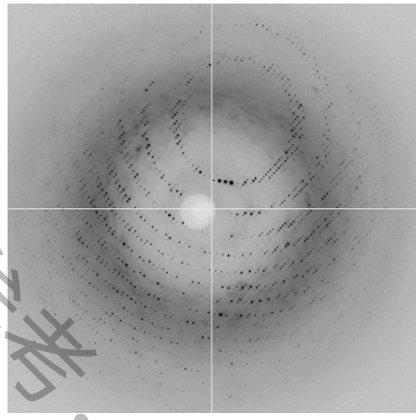
MD: Initial conditions

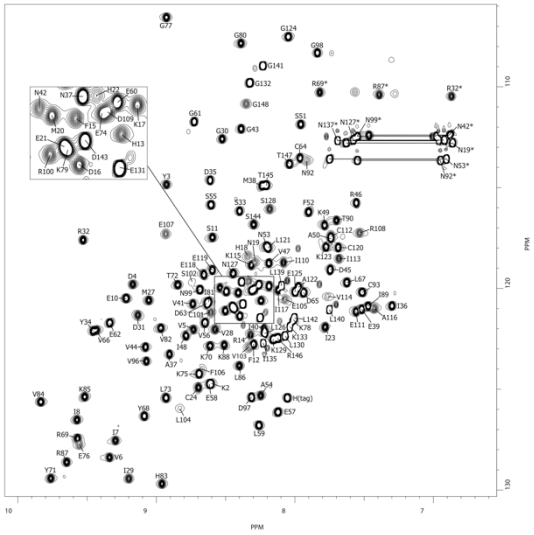
1. Initial positions
2. Initial momenta (speed)
3. Time step
4. Environment parameters

MD: Initial positions

Solids: mainly from expt.

1. Initial positions
2. Initial momenta
3. Time interval
4. Env. param.





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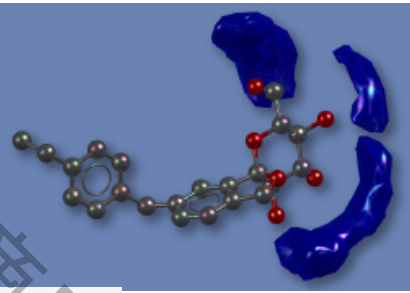

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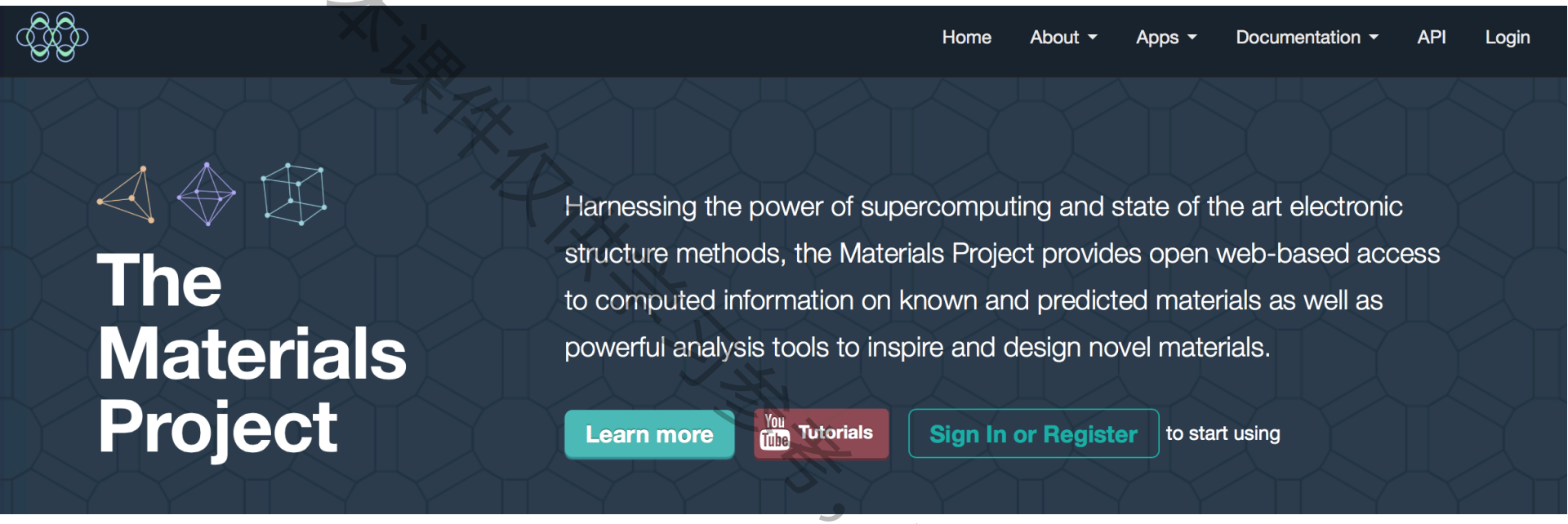

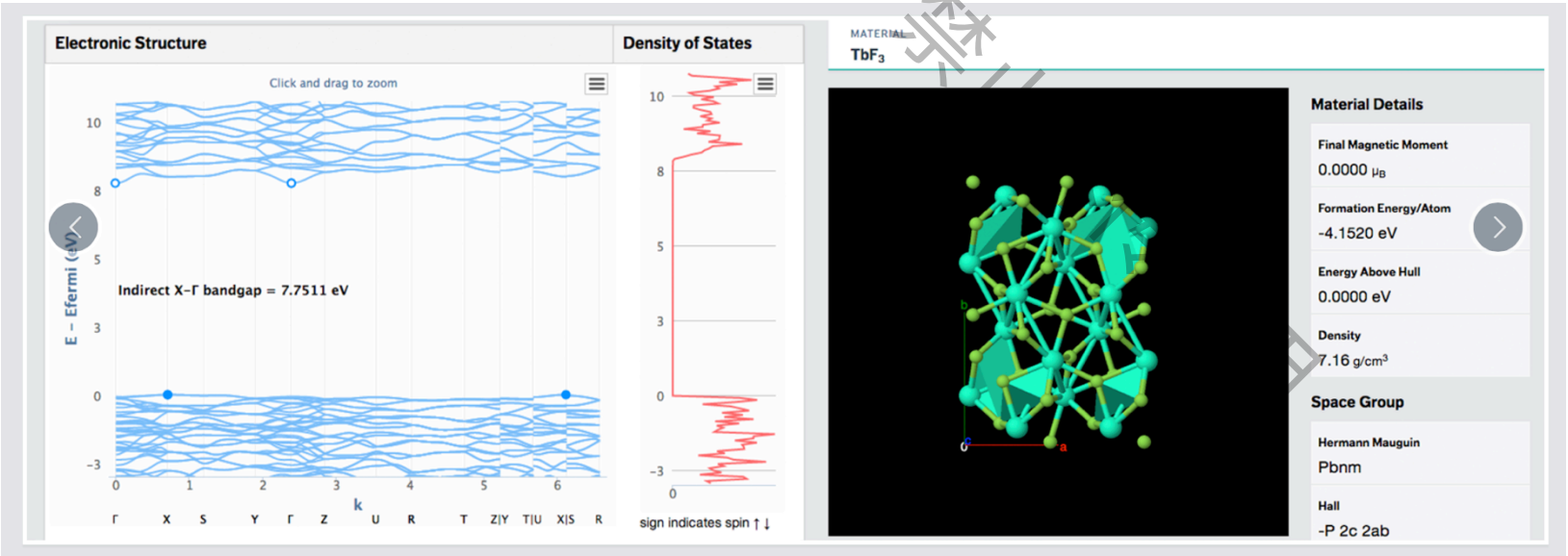

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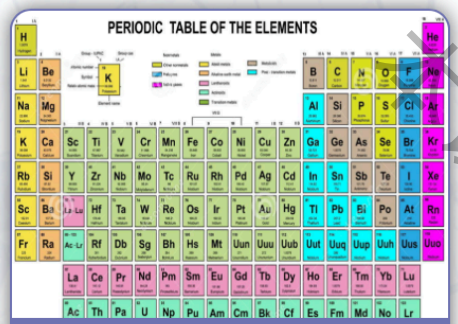
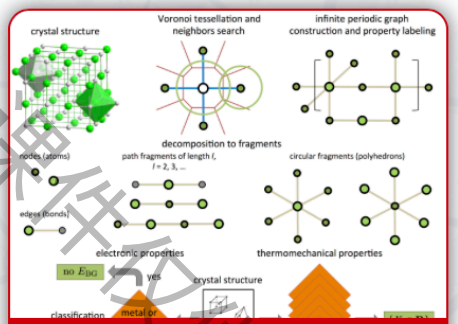
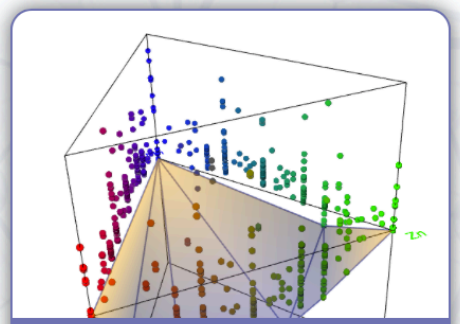


MendeLIB search

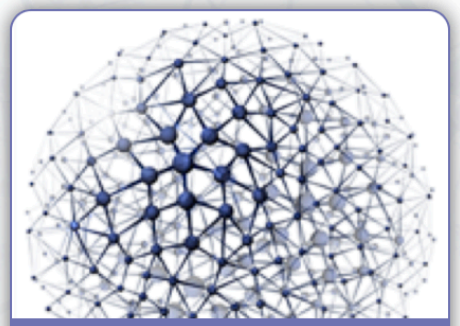


AFLOW-ML

Crystal prototypes



AFLOW hull beta



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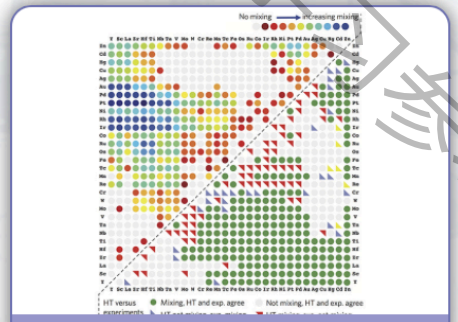
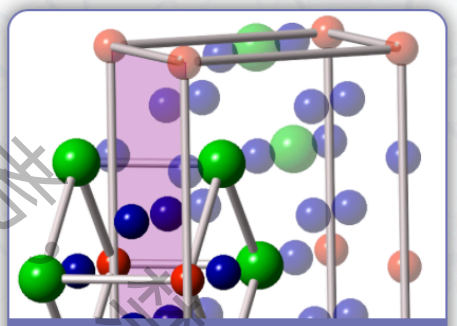


Binary alloy library



Superalloys search

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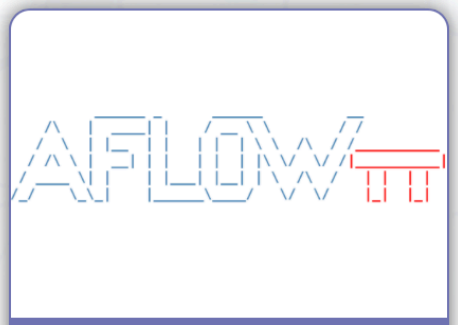

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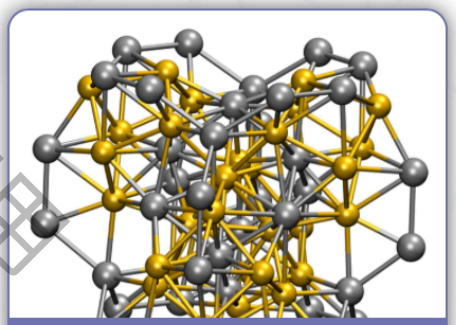
PAOFLOW

Geolocation data



Showcase material

STRUCTURAL SCIENCE
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ISSN 2052-5206

Report on the sixth blind test of organic crystal structure prediction methods

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§ Retired.

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Supporting information: this article has supporting information at journals.iucr.org/b

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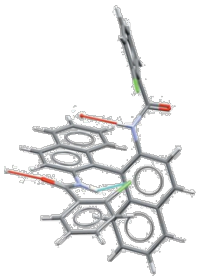

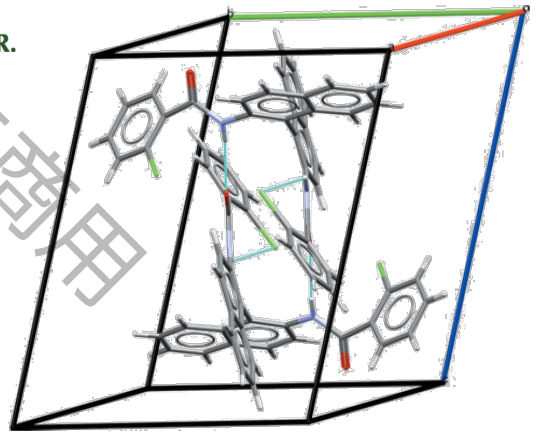

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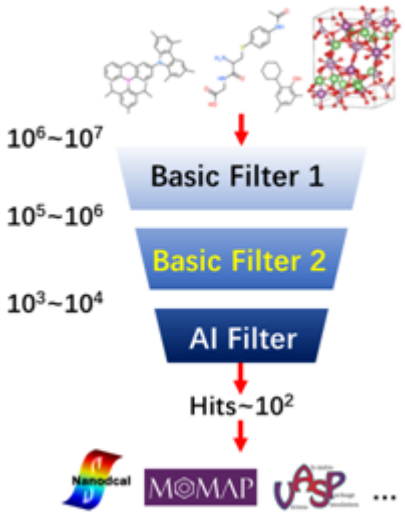

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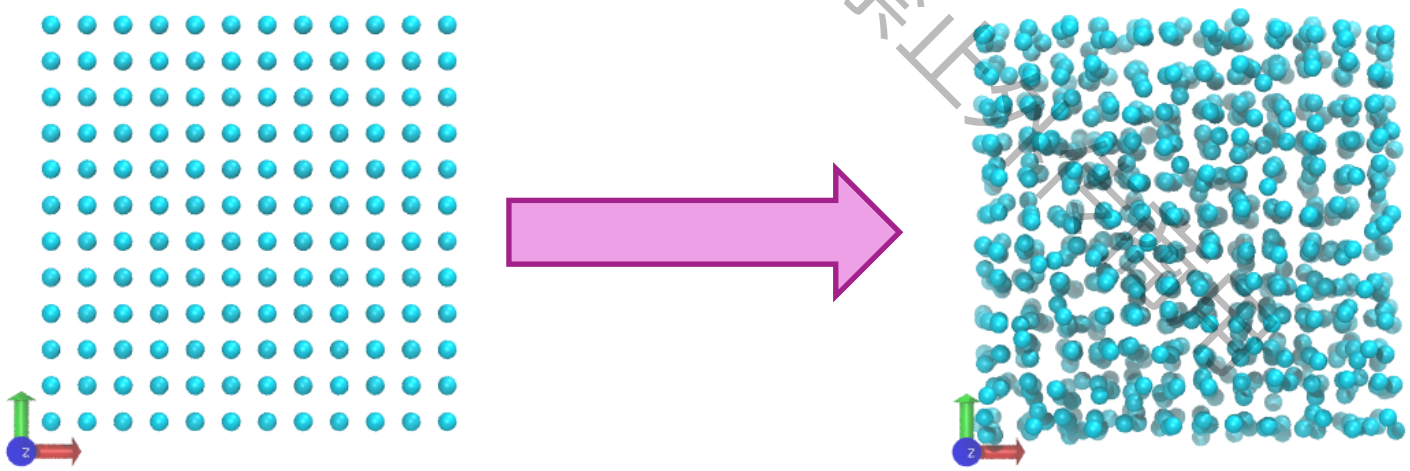
MD: Initial positions

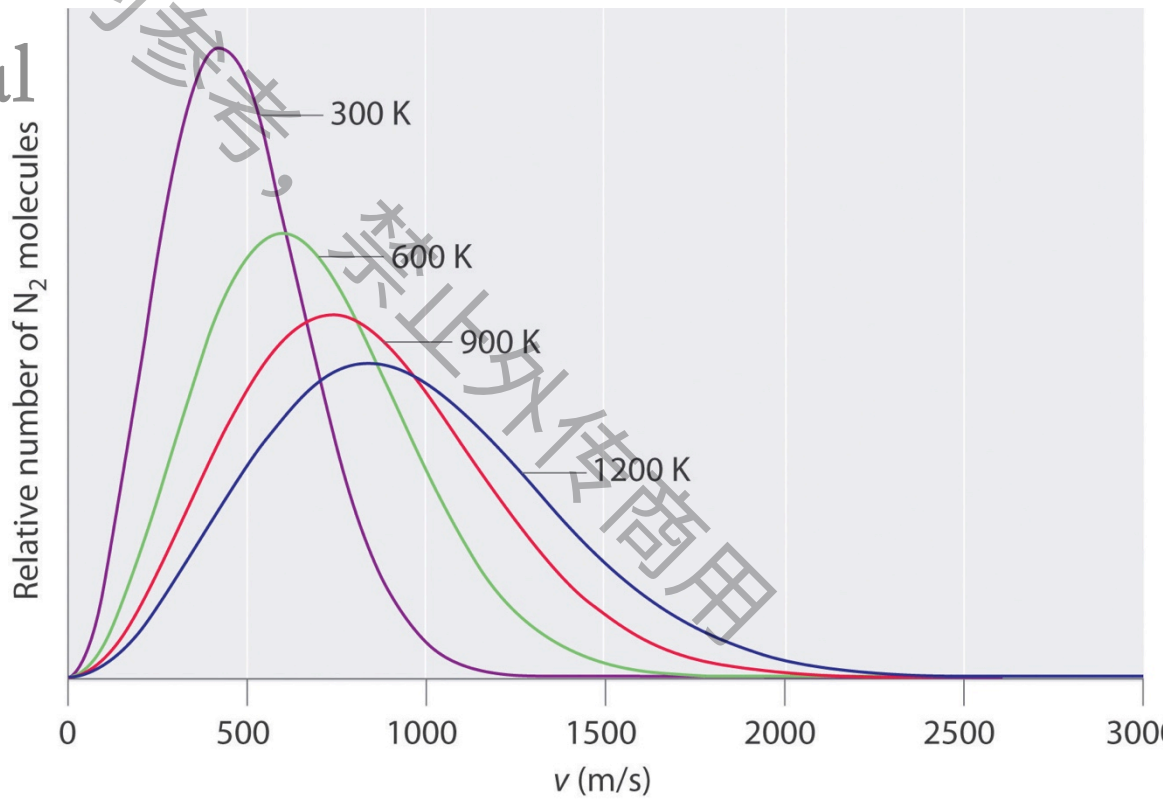
1. Initial positions
2. Initial momenta
3. Time interval
4. Env. param.

Gas, liquids: uniform arranged



MD: Initial momenta

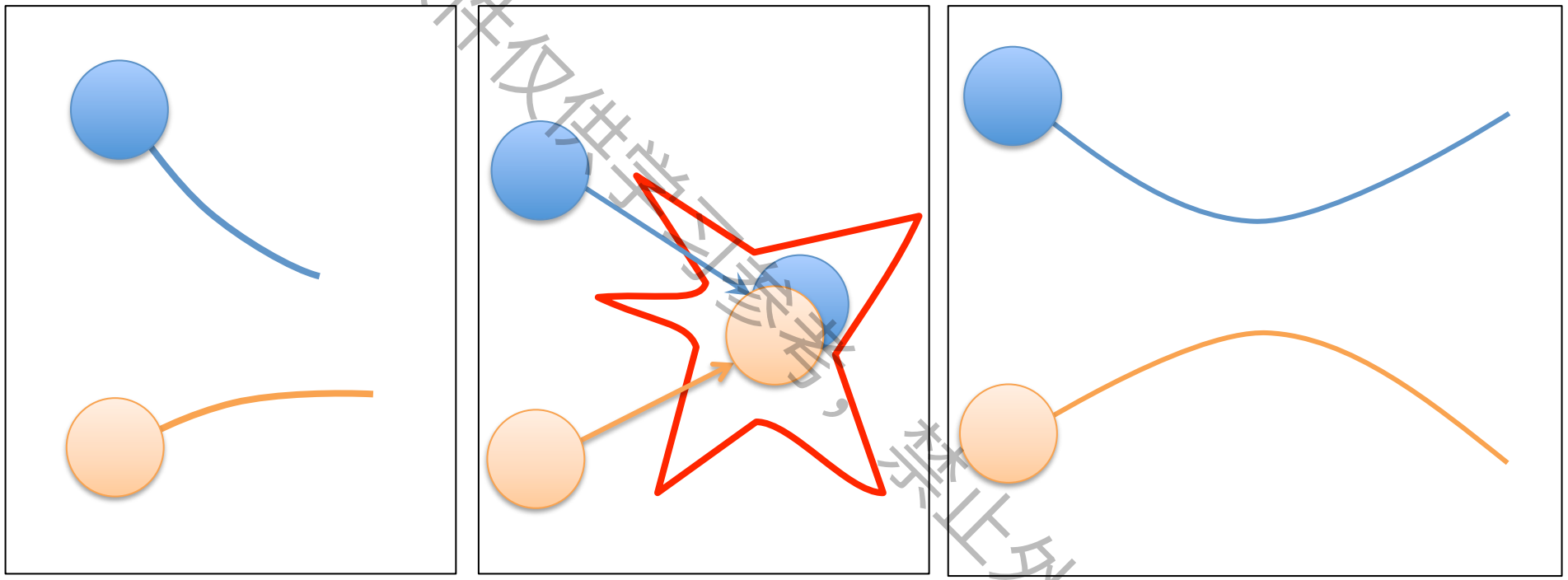
1. Initial positions
2. Initial momenta
3. Time interval
4. Env. param.



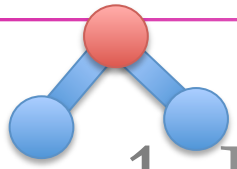
MD: Time interval

1. Initial positions
2. Initial momenta
3. Time interval
4. Env. param.

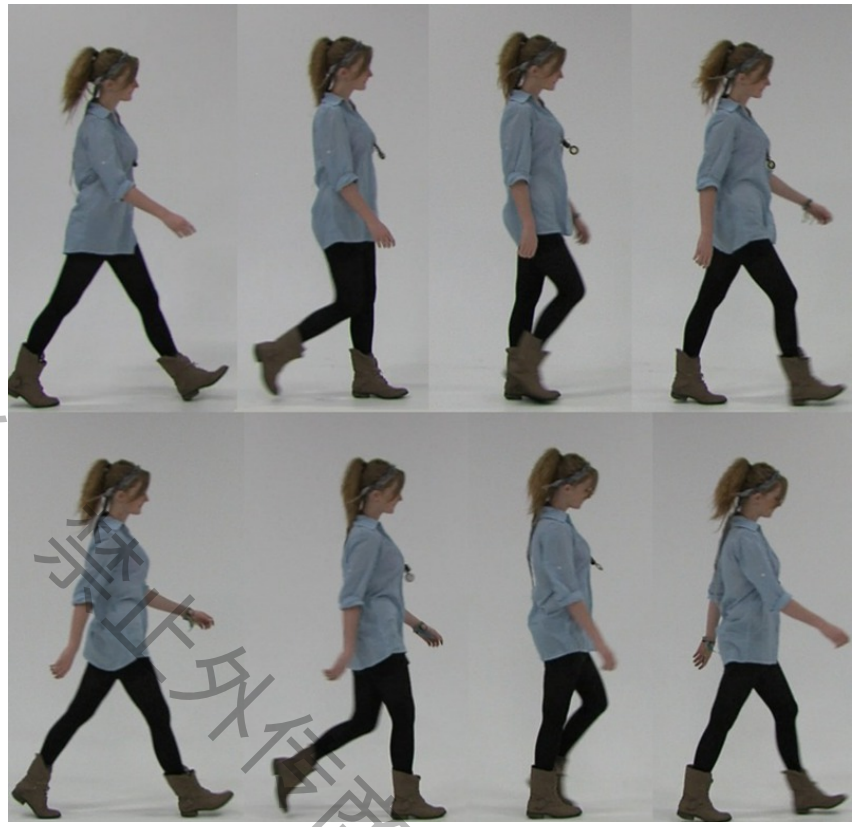
MD: Time interval



MD: Time interval



1. Initial positions
2. Initial momenta
3. Time interval
4. Env. param.



1/10 minimum period

1. O-H: 1.08×10^{14} Hz,

T~9 fs→ dt=0.9 fs

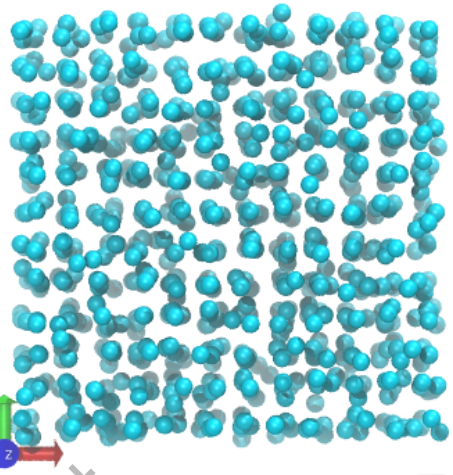
To simulate the absorption of CO_2 on metal surface is easier than H_2O.

2. Ar: 3.44×10^{11} Hz,

T=2.906 ps → dt = 0.29 ps = 290 fs

MD: Environment parameters

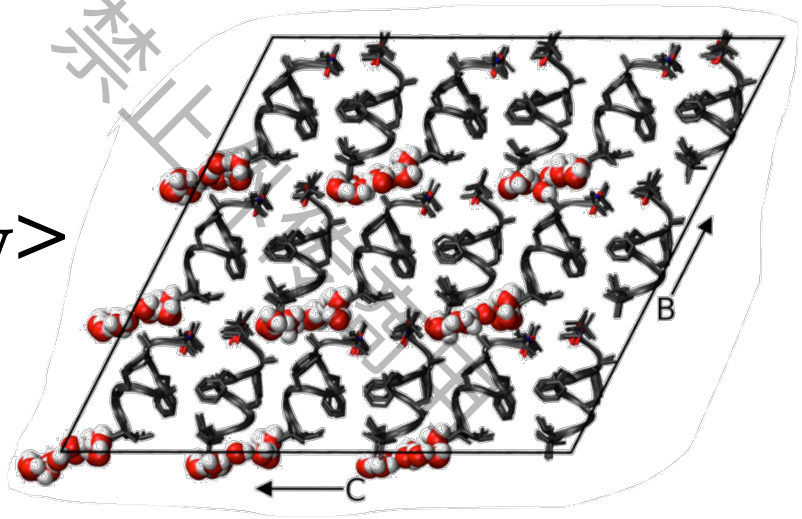
1. Initial positions
2. Initial momenta
3. Time interval
4. Env. param.



Temperature: <velocity>

Pressure: Volume

Boundary condition



MD: Other things

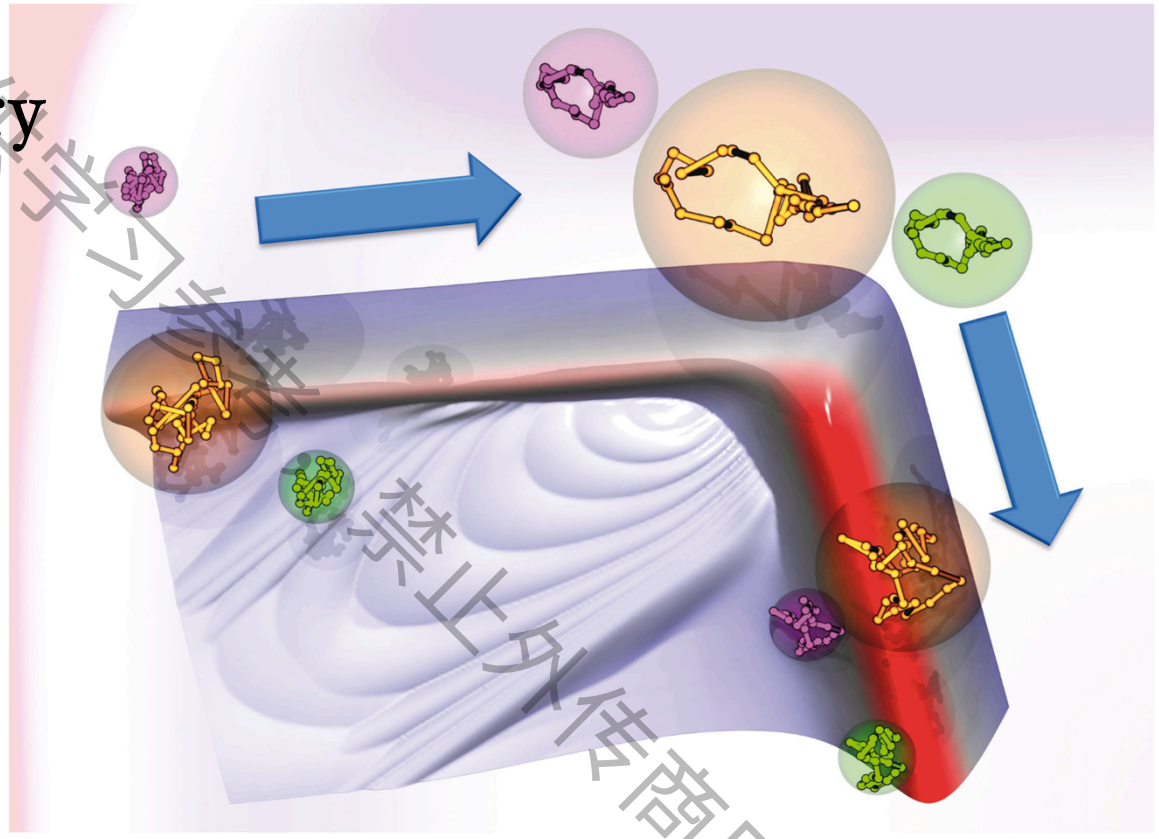
1. Initial positions
2. Initial momenta
3. Time interval
4. Env. param.
5. Interatomic interactions: *ab initio* vs. Force field

MD: Boundary condition

1. No boundary condition: gas phase chemical reactions
2. Finite boundary conditions:
   Solvation models： MM-PB(GB)/SA
3. Spherical boundary: (early) QM/MM MD
4. Periodical boundary condition
   General purpose

MD: Boundary condition

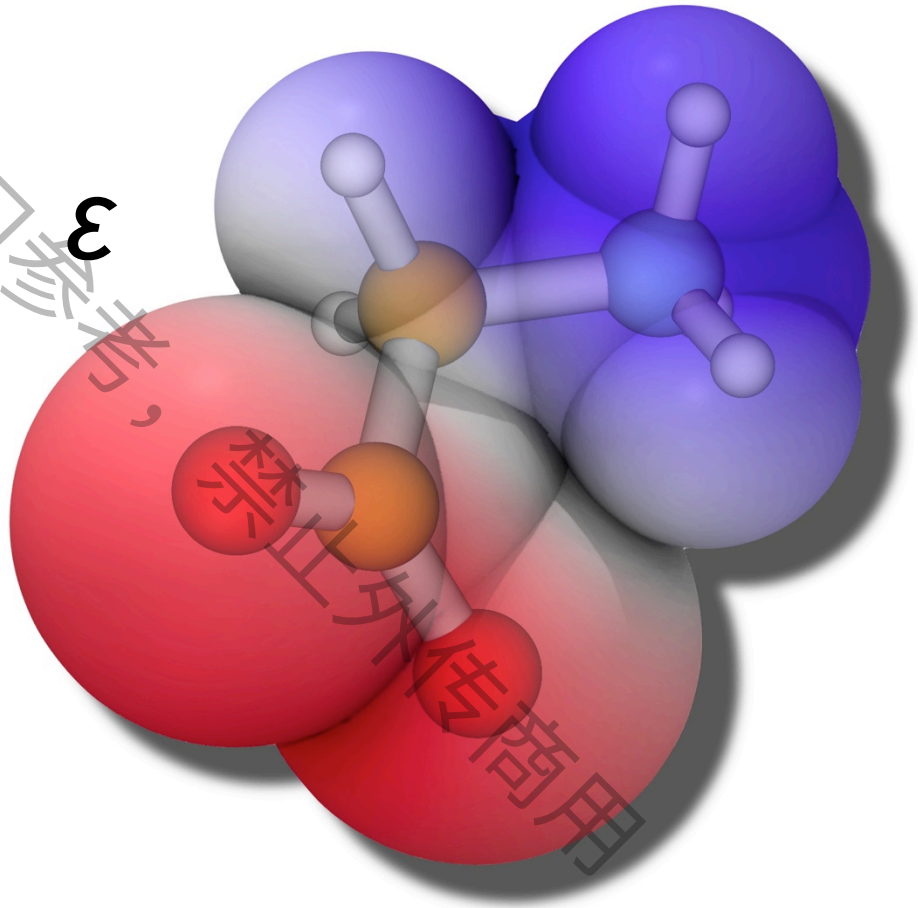
1. No boundary



Bai, M.; Lu, D.; **Li, Y.;** Li, J., *Physical Chemistry Chemical Physics* **2016,** *18*, 32031-32041.

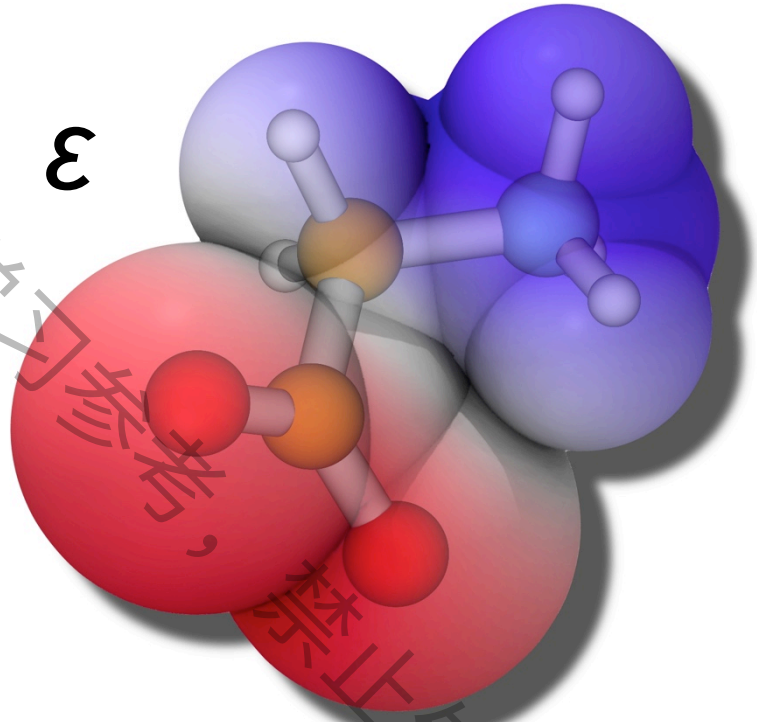
MD: Boundary condition

2. Finite boundary (ε)
   (Self-Consistent Reaction Field, SCRF)



MD: Solvation

ε



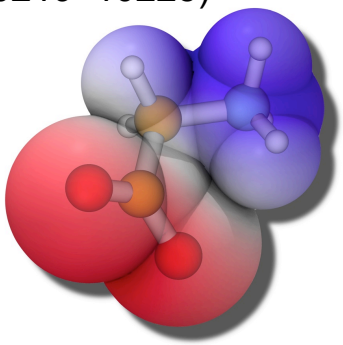
A_{SAS} is the **solvent-accessible surface area.**

$$F_{\mathrm{nonelec}}(\mathbf{r}^N) = F_{\mathrm{vdW}} + F_{\mathrm{cav}}$$
$$\approx \gamma A_{\mathrm{SAS}}(\mathbf{r}^N)$$

MD: Solvation models

Poisson-Boltzmann model: (D. Bashford & M. Karplus, *Biochemistry* **1990**, *29*, 10219–10225)

$$\nabla \cdot \left(\varepsilon(\boldsymbol{r}) \nabla \phi \right) - \kappa \varepsilon(r) \sinh\left(\phi \right) = 4\pi \rho_0(\boldsymbol{r})$$

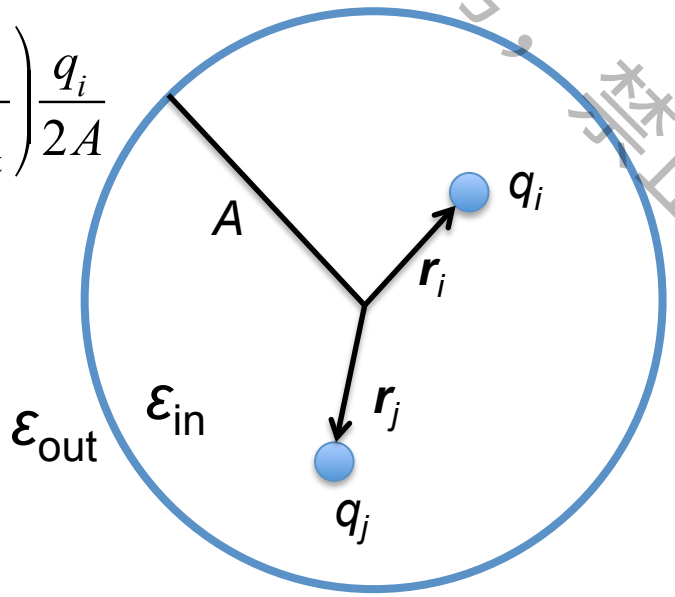


Generalized Born model: A. V. Onufriev & D. Case, *Ann. Rev. Biophys*. **2019**, *48*:275-296

$$\Delta G^{\mathrm{GB}}(R_i) = -\left(1 - \frac{1}{\varepsilon_{\mathrm{out}}}\right)\frac{q_i}{2A}$$

$$R_i = A - \frac{r_i^2}{A}$$

$\varepsilon_{\mathrm{out}}$ is small

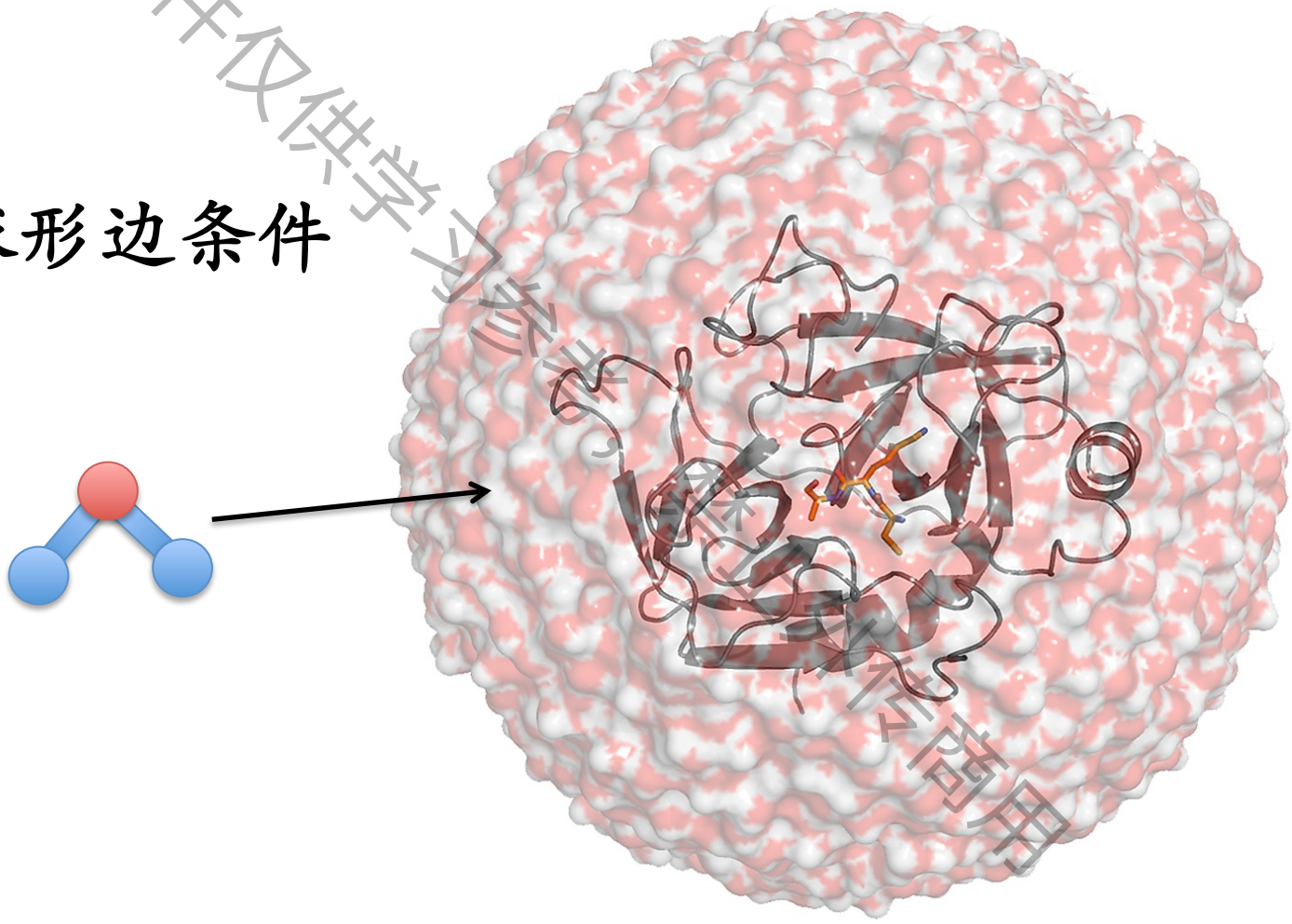


$$\Delta G^{\mathrm{GB}}(R_i) = -\frac{1}{2}\left(\frac{1}{\varepsilon_{\mathrm{in}}} - \frac{1}{\varepsilon_{\mathrm{out}}}\right)\sum_{i,j}\frac{q_i q_j}{\sqrt{r_{ij}^2 + R_i R_j}}$$

$\varepsilon_{\mathrm{out}}$ is large

MD: boundary condition

3. 球形边条件

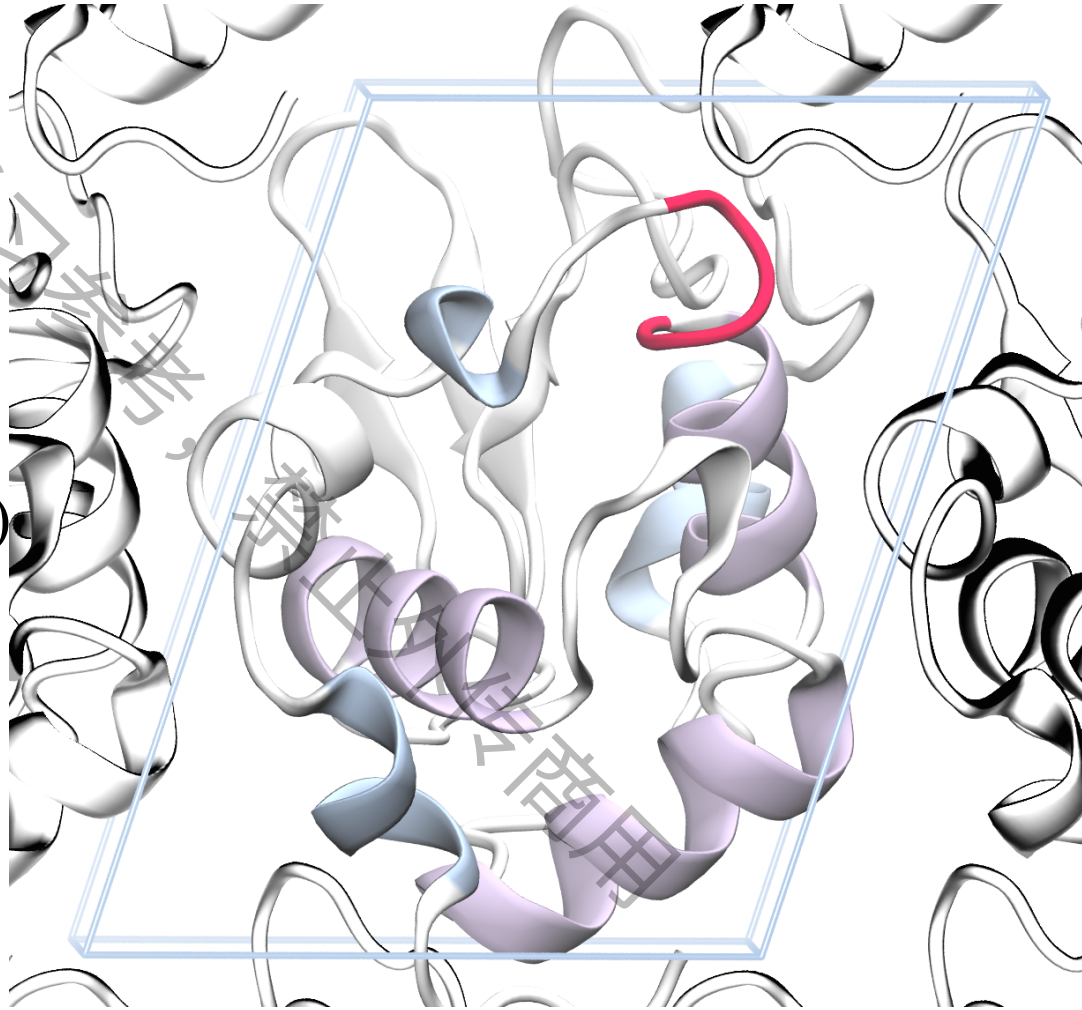


MD: PBC

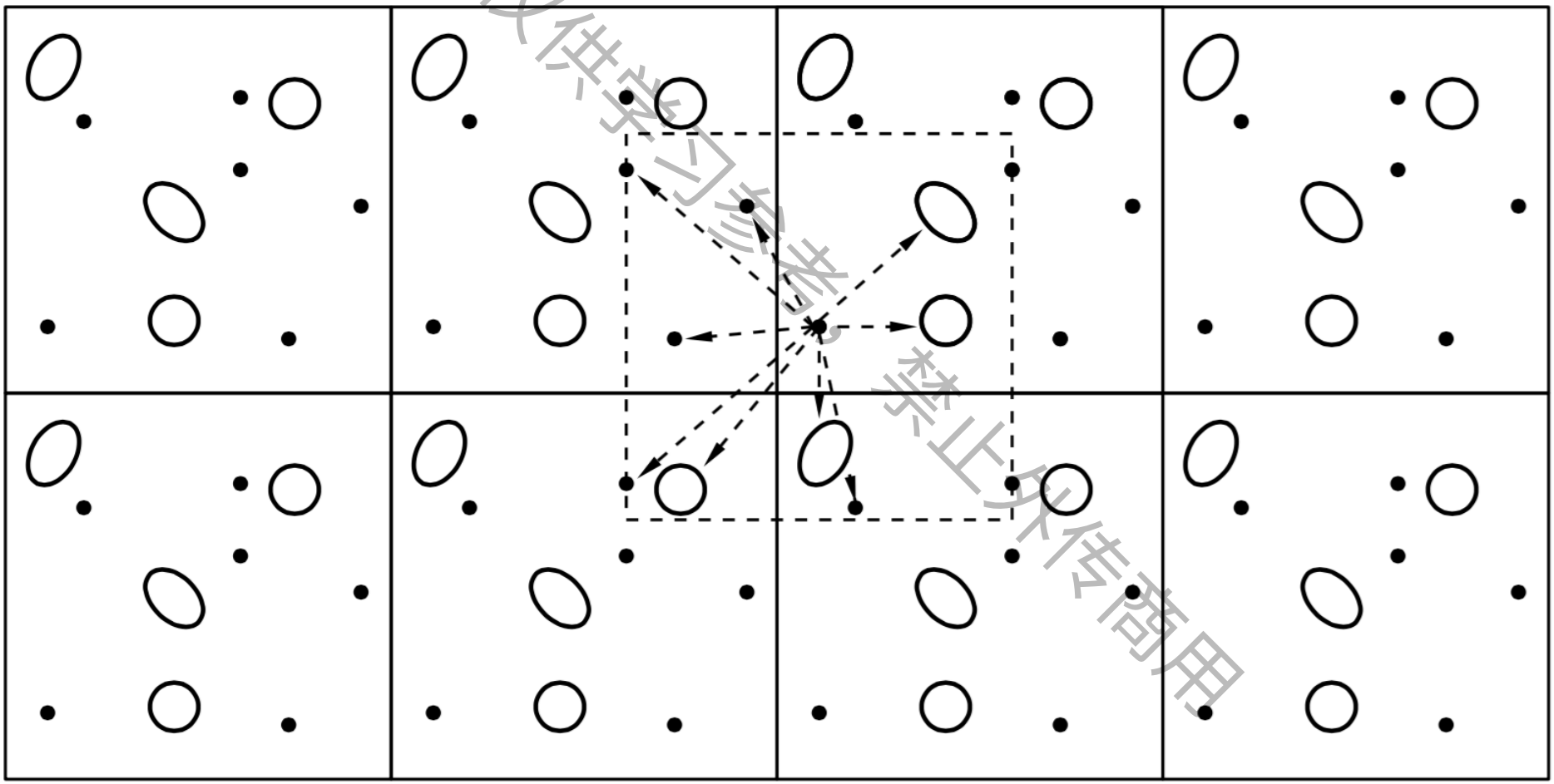
4. Periodical boundary condition (PBC)

$$\vec{F}_{PBC}(\vec{r}_i - \vec{r}_j) = \sum_n \vec{F}(\vec{r}_i - \vec{r}_j + \vec{R}_n)$$

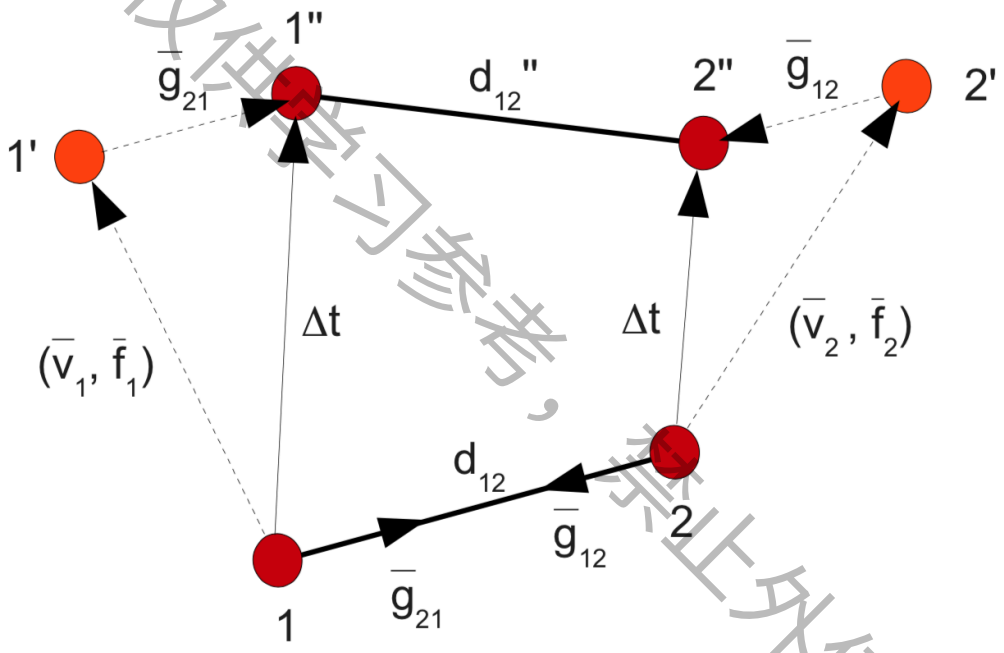
实际操作中，需截断！



PBC: least image



Constraint: SHAKE/RATTLE



Constraint: SHAKE/RATTLE

For a pair of given atoms:

$$\boldsymbol{d}_{12} = d_{12}\tilde{\boldsymbol{r}}_{12}^{0} \qquad \boldsymbol{r}_{12} = \boldsymbol{x}_2 - \boldsymbol{x}_1$$

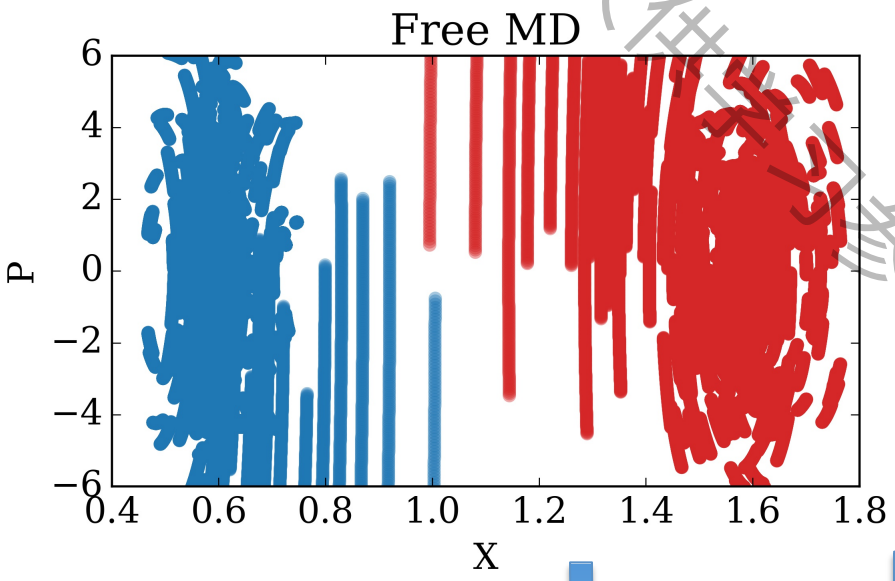
$$g_{12} = -\mu_{12}\frac{\left(r_{12}^2 - d_{12}^2\right)}{\boldsymbol{r}_{12}\cdot\boldsymbol{d}_{12}(\delta t)^2} \qquad h_{12} = -\frac{\boldsymbol{p}_{12}\cdot\boldsymbol{d}_{12}}{d_{12}^2\delta t}$$

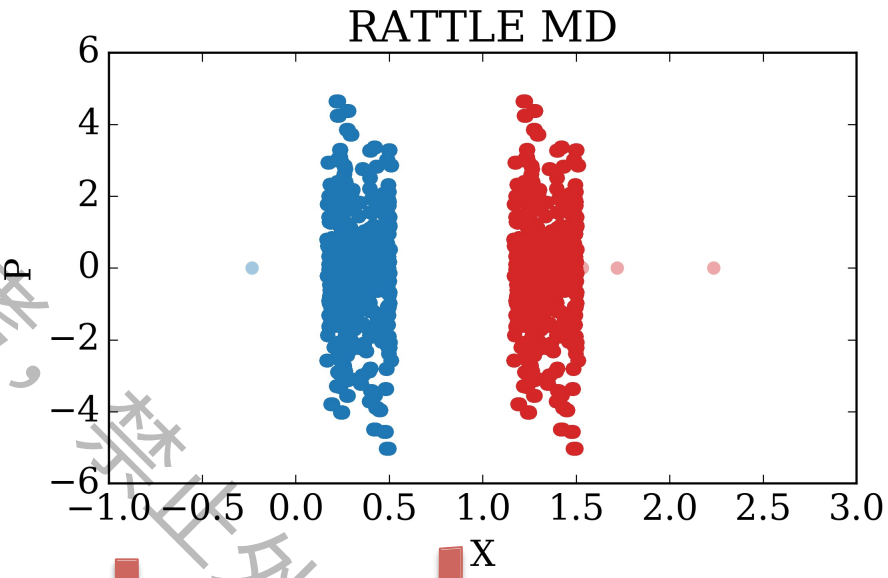
$$g_{21} = -g_{12} \qquad h_{21} = -h_{12}$$

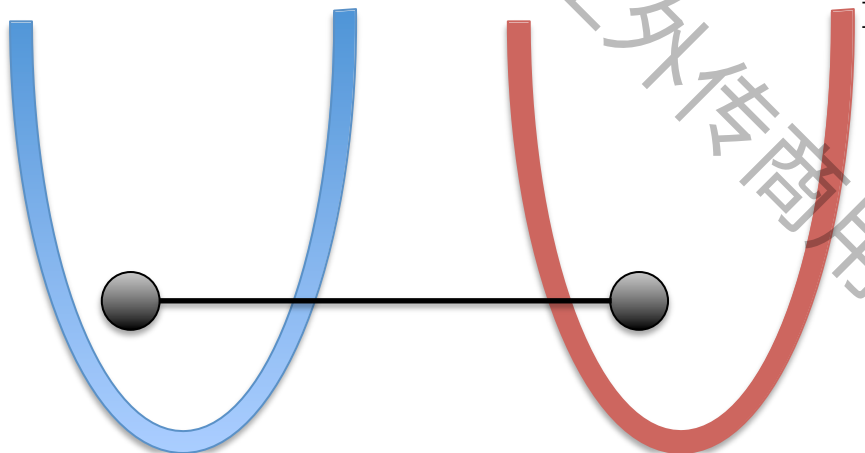
$$\boldsymbol{g}_{12} = g_{12}\boldsymbol{d}_{12} \qquad \boldsymbol{h}_{12} = h_{12}\boldsymbol{d}_{12}$$

$$\boldsymbol{x}_1 = \boldsymbol{x}_1^0 + \boldsymbol{g}_{21}\frac{(\delta t)^2}{2\mu_{12}} \qquad \boldsymbol{p}_1 = \boldsymbol{p}_1^0 + \boldsymbol{h}_{21}\frac{\delta t}{2}$$

$$\boldsymbol{x}_2 = \boldsymbol{x}_2^0 + \boldsymbol{g}_{12}\frac{(\delta t)^2}{2\mu_{12}} \qquad \boldsymbol{p}_2 = \boldsymbol{p}_2^0 + \boldsymbol{h}_{12}\frac{\delta t}{2}$$







```
for istep in range(Nstep):

    x1, x2, p1, p2 = Verlet_step2(x1_init, x2_init, p1_init,p2_init, dt, mass)

    ##### Andersen thermostat.
    if istep % N_andersen == 0:
        p1 = init_p(Temperature) ##### Regenerate new momenta after the Andersen time interval.
        p2 = init_p(Temperature) ##### Regenerate new momenta after the Andersen time interval.

    ##### Constraint.
    dt12 = np.subtract(x2,x1)

    g12 = - mu12 *(np.multiply(dt12,dt12) - np.multiply(d12,d12))/(np.multiply(d12, dt12)*dt**2)
    gf12 = g12*d12
    gf21 = -gf12

    x1 = x1 + gf21*dt**2/(2.0E0*mass) #### New x1 after constraint.
    x2 = x2 + gf12*dt**2/(2.0E0*mass) #### New x2 after constraint.

    p12 = np.subtract(p2,p1)
    h12 = -np.multiply(p12,d12)/(d12**2*dt)
    h21 = -h12

    p1 = p1 + h21*dt/2.0E0 #### New p1 after constraint.
    p2 = p2 + h12*dt/2.0E0 #### New p2 after constraint.

    #####

    x1_init=x1
    x2_init=x2
    p1_init=p1
    p2_init=p2
```

Exercise:

1. How many seconds of the 1 a.u. time? If in femtosecond, how large is it?

2. In our example code, how large the Δt should be?