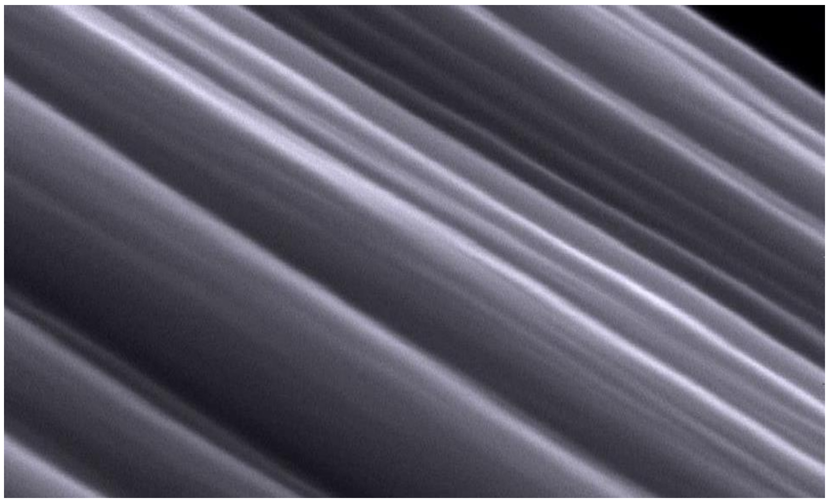
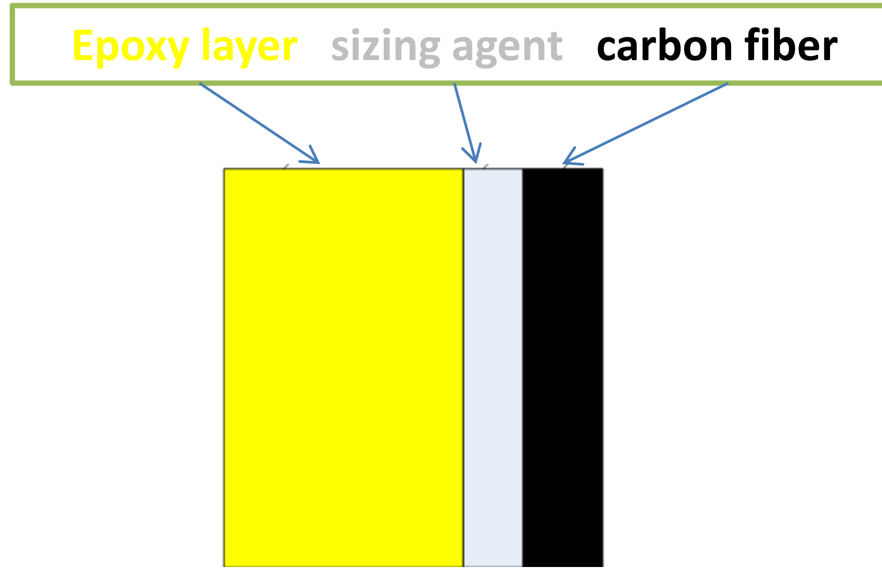
Epoxy layer structure on carbon fiber

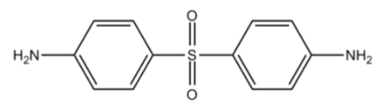




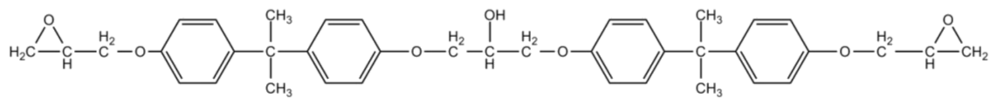
- Carbon fiber has to be protected by epoxy, otherwise too brittle to use.
- Sizing agent is important to increase the affinity between epoxy layer and carbon fiber.
- In experiments, it's difficult to characterize structures and mechanical properties of this complex.

Chemicals in epoxy and sizing agent

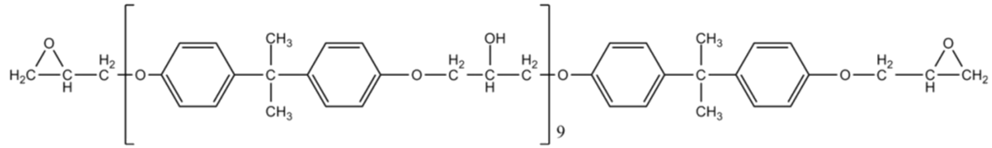
DDS:



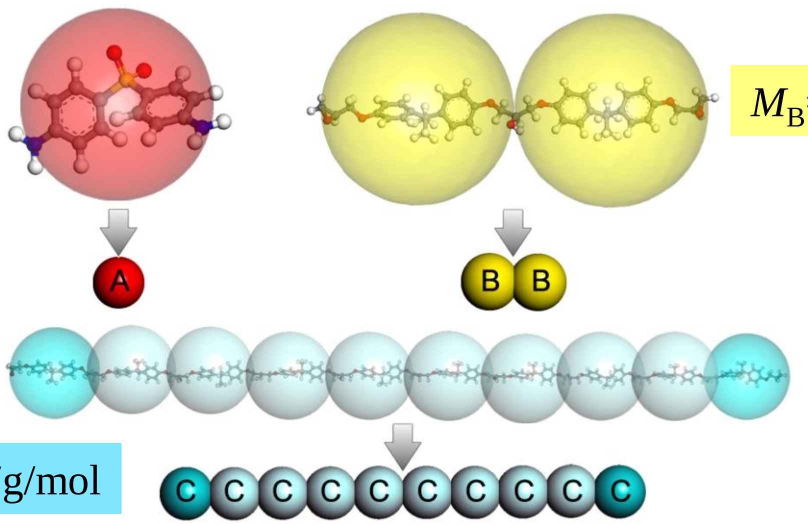
DGEBA (RA):



Sizing agent (SA):



M_A=248.30g/mol



M_B=312.40g/mol

M_C=289.97g/mol

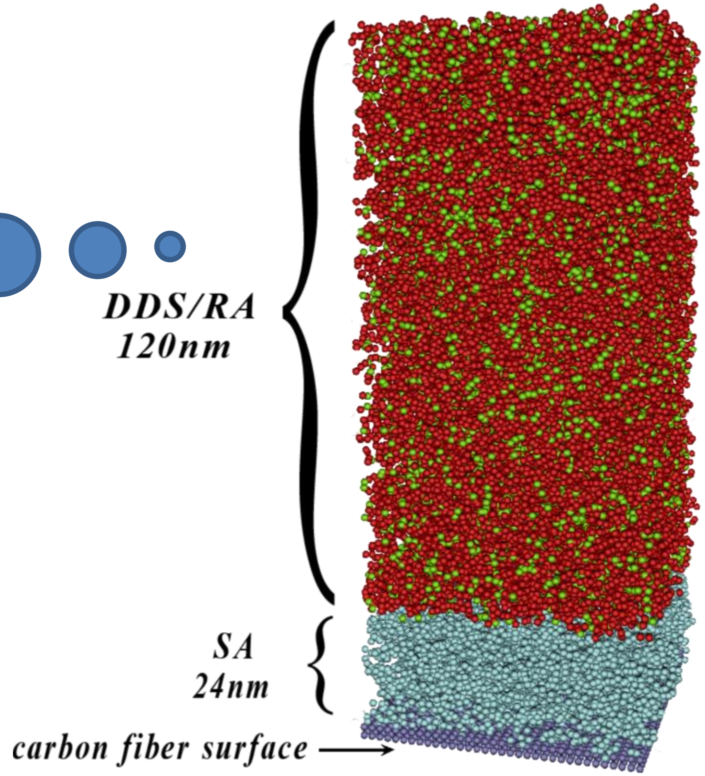
$\overline{M} = \sum_{i=A\sim C}(\phi_i M_i)$ =266.28g/mol

$\bar{v} = 409.42\text{A}^3$

Length scale: L=1.07nm

Carbon fiber-epoxy complex

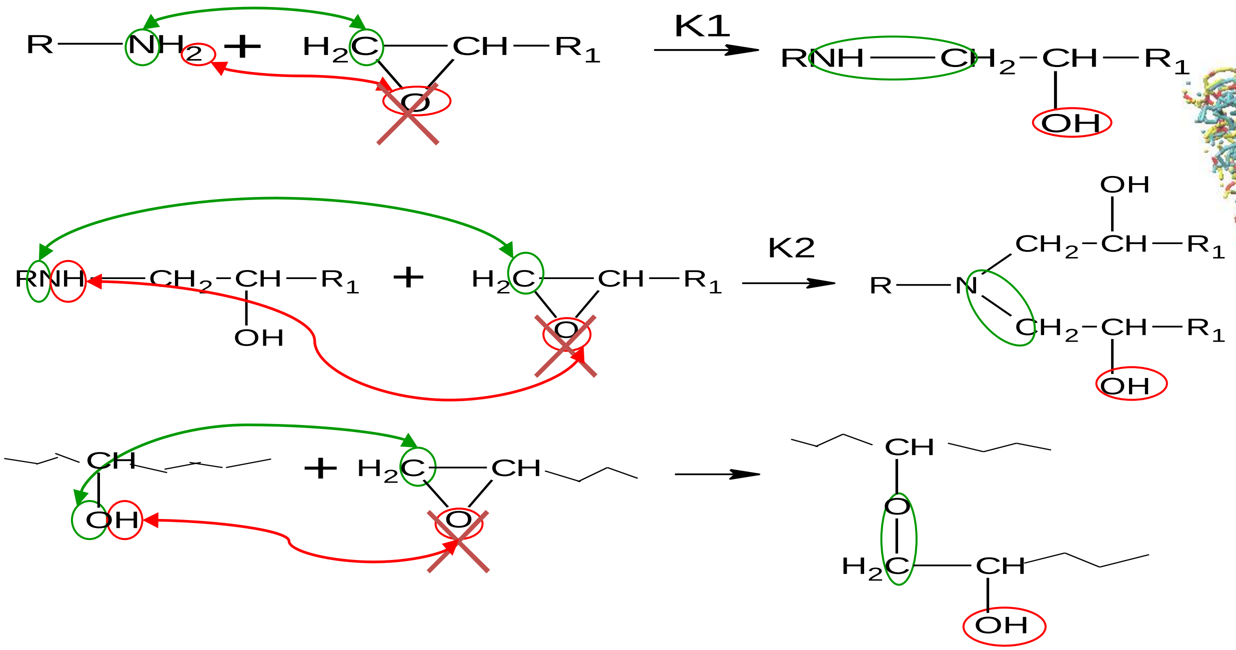
The coarse grained model represents a system with more than 10,000,000 atoms

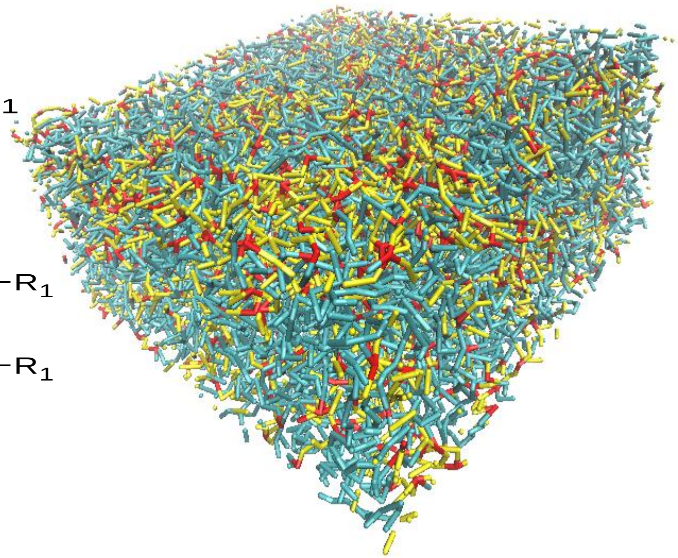


We use DPD to study the influence of reaction on the distribution of different chemicals. The interaction parameters between them are obtained from their χ parameters.

Reaction kinetics

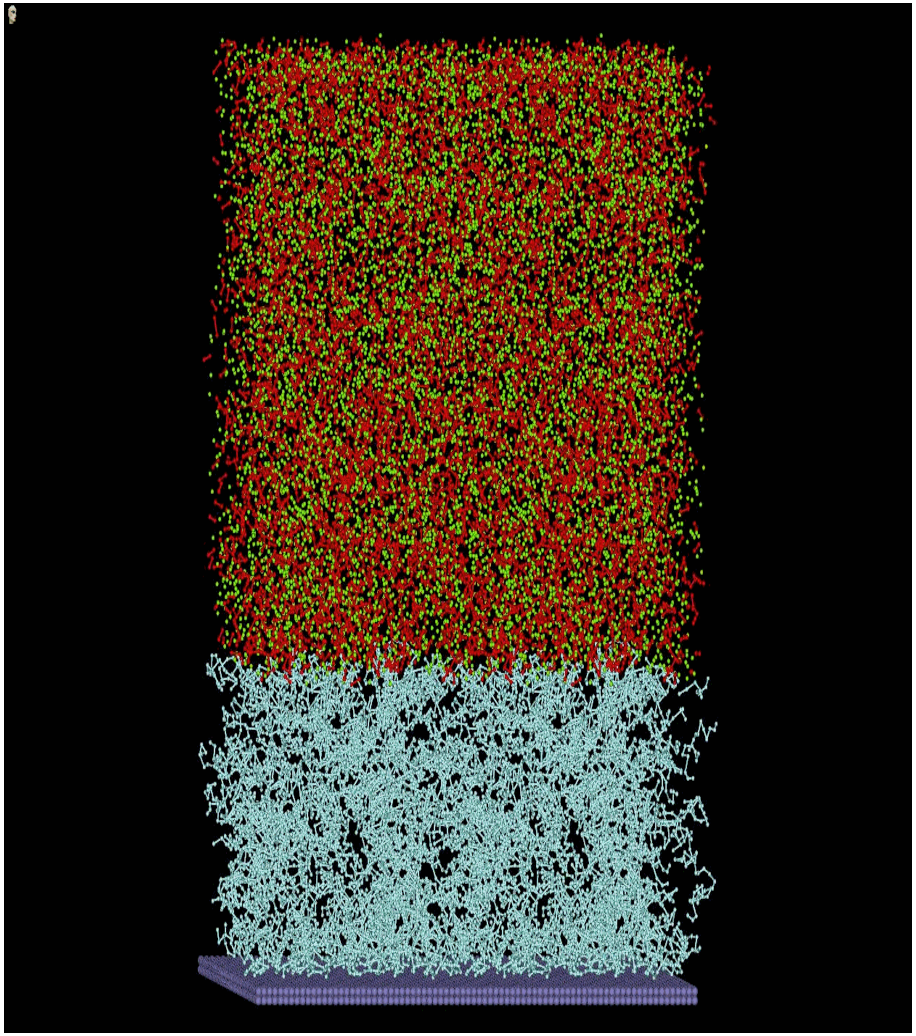
Reaction kinetics:

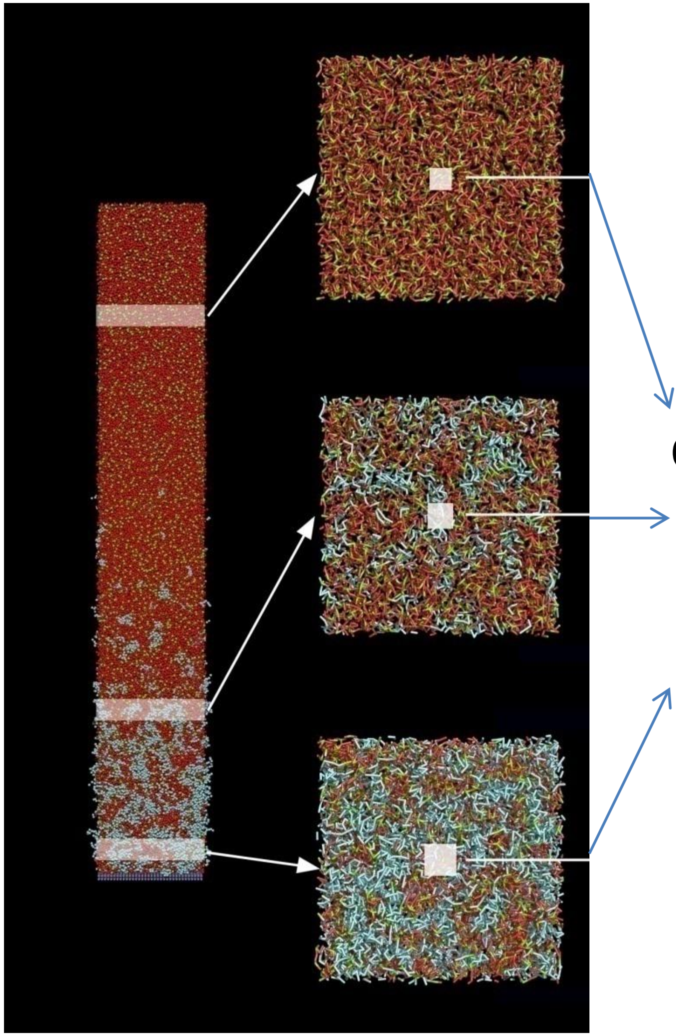




Typical network structure formed in curing process

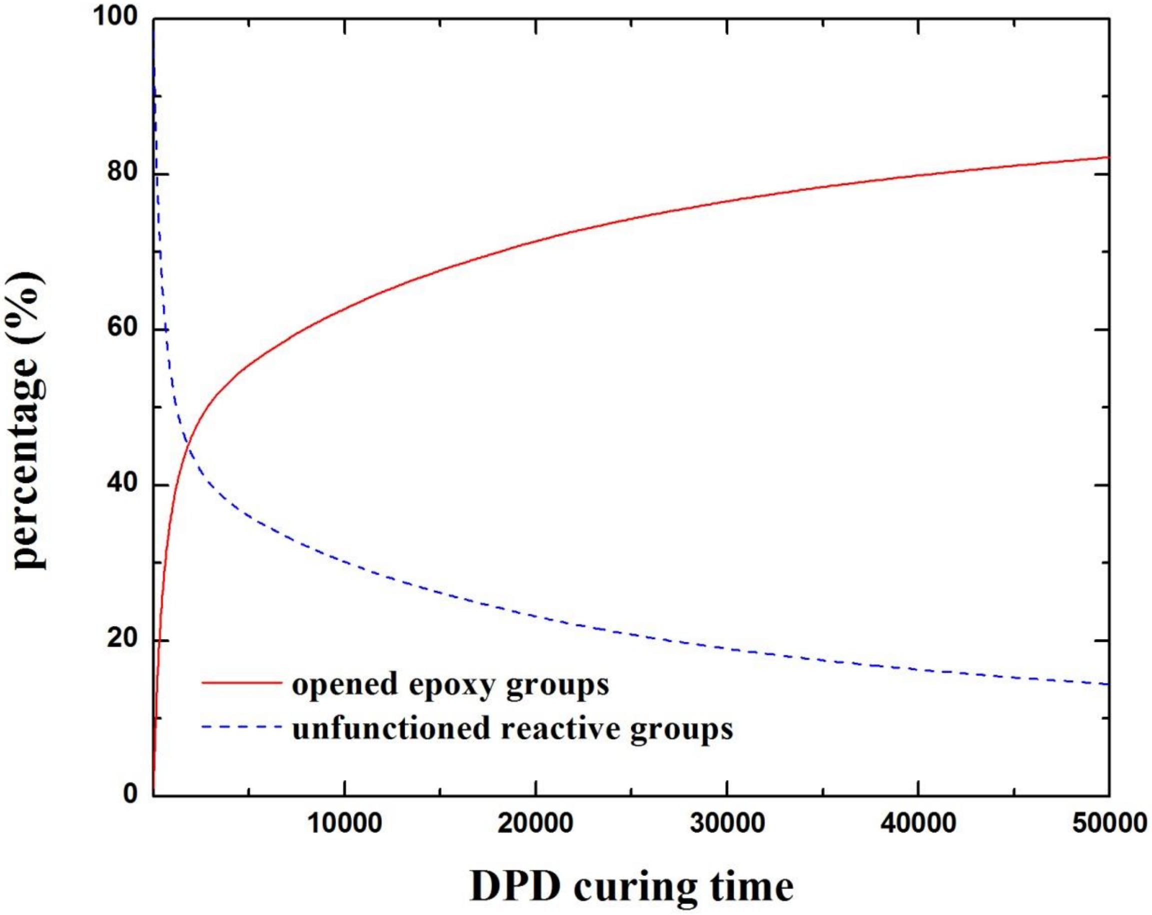
Reaction+diffusion





Composition of different chemicals in these layers

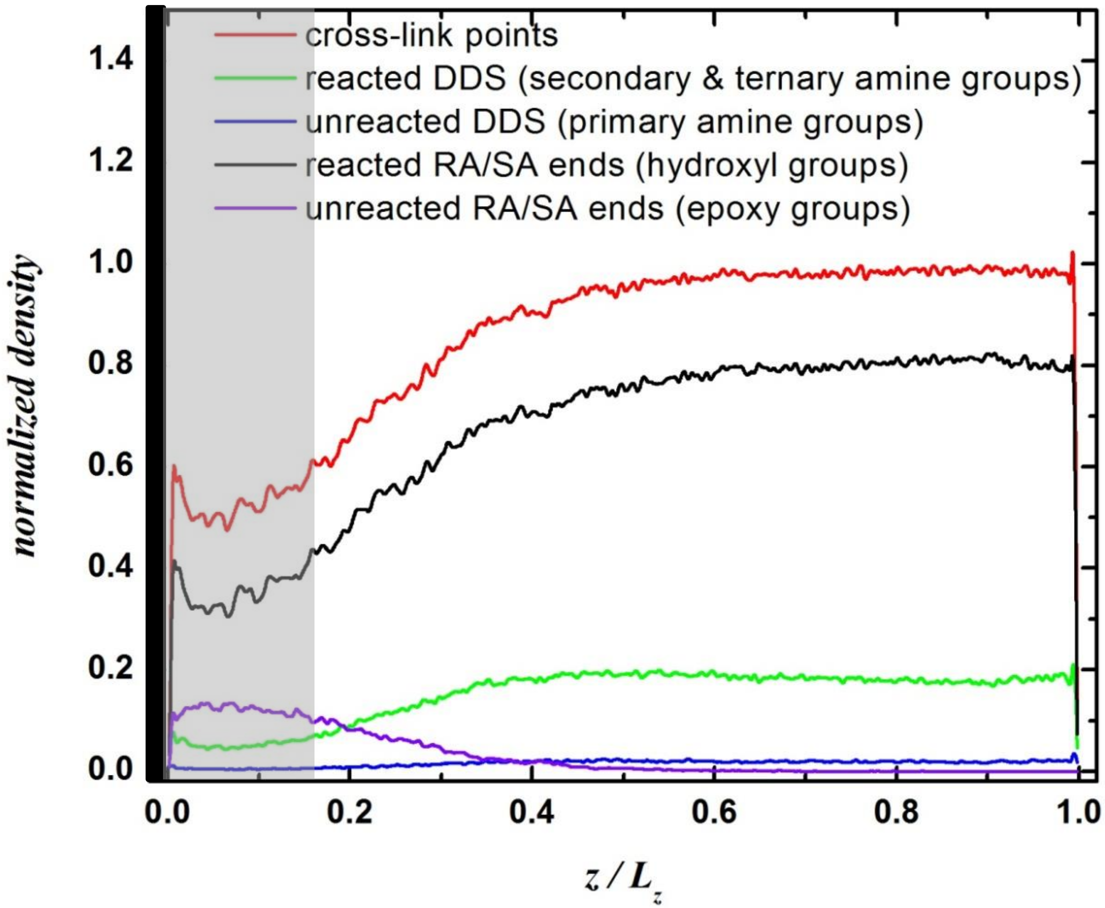
Time evolution of epoxy groups



Curing process slows down with time, because the number of functional groups deceases largely with time and "big" molecules are difficult to move.

Chemical distribution

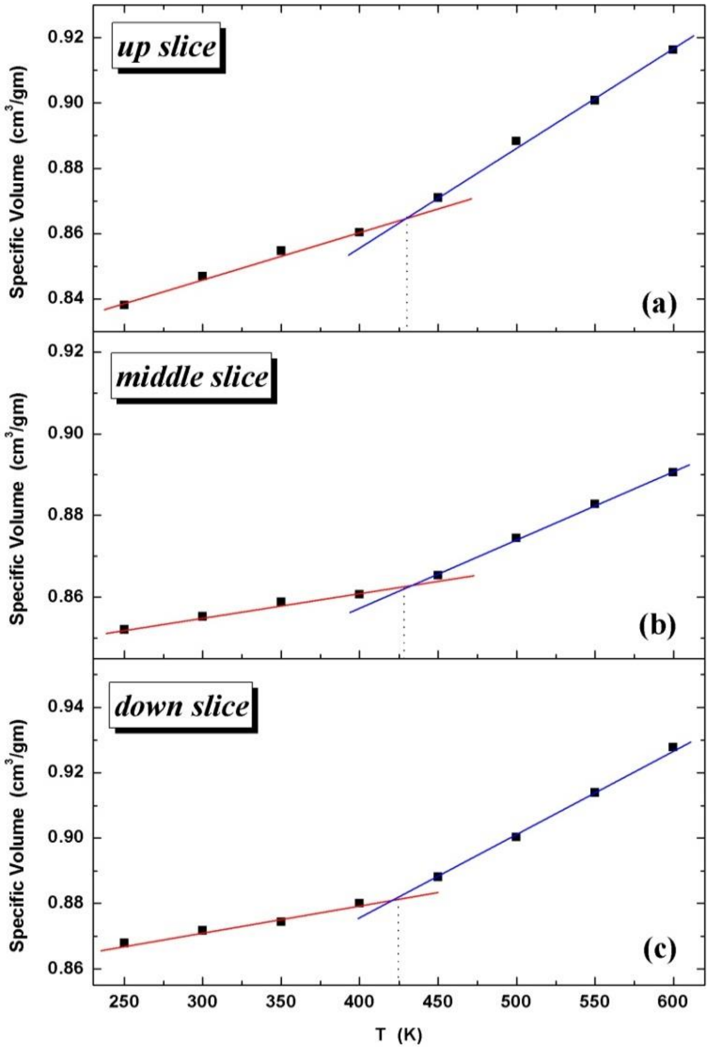
Chemical distribution along the normal direction of carbon fiber surface.



Mechanical properties

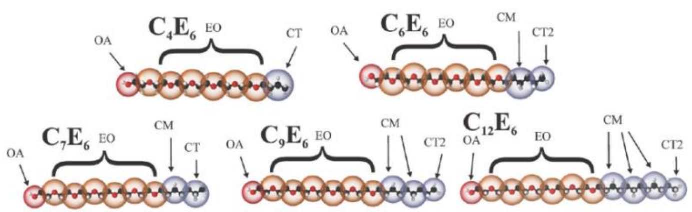
- Generate all-atom model based on the chemical distribution in different layers;
- Run MD simulations and calculate mechanical properties.

sample	Up slice	Middle slice	Down slice
Shear Modulus (GPa)	1.217±0.244	0.804±0.461	0.527±0.385

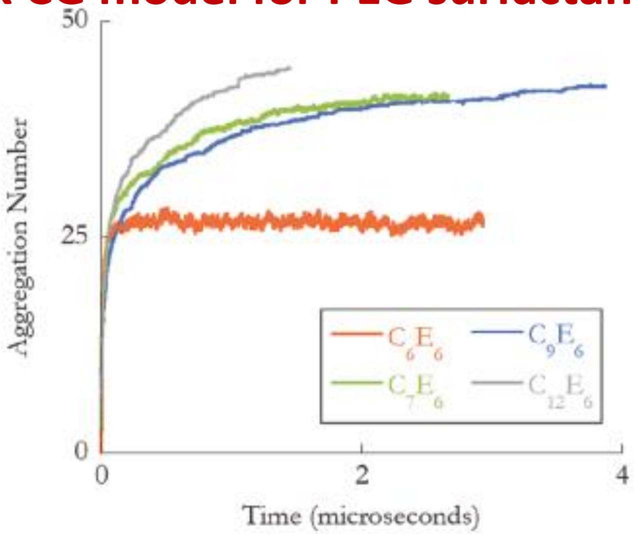


Timescales (Sampling)

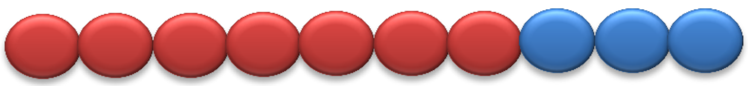
It is still difficult to approach equilibrium even with CG representation.



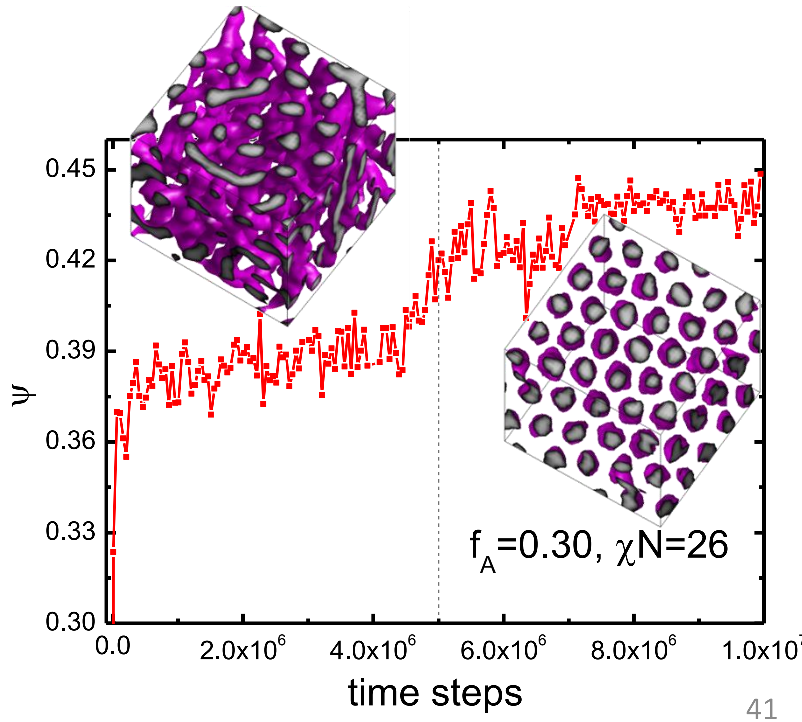
SDK CG model for PEG surfactants.



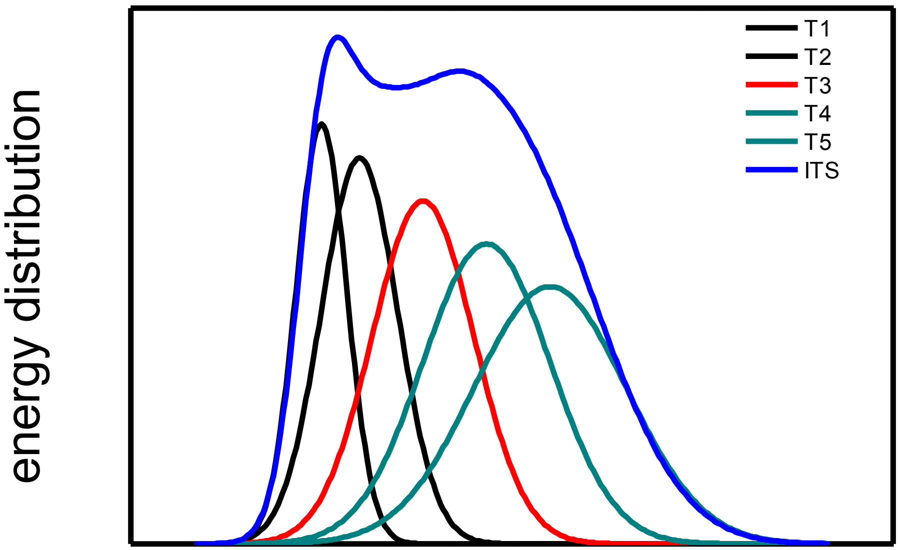
Klein et al., JCTC, 7, 4135, 2011



A7B3 block copolymer model.



Integrated tempering sampling (ITS)



Generalized distribution:

$$W(r) = \int_{\beta'} f(\beta') e^{-\beta' U(r)} dr$$

$$f(\beta') = \sum_k n_k \delta(\beta - \beta')$$

$$W(r) = \sum_k n_k e^{-\beta_k U(r)} \qquad k = 1, 2, \ldots, N\,.$$

Implementation of ITS

$$e^{-\beta U'(r)} \equiv W(r) = \sum_k n_k e^{-\beta_k U(r)}$$

$$U'(r) = -\frac{1}{\beta} \ln \sum_k n_k e^{-\beta_k U(r)}$$

$$F_b = -\frac{\partial U'(r)}{\partial r} = -\frac{\partial U'(r)}{\partial U(r)} \frac{\partial U(r)}{\partial r} = \frac{\sum_k n_k \beta_k e^{-\beta_k U(r)}}{\beta \sum_k n_k e^{-\beta_k U(r)}} F$$

For $T_j \in [T_1, T_N]$**:**

$$\langle A \rangle_{\beta_j} = \frac{\int A(r) e^{-\beta_j U(r)} dr}{\int e^{-\beta_j U(r)} dr} = \frac{\int \frac{A(r) e^{-\beta_j U(r)}}{W(r)} W(r) dr}{\int \frac{e^{-\beta_j U(r)}}{W(r)} W(r) dr} = \frac{\left\langle \frac{A(r) e^{-\beta_j U(r)}}{W(r)} \right\rangle_W}{\left\langle \frac{e^{-\beta_j U(r)}}{W(r)} \right\rangle_W}$$

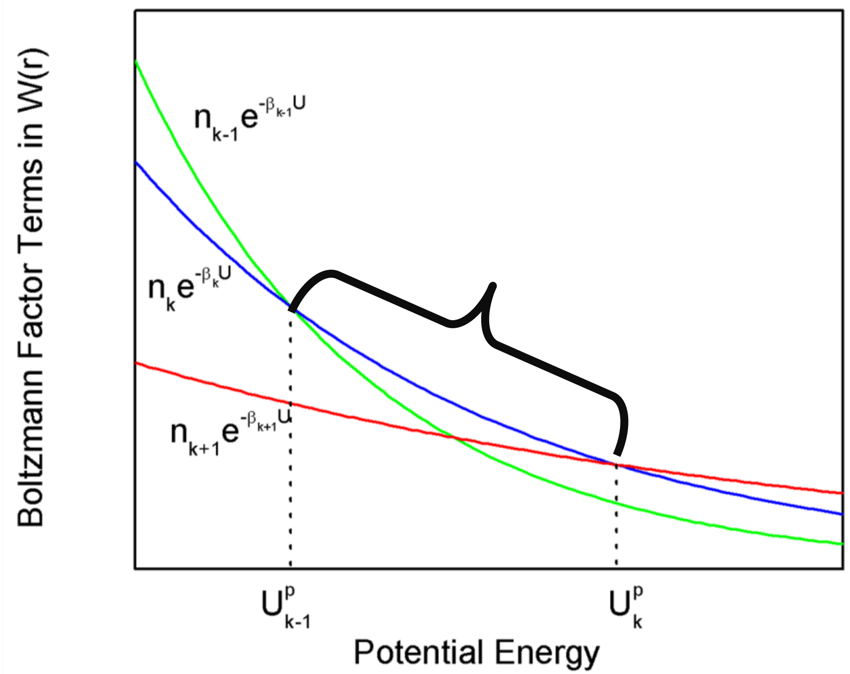
How to obtain n_k?

Define the energy U_k^p, at which the values of two adjacent terms in *W(r)* are equal:

$$n_k e^{-\beta_k U_k^p} = n_{k+1} e^{-\beta_{k+1} U_k^p}$$

Therefore

$$U_k^p = \frac{\ln n_k - \ln n_{k+1}}{\beta_k - \beta_{k+1}}$$



For energy $U_{k-1}^p < U < U_k^p$

$$n_1 e^{-\beta_1 U} < n_2 e^{-\beta_2 U} < \ldots < n_k e^{-\beta_k U} > \ldots > n_N e^{-\beta_N U}$$

The value of *W(r)* is dominated by its *k*-th term.

How to obtain n_k?

Define the energy U_k^q, at which the potential energy distribution of the canonical ensemble at temperature T_k is equal to that of the canonical ensemble at temperature T_{k+1} .

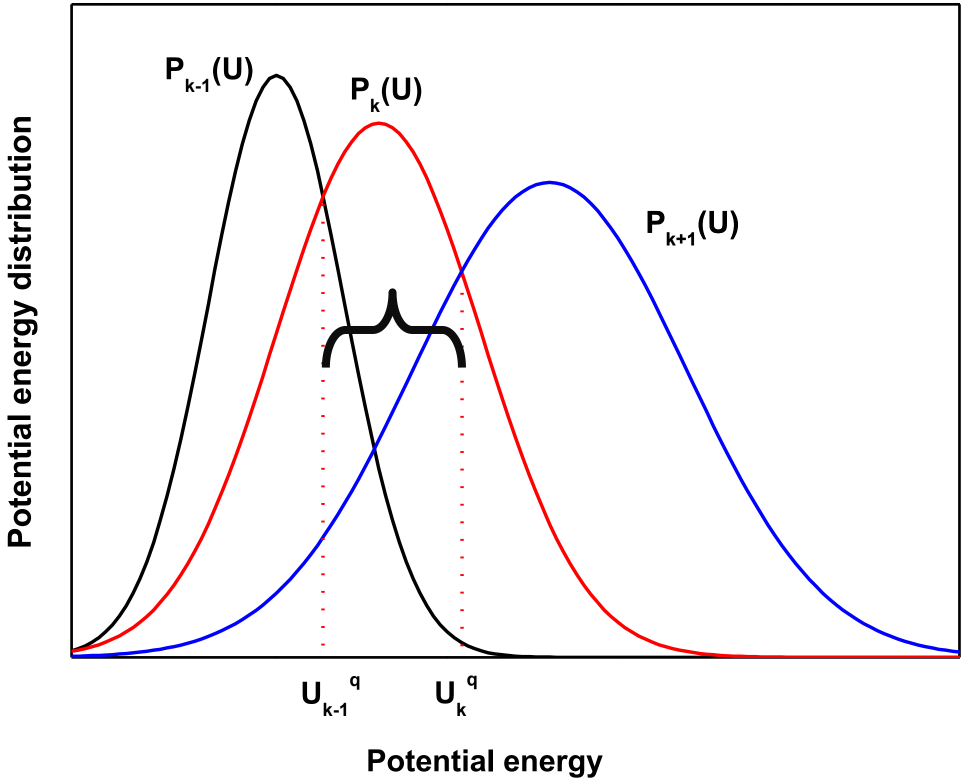
$$P_k(U_k^q) = P_{k+1}(U_k^q)$$

Since $P_k(U) = \dfrac{n(U)e^{-\beta_k U}}{Q_k}$

So $U_k^q = \dfrac{\ln Q_{k+1} - \ln Q_k}{\beta_k - \beta_{k+1}}$

For energy $U_{k-1}^q < U < U_k^q$

there is a maximum for function $P_k(U)$.



How to obtain n_k?

To optimize the energy distribution generated in ITS simulation, when *W(r)* is dominated by the *k*-th term in the range of $U_{k-1}^p < U < U_k^p$, the maximum of the potential energy distribution should be in the same range: $U_k^p = U_k^q$

Thus $$\ln n_k - \ln n_{k+1} = U_k^q(\beta_k - \beta_{k+1})$$

The slope of a secant line is approximated by average of the slopes of tangent lines at two line terminals.

$$U_k^q = \frac{\ln Q_{k+1} - \ln Q_k}{\beta_k - \beta_{k+1}} \approx -\frac{1}{2}\left(\frac{\partial \ln Q_k}{\partial \beta_k} + \frac{\partial \ln Q_{k+1}}{\partial \beta_{k+1}}\right) = \frac{1}{2}\left(\langle U \rangle_k + \langle U \rangle_{k+1}\right)$$

The temperature distribution

Define overlap factor *t*, which gives the ratio between energy distributions at two adjacent temperatures.

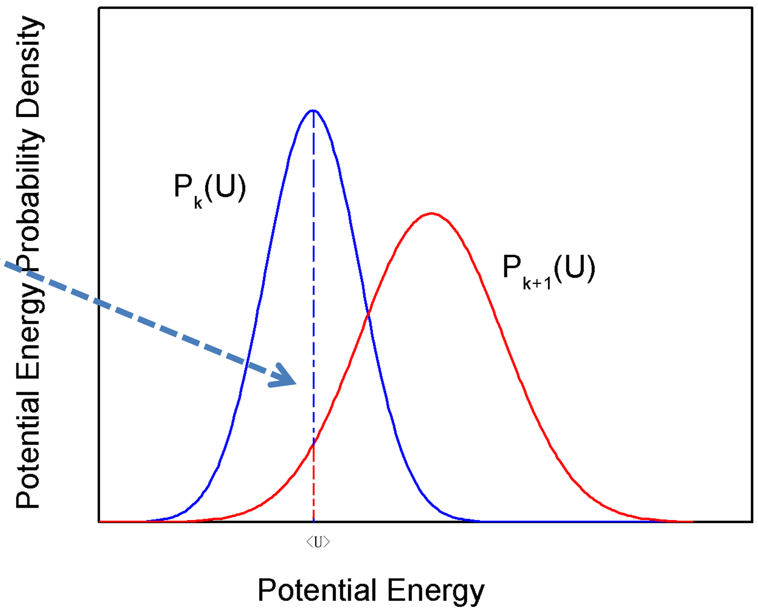
$$\frac{P_k(\langle U \rangle_k)}{P_{k+1}(\langle U \rangle_k)} = t$$

Thus:

$$\frac{\dfrac{n(\langle U \rangle_k) e^{-\beta_k \langle U \rangle_k}}{Q_k}}{\dfrac{n(\langle U \rangle_k) e^{-\beta_{k+1} \langle U \rangle_k}}{Q_{k+1}}} = t$$

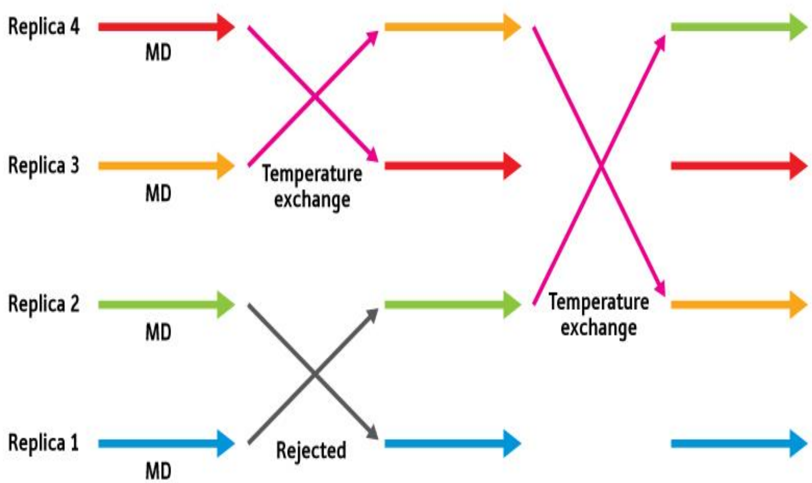
Finally we have:

$$\beta_k - \beta_{k+1} = \frac{\ln t}{U_k^q - \langle U \rangle_k}$$



The temperature distribution

Compare to replica exchange method:



$$P_{acc}(U_k, \beta_k \leftrightarrow U_{k+1}, \beta_{k+1}) = \min\{1, e^{(\beta_{k+1}-\beta_k)(U_{k+1}-U_k)}\}$$

In ITS:

$$\beta_k - \beta_{k+1} = \frac{\ln t}{U_k^q - \langle U \rangle_k}$$

$$U_k^q = \frac{1}{2}(\langle U \rangle_k + \langle U \rangle_{k+1})$$

$$\beta_k - \beta_{k+1} = \frac{2 \ln t}{\langle U \rangle_{k+1} - \langle U \rangle_k}$$

$$e^{(\beta_{k+1}-\beta_k)(\langle U \rangle_{k+1} - \langle U \rangle_k)} = t^{-2}$$

If a set of temperatures could give a reasonable acceptance ratio in REM simulations, there should be enough overlap between adjacent temperatures in ITS.

Simulation procedure

$$\ln n_k - \ln n_{k+1} = U_k^q(\beta_k - \beta_{k+1})$$

$$U_k^q = \frac{\ln Q_{k+1} - \ln Q_k}{\beta_k - \beta_{k+1}} \approx -\frac{1}{2}\left(\frac{\partial \ln Q_k}{\partial \beta_k} + \frac{\partial \ln Q_{k+1}}{\partial \beta_{k+1}}\right) = \frac{1}{2}\left(\langle U \rangle_k + \langle U \rangle_{k+1}\right)$$

po-

the

by

$$\beta_k - \beta_{k+1} = \frac{\ln t}{U_k^q - \langle U \rangle_k}$$

3. Determine the ITS tem

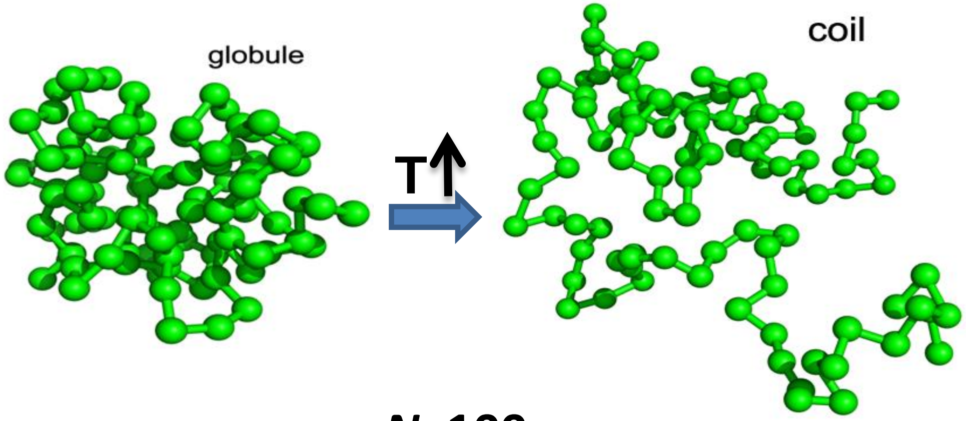
ing factors n_k through

$$F_b = -\frac{\partial U'(r)}{\partial r} = -\frac{\partial U'(r)}{\partial U(r)}\frac{\partial U(r)}{\partial r} = \frac{\sum_k n_k \beta_k e^{-\beta_k U(r)}}{\beta \sum_k n_k e^{-\beta_k U(r)}} F$$

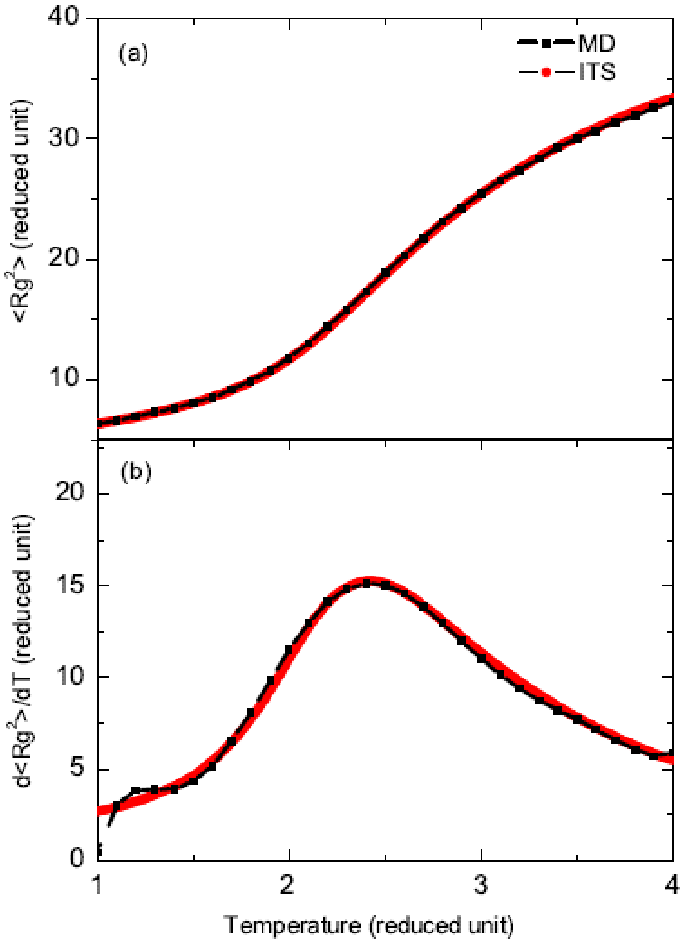
4. $$\langle A \rangle_{\beta_j} = \frac{\int A(r) e^{-\beta_j U(r)} dr}{\int e^{-\beta_j U(r)} dr} = \frac{\int \frac{A(r) e^{-\beta_j U(r)}}{W(r)} W(r) dr}{\int \frac{e^{-\beta_j U(r)}}{W(r)} W(r) dr} = \frac{\left\langle \frac{A(r) e^{-\beta_j U(r)}}{W(r)} \right\rangle_W}{\left\langle \frac{e^{-\beta_j U(r)}}{W(r)} \right\rangle_W}$$ hich

5. After ITS simulation, the canonical ensemble properties can be calculated by reweighting.

Coil-to-globule transition



***N*=100**



In ITS:
t=exp(0.5)
T=1.0-4.35
Simulate 1.0X10^9 steps

In conventional MD: 31 temperatures

GPU simulation package

GALAMOST: GPU-accelerated large-scale molecular simulation toolkit

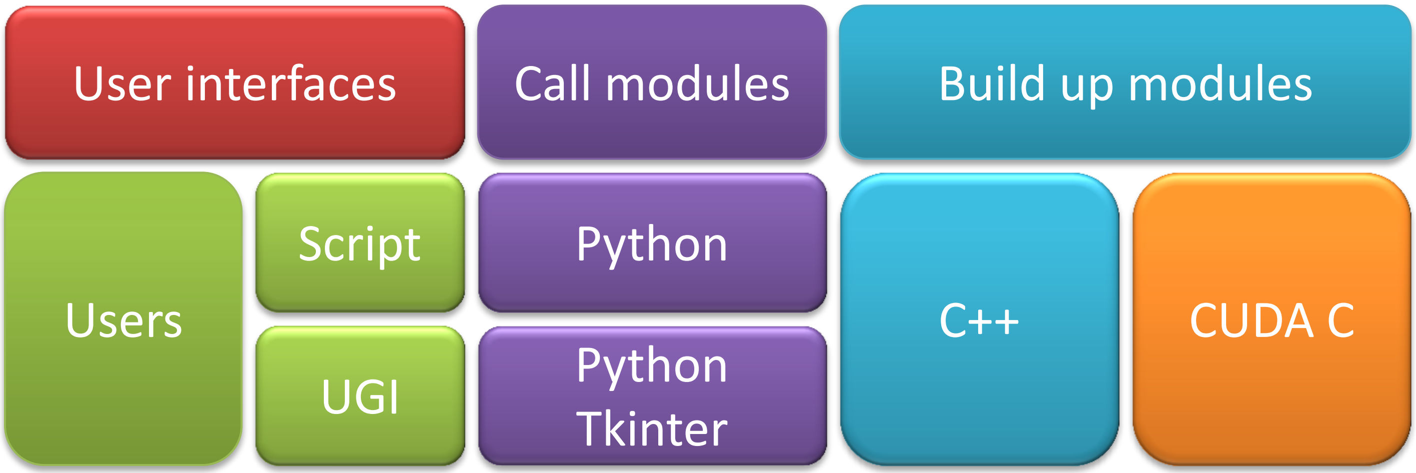
http://galamost.com/

Free to download!

Functions:

- **CGMD; Brownian Dynamics; Dissipative Particle Dynamics;**
- **Particle-field coupling (MDSCF);**
- **Numerical potential (e.g. from iterative Boltzmann inversion & inverse Monte Carlo);**
- **NVE; NVT; NPT (Nose-Hoover; Andersen);**
- **Anisotropic soft particle model;**
- **Stochastic polymerization model;**
- **Integrated tempering sampling.**

GALAMOST: Structures



More characteristics of this package:

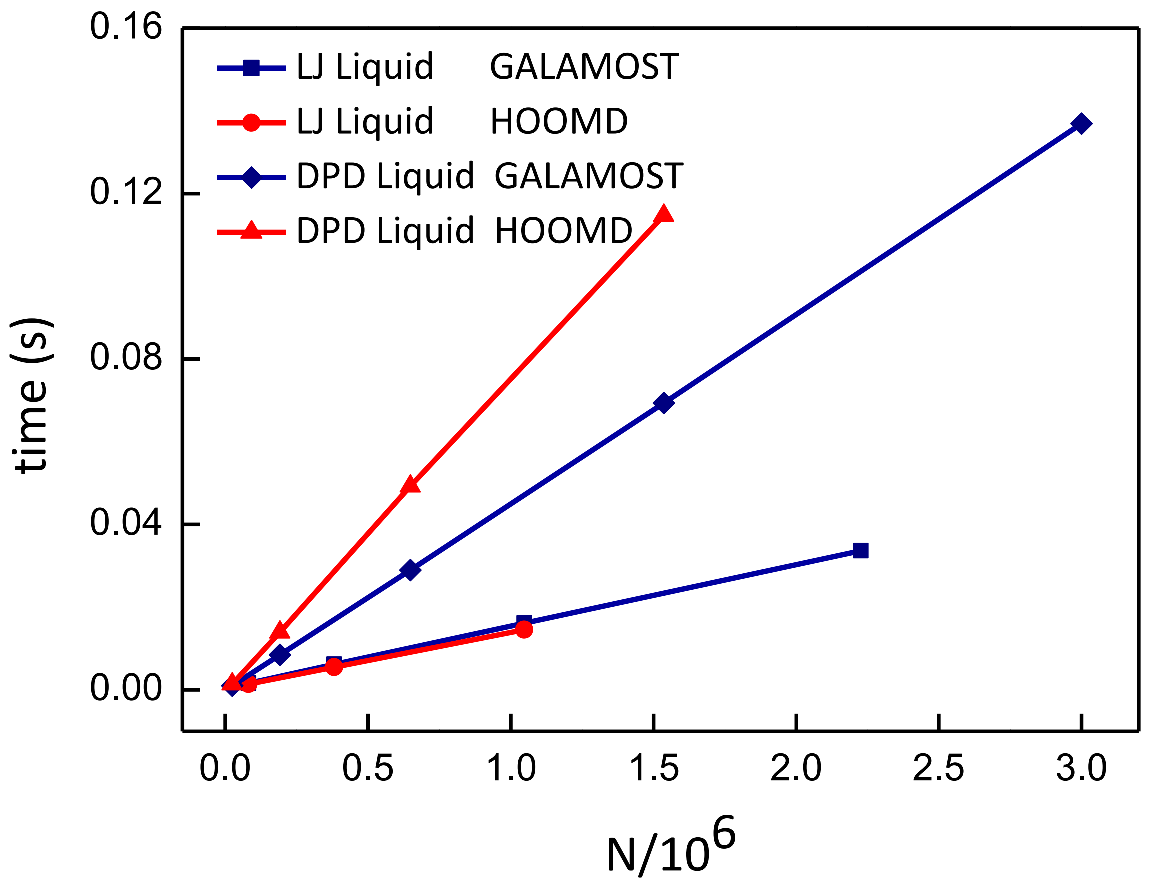
Specifically designed for running on GPUs only

Standard format of input and output file: xml, mol2, dcd ...

GALAMOST: Performances

Performances: the average costing time per time step of GALAMOST and HOOMD.

System size: up to 2.2 M LJ liquid particles or 3.0 M DPD liquid particles on GTX 580 with 1.5 GB device memory.



DPD: ~1.5 days for 3.0M particles×1.0M steps.

Summary

Approaching larger spatiotemporal scales in polymer simulations:

Generic polymer model | Stochastic polymerization model | Soft patchy-particle model

Enhanced sampling (ITS) + DPD + Kinetic network analysis

DPD with SCF treatment | Numerical potential with DPD thermstating | DPD with electrostatics

Acknowledgement

- Financial supports from National Natural Science Foundation of China.
- Financial supports from Ministry of Science and Technology of China.
- All my group members!
- Collaborators:
  - Prof. *Zhao-Yan Sun* and Prof. *Lijia An* @ Changchun Inst. Appl. Chem.
  - Prof. *De-Yue Yan* and Prof. *Yongfeng Zhou* @ Shanghai Jiaotong U.
  - Prof. *Aatto Laaksonen* @ Stockholm U.
  - Prof. *Florian Mueller-Plathe* @ TUDarmstadt
  - Prof. *Giuseppe Milano* @ Salerno U.
  - Prof. *Yi-Qin Gao* @ Peking U.
  - Prof. *An-Chang Shi* @ McMaster U.
  - Prof. *Zhihong Nie* @ Maryland U.
  - Prof. *Xuhui Huang* @ HKUST ……

Thank you for your attention!