前沿化学实验13——理论与计算化学

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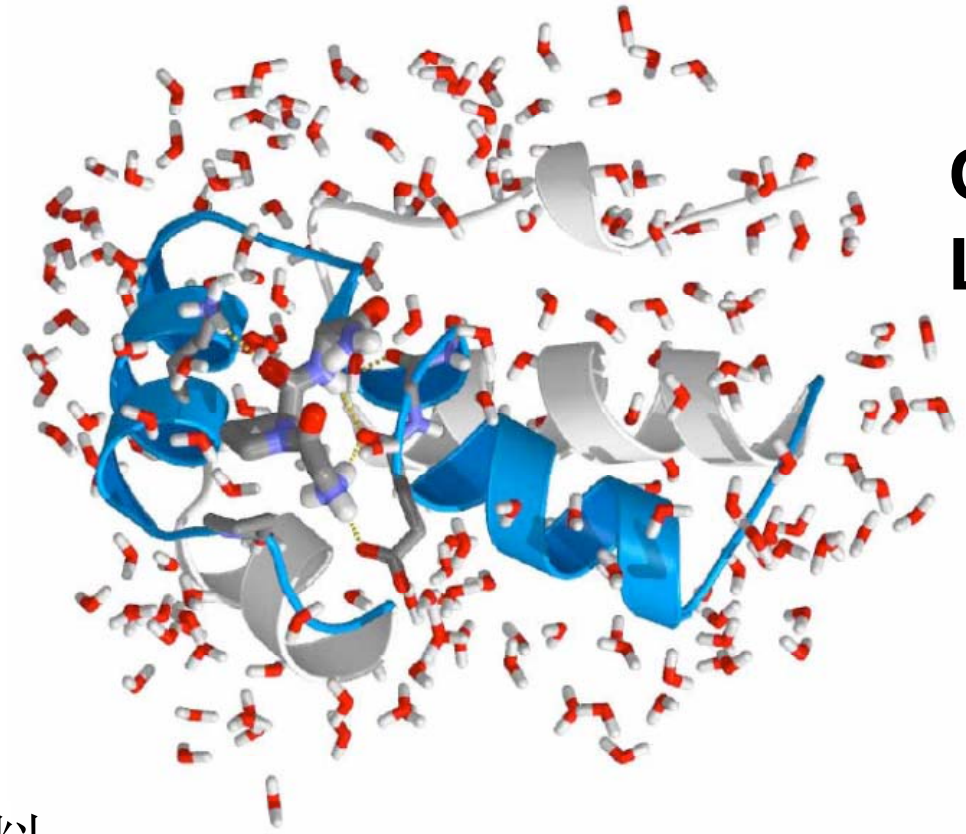
中国科学院大学前沿化学实验，2020.9.25

3. 分子动力学模拟简介

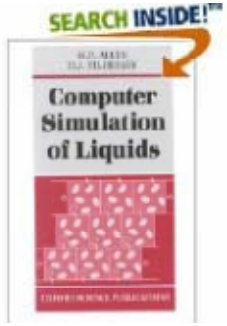


Gromacs Logo

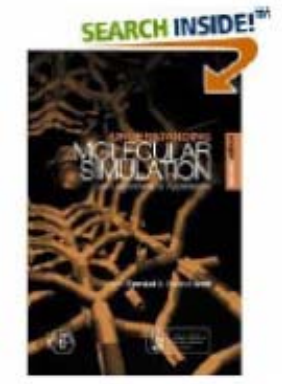
主要参考资料：

Emppu Salonen Helsinki University of Technology
Molecular Dynamics Simulation - Michel Cuendet - EMBL 2008

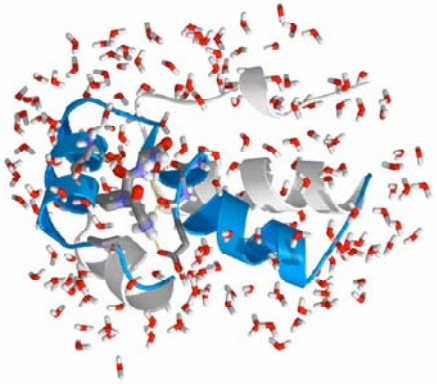
参考书目



M. P. Allen and D. J. Tildesley, Computer Simulation of Liquids
(Clarendon Press, Oxford, 1987)

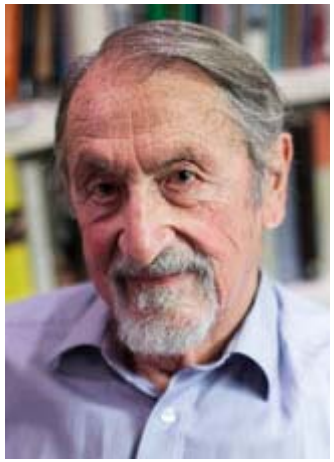


D. Frenkel and B. Smit, Understanding Molecular Simulation
(Academic Press, San Diego, 2002)



Gromacs User Manual

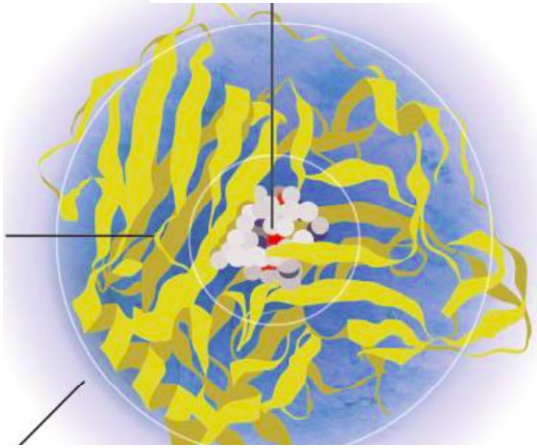
2013诺贝尔化学奖：分子动力学模拟，多尺度模型



Martin Karplus Michael Levitt Arieh Warshel

量子力学

经典力学

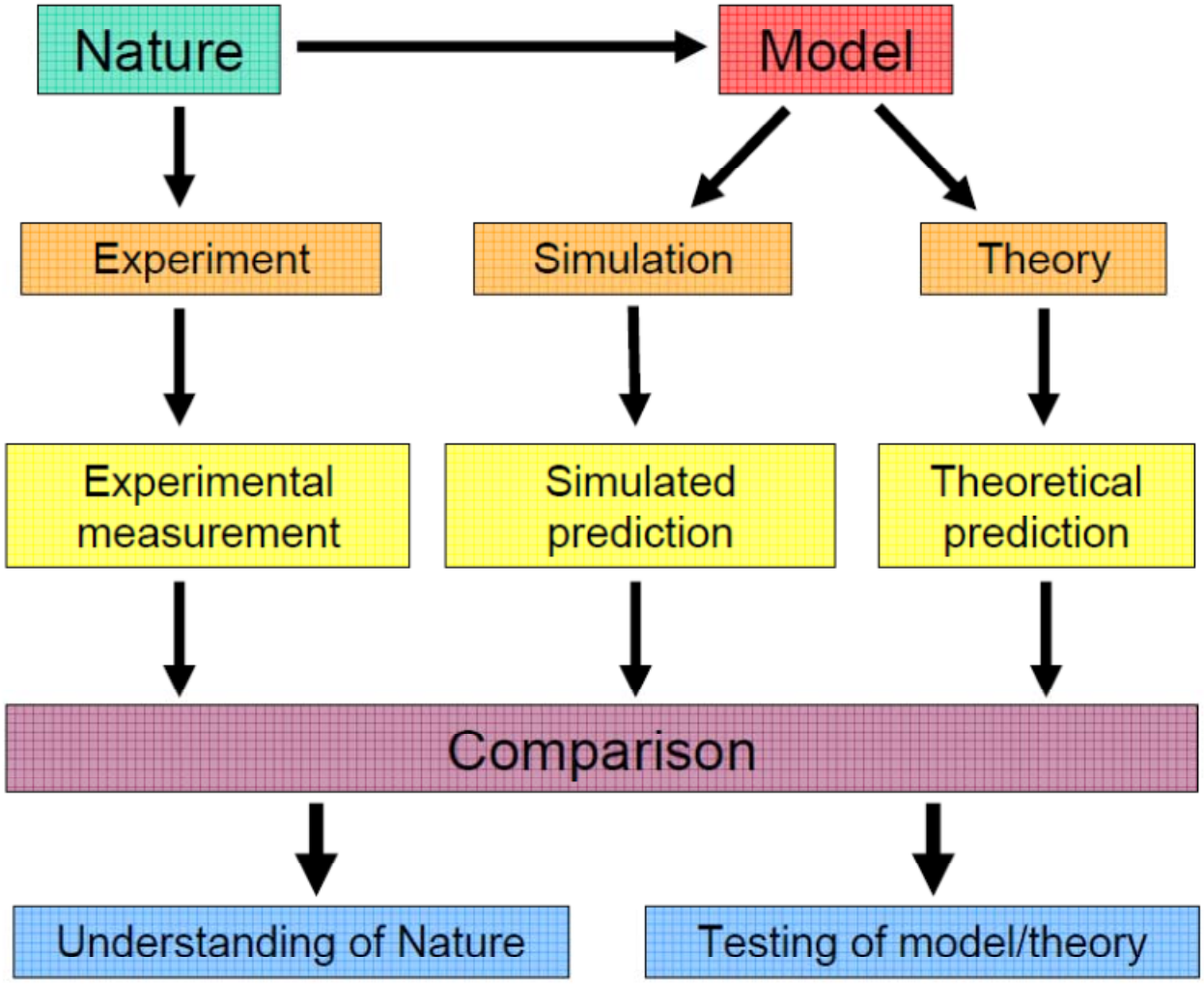


连续介质模型

“发展了用于研究复杂化学体系的多尺度模型”

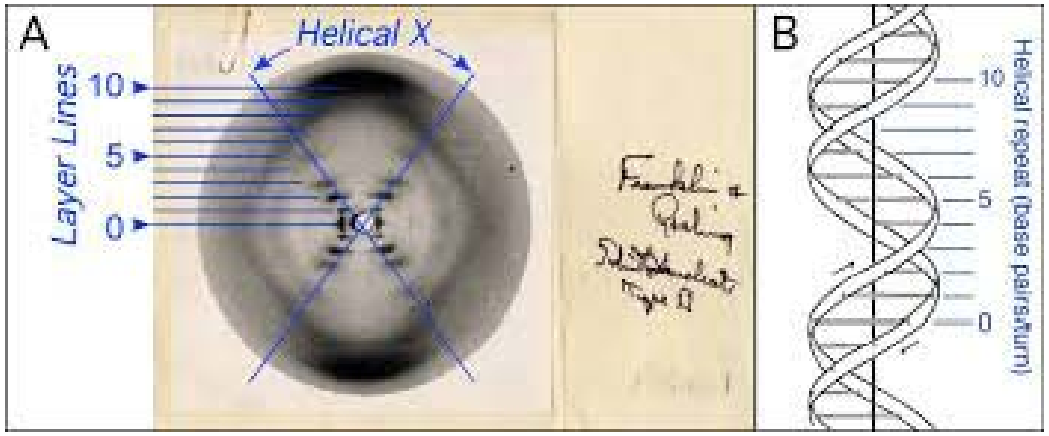
“这些在计算机上进行的实验极大地加深了人们对化学过程的认识”

理论模型的作用

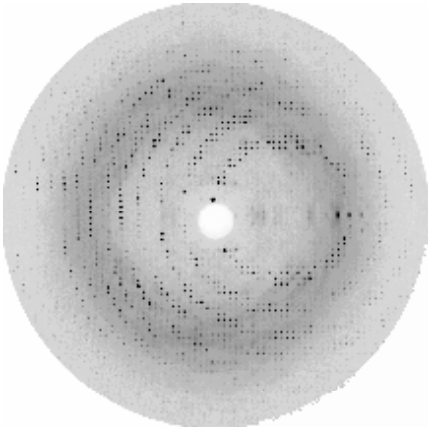


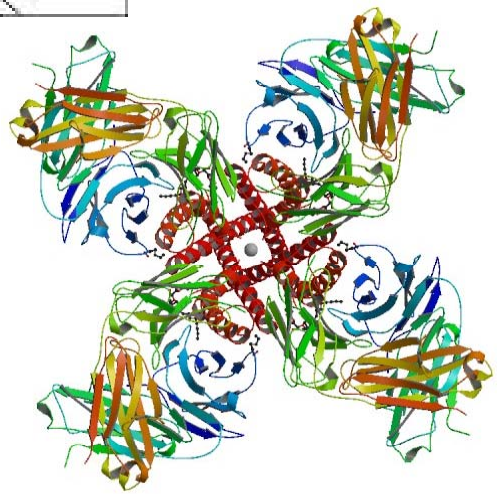
好的理论模型对于认识和预测实验现象作用巨大

例子：X射线衍射



DNA Structure, 1962 Nobel Prize in Physiology or Medicine





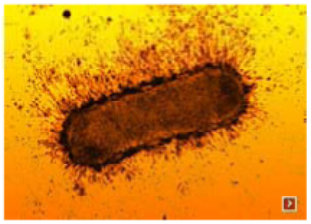
R. MacKinnon, 2002 Nobel Prize in Chemistry

背后的理论化学模型：力场模型、结构优化

时间与空间尺度

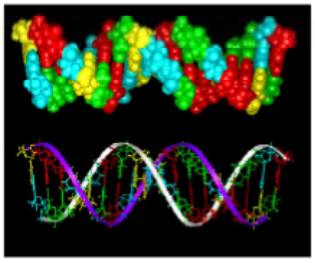
Macroscale

- Time > 1 *s*
- Lengthscale > 1μ
- Phase field models, FEM



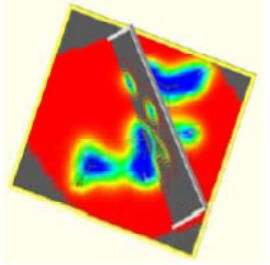
Mesoscale

- Time ~ 10^{-8} – 10^{-2} *s*
- Lengthscale ~ 10-1000 nm
- DPD, coarse-graining



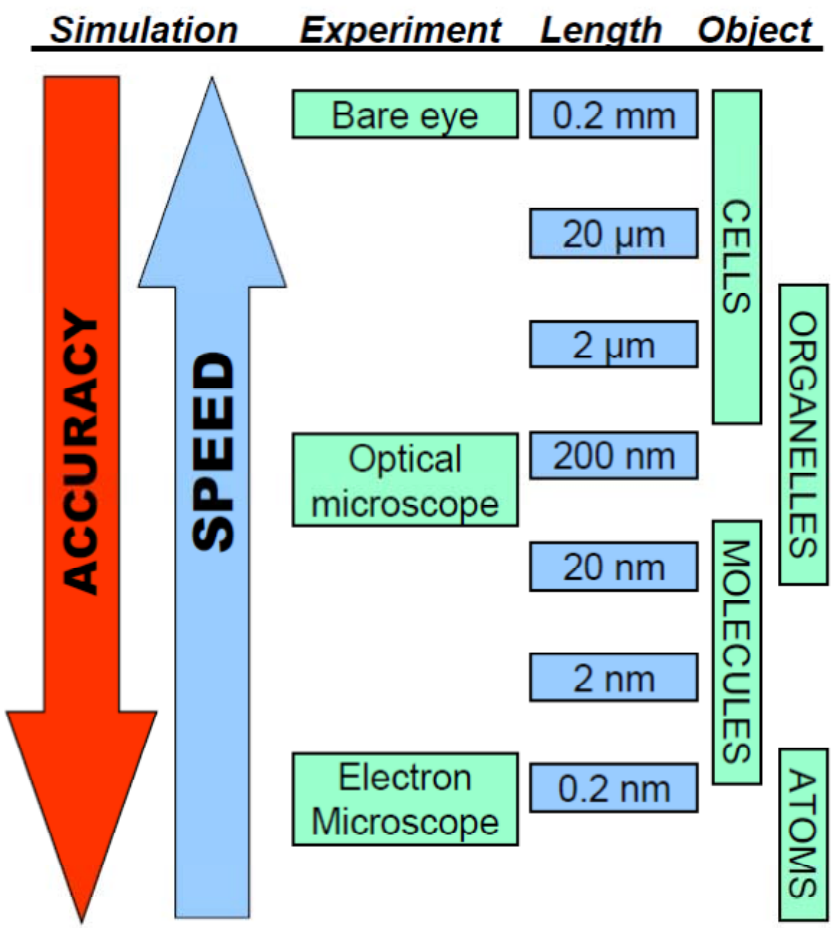
Nanoscale

- Time ~ 10^{-15} – 10^{-9} *s*
- Lengthscale ~ 0.1 - 10 nm
- Molecular dynamics, Monte Carlo



Subatomic scale

- Electronic structures
- *Ab initio*



所有模拟都是精度和计算可行性的折中

经典还是量子动力学

1. polypeptide folding
2. biomolecular association
3. partitioning between solvents
4. membrane/micelle formation

} *thermodynamic equilibria governed by weak (non-bonded) forces*

5. chemical reactions, enzyme catalysis
6. enzyme catalysis
7. photochemical ractions, electron transfer

} *chemical transformations governed by strong forces*

***characteristics** (1-4)*:

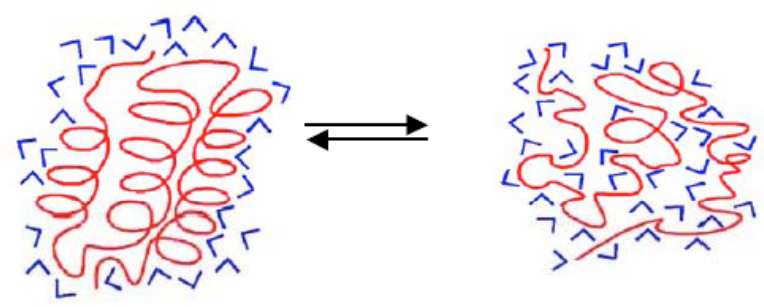
- degrees of freedom: atomic (solute + solvent) → classical MD
- equations of motion: classical dynamics
- governing theory: statistical mechanics

***characteristics** (5-7)*: → quantum MD

- degrees of freedom: electronic, nuclear
- equations of motion: quantum dynamics
- governing theory: quantum statistical mechanics

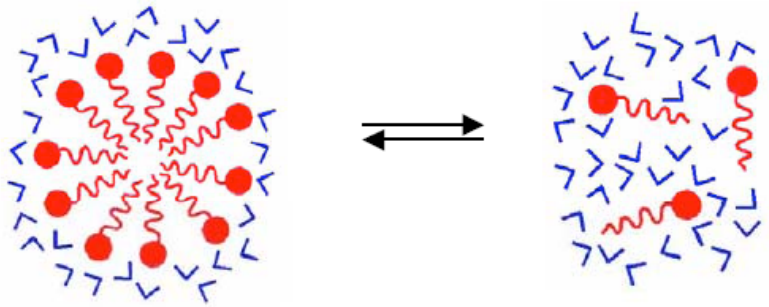
Folding

folded/native ⇌ denatured



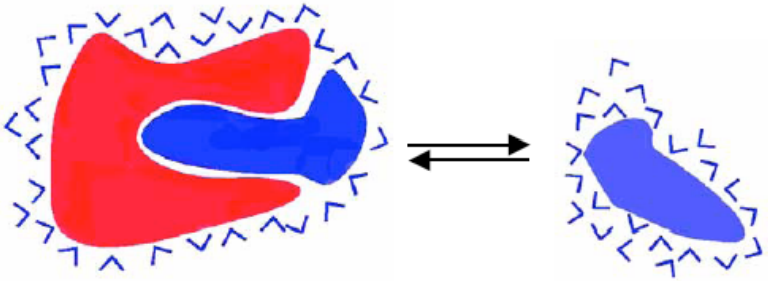
Micelle Formation

micelle ⇌ mixture



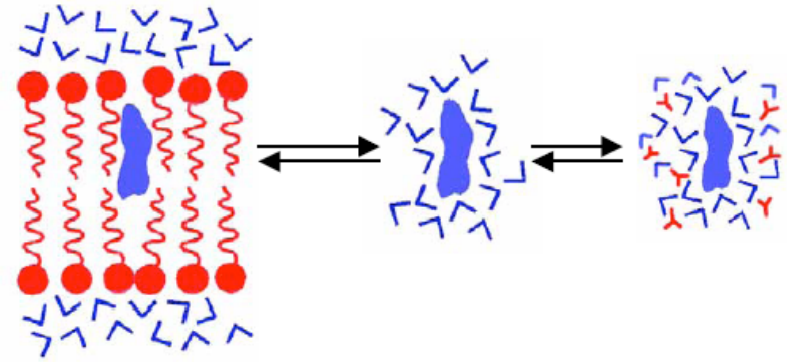
Complexation

bound ⇌ unbound

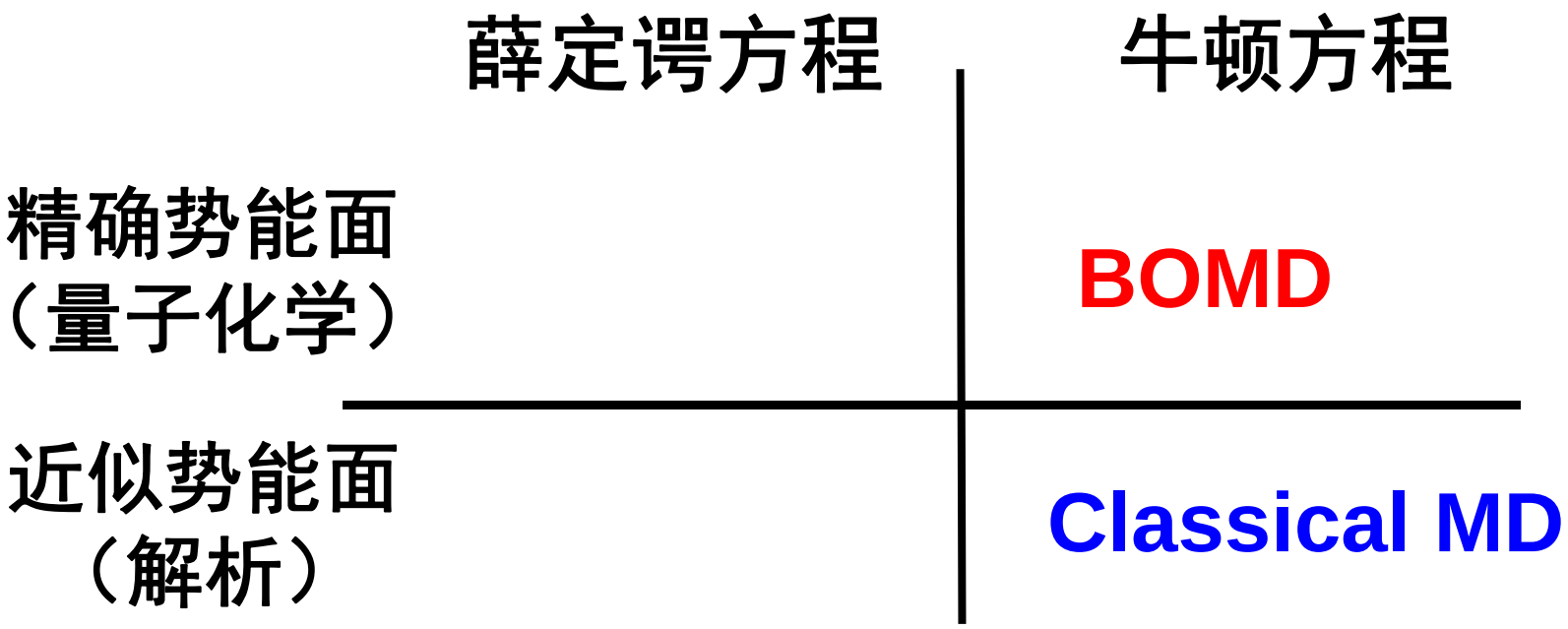


Partitioning

in membrane ⇌ in water ⇌ in mixtures



经典分子动力学模拟

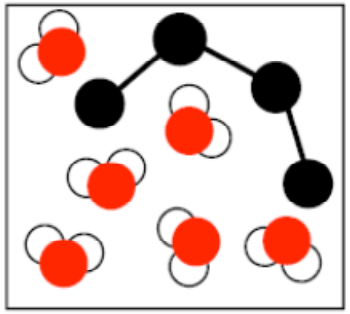


其它：QM/MM, non-adiabatic MD,…

经典分子动力学模拟的基本要素

Every molecule consists of atoms that are very strongly bound to each other

如何描述分子

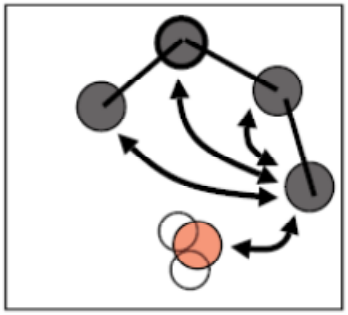


Degrees of freedom: atoms as elementary particles + topology

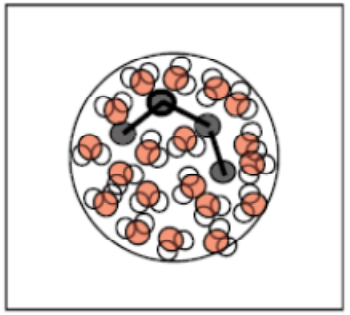
Forces or interactions between atoms

如何模拟外界条件

Boundary conditions



MOLECULAR MODEL

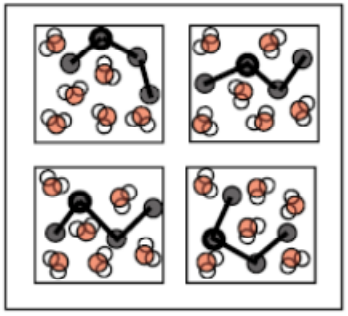


Force field = physico-chemical knowledge

相互作用

Methods to generate configurations of atoms: Newton

随时间演化



system
temperature
pressure
walls
external forces

分子模型：质点、弹簧...