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):

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

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

\[ \vec{F}^d_{ij} = -\gamma \omega^D(r_{ij}) (\vec{V}_{ij} \cdot \hat{r}_{ij}) \hat{r}_{ij} \]

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

\[ a \rho = 75 \]

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

\[ \omega^D(r) = \omega^R^2(r) \]

\[ \sigma = (2k_B T \gamma)^{1/2} \]
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%).

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


Network morphology

Materials science: Continuity through dispersity

Richard A Register

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- 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:

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

\[ \delta = \frac{N}{N_n}, \quad \text{PDI} = \frac{N_w}{N_n} = \frac{1+u}{u} \]

Simulated systems:

<table>
<thead>
<tr>
<th>System</th>
<th>PDI_A</th>
<th>PDI_B</th>
</tr>
</thead>
<tbody>
<tr>
<td>Asymmetric PDI</td>
<td>1.0</td>
<td>1.5 (SZ)</td>
</tr>
<tr>
<td>Symmetric PDI</td>
<td>1.5 (SZ)</td>
<td>1.5 (SZ)</td>
</tr>
</tbody>
</table>

\[ A_x B_{N-2x} A_x, \quad N_n = 8~18 \]

\[ V_{box} = 40 \times 40 \times 40 \]
Network morphology

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

\[ \text{PDI}_A = 1.00, \text{PDI}_B = 1.50 \text{ (SZ)} \]

irregular bicontinuous phase (BIC) \( \sim 10\% \)
Network morphology

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

$\text{PDI}_A = 1.50 \text{ (SZ)}, \text{PDI}_B = 1.50 \text{ (SZ)}$

irregular bicontinuous phase (BIC) $\sim 20\%$
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 ($\text{PDI}_A=1.00$, $\text{PDI}_B=1.50$): $f_B=0.375$, $\chi N=62.04$

Take a part of the network structure
Show polymer beads
Selective distribution of blocks with different chain lengths can stabilize the BIC phase.
Soft Janus 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:

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

\[ k_B T = 1.0 \quad \text{as the units.} \]

\[ r_c = 1.0 \]
Soft colloidal particle model

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

\[ \alpha_{ij}^R = \frac{EV}{k_B T} \]

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

\[ d = \frac{\alpha_{ij}^R + \alpha_{ij}^A/2}{\alpha_{ij}^R + \alpha_{ij}^A} \]

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

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

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

\(E\): elastic modulus

\(d\): diameter of colloidal particle

\(\delta d\): the range of attraction

\(G\): potential well depth
Soft colloidal particle model

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

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

Suppose:
- nanoparticle diameter \(d = 20\) nm
- Elastic modulus \(E = 8.3 \times 10^7\) Pa
- Attraction range \(\delta d = 0.4\) nm
- Attraction well depth \(G = 2\ k_B T\)

\[ \alpha_{ij}^R \approx 10000 \]
\[ \alpha_{ij}^A \approx 400 \]
\[ r_c = 1.0 (\approx 20.5\ nm) \]
Describe the patch size

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

\[
f = \cos \theta_i' \cos \theta_j'
\]

for \(|\cos \theta_i| \geq \cos \beta\) and \(|\cos \theta_j| \geq \cos \beta\)

\[
\theta_i' = \arccos(|\cos \theta_i|) \quad \theta_j' = \arccos(|\cos \theta_j|)
\]

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

The patch parts are hydrophobic.
Patchy particle self-assembly

We then focus on the soft two-patch particle with diameter $d \sim 20$ nm and modulus $E \sim 4.1 \times 10^6$ Pa:

$G=2.0 \ k_B T; \ \beta=30^\circ$

$G=9.8 \ k_B T; \ \beta=30^\circ$
Patchy particle self-assembly

G=2.0 k_BT; \( \beta = 60^\circ \)

G=9.8 k_BT; \( \beta = 60^\circ \)
Describe patchy particle

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

- The middle part is hydrophobic.

\[ f = \begin{cases} 
\cos \frac{\pi}{2} \left(\frac{\pi/2 - \theta'_i}{\pi/2 - \beta}\right) \cos \frac{\pi}{2} \left(\frac{\pi/2 - \theta'_j}{\pi/2 - \beta}\right) & \text{if } |\cos \theta_i| \leq \cos \beta \text{ and } |\cos \theta_j| \leq \cos \beta \\
0 & \text{otherwise.} 
\end{cases} \]

\[ \theta'_i = \arccos(|\cos \theta_i|) \quad \theta'_j = \arccos(|\cos \theta_j|) \]

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

The middle part is hydrophobic.
Patchy particle self-assembly

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

Loosely packed hexagonal membrane

Tetragonal membrane

Kagome membrane

densely packed hexagonal membrane
Multi-patch particle model

\[ U_{ij} = \begin{cases} \frac{\alpha^R_{ij} d_{ij}}{2} \left(1 - \frac{r_{ij}}{d_{ij}}\right)^2 - \sum_{\kappa=1}^{M_i} \sum_{\lambda=1}^{M_j} f^{\nu} \left( n_{i}^{\kappa}, n_{j}^{\lambda}, r_{ij} \right) \frac{\alpha^A_{ij} d_{ij}}{2} \left[ \frac{r_{ij}}{d_{ij}} - \left(\frac{r_{ij}}{d_{ij}}\right)^2 \right] & \text{if } r_{ij} \leq d_{ij} \\ 0 & \text{if } r_{ij} > d_{ij}, \end{cases} \]  

(1)

\[ f \left( n_{i}^{\kappa}, n_{j}^{\lambda}, r_{ij} \right) = \begin{cases} \cos \frac{\pi \theta_{i}^{\kappa}}{2 \theta_{m}^{\kappa}} \cos \frac{\pi \theta_{j}^{\lambda}}{2 \theta_{m}^{\lambda}} & \text{if } \cos \theta_{i}^{\kappa} \geq \cos \theta_{m}^{\kappa} \text{ and } \cos \theta_{j}^{\lambda} \geq \theta_{m}^{\lambda} \\ 0 & \text{otherwise.} \end{cases} \]  

(2)
Multi-patch particle model

\[ F_{ij} = -\frac{\partial U_{ij}}{\partial r_{ij}} \]

\[ = \alpha_{ij}^R \left( 1 - \frac{r_{ij}}{d_{ij}} \right) \frac{r_{ij}}{r_{ij}} + \sum_{\kappa=1}^{M_i} \sum_{\lambda=1}^{M_j} \frac{\alpha_{ij}^A f^\nu (n_i^\kappa, n_j^\lambda, r_{ij})}{2} \left( \frac{1}{2} - \frac{r_{ij}}{d_{ij}} \right) \frac{r_{ij}}{r_{ij}} - \frac{\alpha_{ij}^A}{2} \left[ \frac{r_{ij}}{d_{ij}} - \left( \frac{r_{ij}}{d_{ij}} \right)^2 \right] \]

\[ \nu f^{\nu - 1} (n_i^\kappa, n_j^\lambda, r_{ij}) \left( \frac{\pi}{2 \theta_m^\kappa} \sin \frac{\pi \theta_i^\kappa}{2 \theta_m^\kappa} \frac{\partial \theta_i^\kappa}{\partial \cos \theta_i^\kappa} \cos \frac{\pi \theta_j^\lambda}{2 \theta_m^\lambda} + \frac{\pi}{2 \theta_m^\lambda} \sin \frac{\pi \theta_j^\lambda}{2 \theta_m^\lambda} \frac{\partial \theta_j^\lambda}{\partial \cos \theta_j^\lambda} \right) \left( \frac{\partial \cos \theta_j^\lambda}{\partial r_{ij}} \cos \frac{\pi \theta_i^\kappa}{2 \theta_m^\kappa} \right), \]

\[ \tau_{ij} = \sum_{\kappa=1}^{M_i} -\frac{\partial U_{ij}}{\partial n_i^\kappa} \]

\[ = \sum_{\kappa=1}^{M_i} \sum_{\lambda=1}^{M_j} \frac{\pi \alpha_{ij}^A d_{ij}}{4 \theta_m^\kappa} \left[ \frac{r_{ij}}{d_{ij}} - \left( \frac{r_{ij}}{d_{ij}} \right)^2 \right] \nu f^{\nu - 1} (n_i^\kappa, n_j^\lambda, r_{ij}) \sin \frac{\pi \theta_i^\kappa}{2 \theta_m^\kappa} \frac{\partial \theta_i^\kappa}{\partial \cos \theta_i^\kappa} \cos \frac{\pi \theta_j^\lambda}{2 \theta_m^\lambda} \frac{r_i}{r_{ij}}. \]

We use quaternion method to integrate equations of motion.
Multi-patch particle model
Multi-patch particle model
Multi-patch particle model
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

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

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

If $P \leq P_r$, connect;
Else if $P > P_r$, do not connect.
Stochastic reaction in a cutoff
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):

\[ M_A = 248.30 \text{g/mol} \]

\[ M_B = 312.40 \text{g/mol} \]

\[ M_C = 289.97 \text{g/mol} \]

\[ \bar{M} = \sum_{i=A-C} (\phi_i M_i) = 266.28 \text{g/mol} \]

\[ \bar{v} = 409.42 \text{Å}^3 \]

Length scale: \( L = 1.07 \text{nm} \)
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 $\chi$ parameters.
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 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.

<table>
<thead>
<tr>
<th>sample</th>
<th>Up slice</th>
<th>Middle slice</th>
<th>Down slice</th>
</tr>
</thead>
<tbody>
<tr>
<td>Shear Modulus (GPa)</td>
<td>1.217 ± 0.244</td>
<td>0.804 ± 0.461</td>
<td>0.527 ± 0.385</td>
</tr>
</tbody>
</table>
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

<table>
<thead>
<tr>
<th>Aggregation Number</th>
</tr>
</thead>
<tbody>
<tr>
<td>Time (microseconds)</td>
</tr>
<tr>
<td>0</td>
</tr>
<tr>
<td>2</td>
</tr>
<tr>
<td>4</td>
</tr>
</tbody>
</table>

A7B3 block copolymer model.

- $f_A = 0.30$, $\chi N = 26$
Integrated tempering sampling (ITS)

Generalized distribution:

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

\[
f(\beta') = \sum_{k} n_k \delta(\beta - \beta')
\]

\[
W(r) = \sum_{k} n_k e^{-\beta_k U(r)} \quad k = 1, 2, \ldots, N.
\]
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 \( T_{j} \in [T_{1}, T_{N}] \):

\[ \langle A \rangle_{\beta_{j}} = \frac{\int A(r) e^{-\beta_{j} U(r)} dr}{\int e^{-\beta_{j} U(r)} dr} = \frac{\int \frac{A(r) e^{-\beta_{j} U(r)}}{W(r)} W(r) dr}{\int \frac{e^{-\beta_{j} U(r)}}{W(r)} W(r) dr} = \frac{\langle \frac{A(r) e^{-\beta_{j} U(r)}}{W(r)} \rangle_{W}}{\langle \frac{e^{-\beta_{j} U(r)}}{W(r)} \rangle_{W}} \]
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 \[ P_k(U) = \frac{n(U)e^{-\beta_kU}}{Q_k} \]

So \[ U_k^q = \frac{\ln Q_{k+1} - \ln Q_k}{\beta_k - \beta_{k+1}} \]

For energy \[ U_{k-1}^q < U < U_k^q \]

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

Potential energy distribution

Potential energy

$P_{k-1}(U)$ $P_k(U)$ $P_{k+1}(U)$
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.

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

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

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:

In ITS:

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

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

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

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

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

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

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

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

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

3. Determine the ITS temperature factors \( t \) through:

\[ F_b = -\frac{\partial U'(r)}{\partial r} = -\frac{\partial U'(r)}{\partial U(r)} \frac{\partial U(r)}{\partial r} = \frac{\sum_k n_k \beta_k e^{-\beta_k U(r)}}{\beta \sum n_k e^{-\beta_k U(r)}} \]

4. \[ \langle A \rangle_{\beta_j} = \frac{\int A(r) e^{-\beta_j U(r)} dr}{\int e^{-\beta_j U(r)} dr} = \frac{\int \frac{A(r) e^{-\beta_j U(r)}}{W(r)} W(r) dr}{\int \frac{e^{-\beta_j U(r)}}{W(r)} W(r) dr} = \frac{\left\langle A(r) e^{-\beta_j U(r)} \right\rangle}{\left\langle e^{-\beta_j U(r)} \right\rangle} \]

5. After ITS simulation, the canonical ensemble properties can be calculated by reweighting.
Coil-to-globule transition

In ITS:
$t = \exp(0.5)$
$T = 1.0 - 4.35$
Simulate $1.0 \times 10^9$ 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
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  - 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!

Changbai mountain in Jilin province