Computational Simulations : molecular dynamics (MD) and DFT

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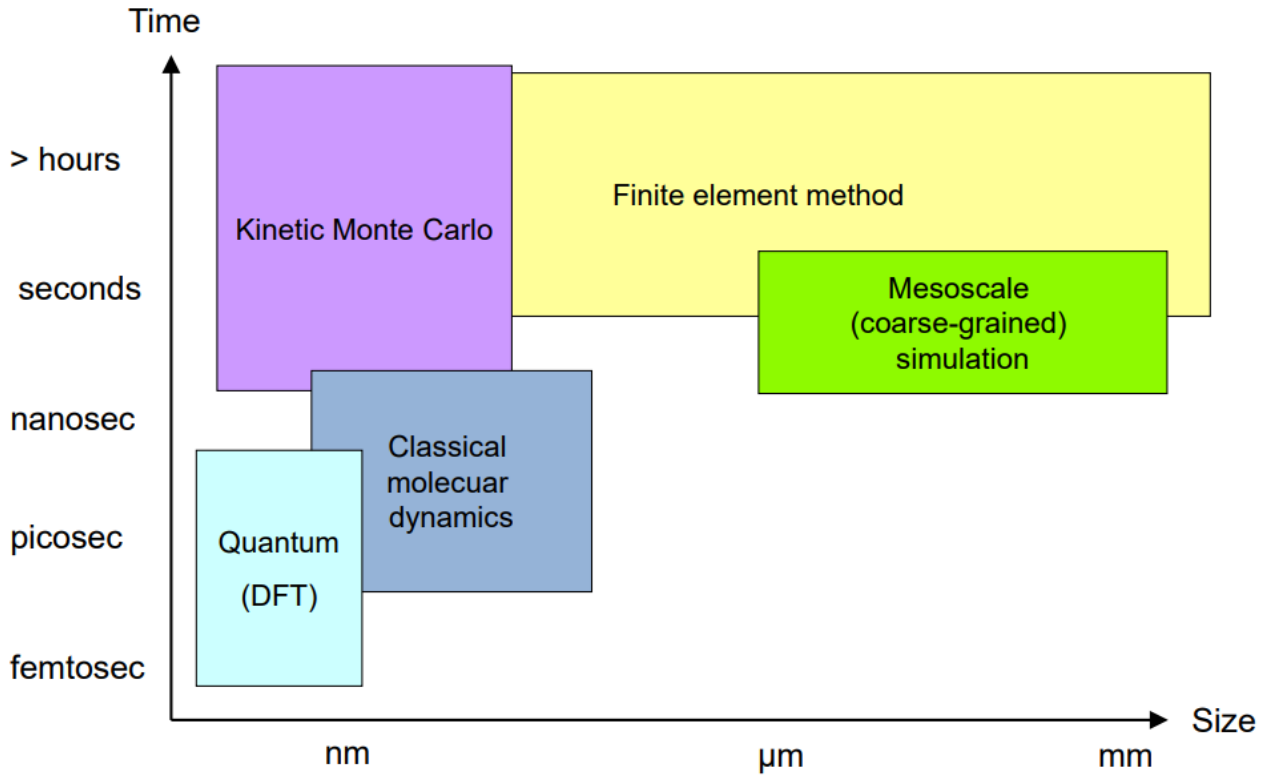
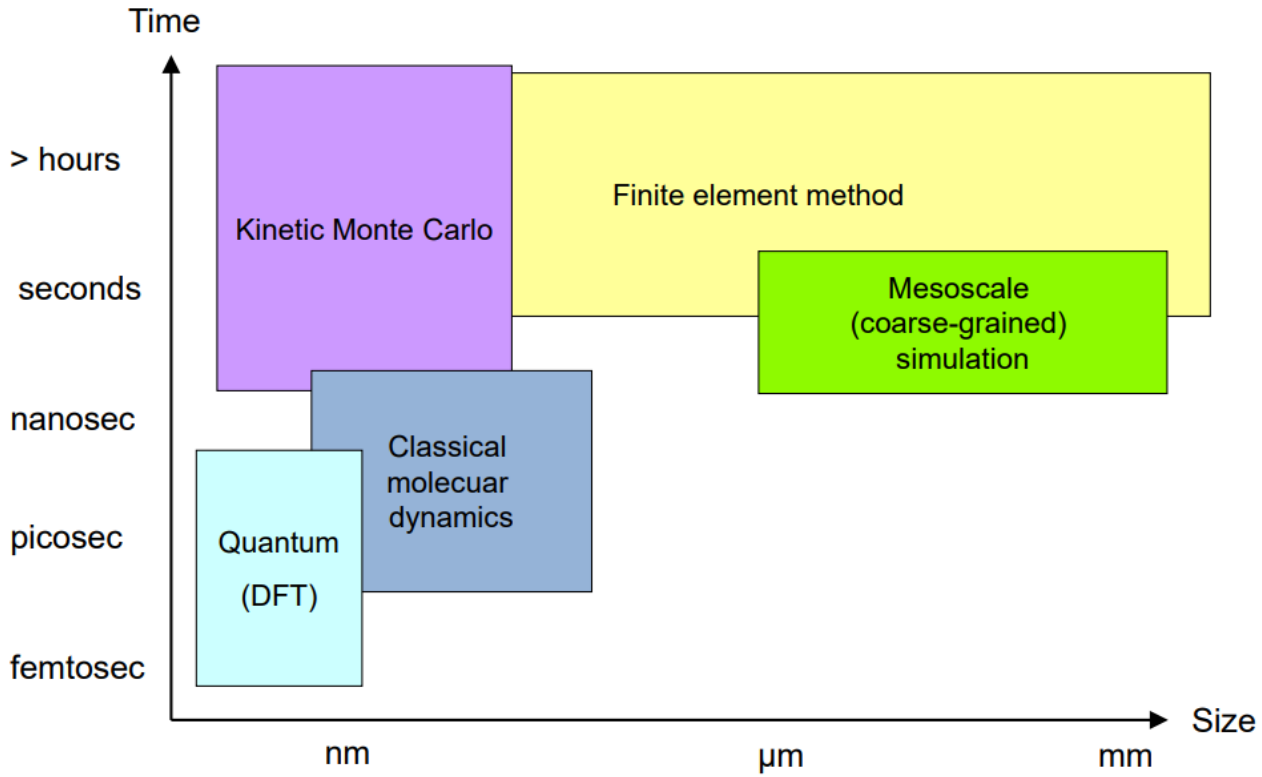
Introduction

Computational modeling



Computational materials science : analysis and prediction of mechanical, electronic, transport, growth and thermodynamics properties of materials based on the solution of basic equations for the model systems that mimic the real materials.

Computational modeling



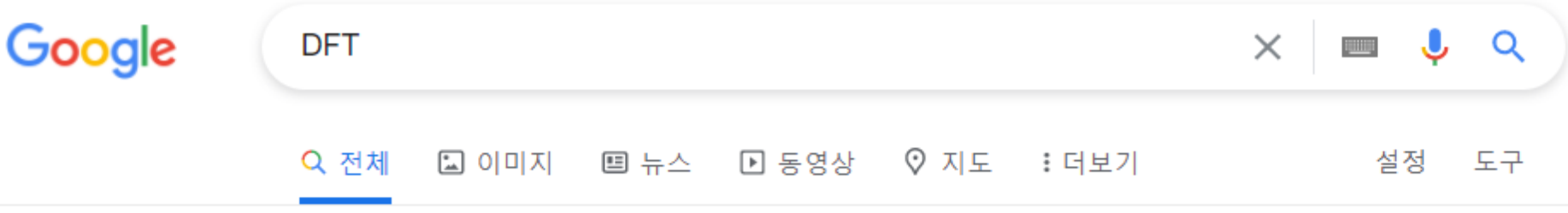
Finite element method : ex) TCAD

Classical molecular dynamics : ex) LAMMPS

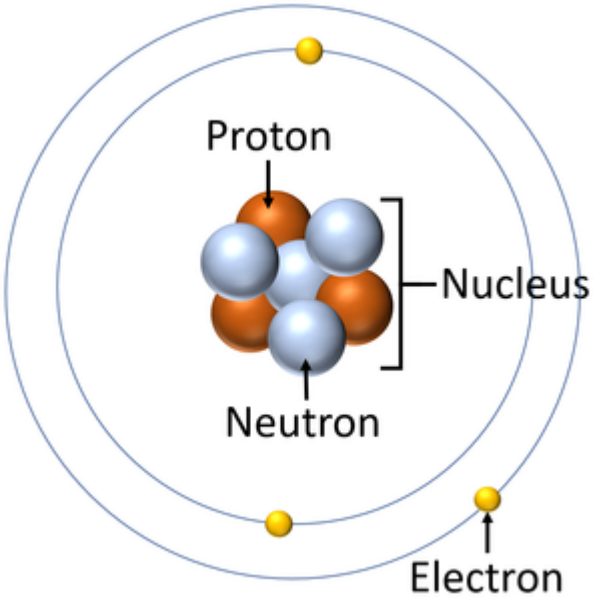
DFT : ex) VASP

Computational simulations

DFT


Google
DFT
전체
이미지
뉴스
동영상
지도
더보기
설정
도구
검색결과 약 22,800,000개 (0.46초)
https://angeloyeo.github.io › 2019/07/14 › Freq_Sampling
주파수 샘플링과 DFT - 공돌이의 수학정리노트
이다. DEFINITION: inverse Discrete Fourier Transform (iDFT). 전체 신호의 길이가 N인 이산 주파수 성분 ...
2019. 7. 14. · 업로더: 공돌이의 수학정리노트
Sampling DTFT · 예제를 통해 DFT를 조금 더... · 주파수 샘플링된 주파수 응답...
https://en.wikipedia.org › wiki › Discrete_Fourier_trans...
Discrete Fourier transform - Wikipedia
In mathematics, the discrete Fourier transform (DFT) converts a finite sequence of equally-spaced samples of a function into a same-length sequence of ...
DFT matrix · Discrete-time Fourier transform · Number-theoretic transform

DFT



https://keystagewiki.com/index.php/Electron

Schrödinger equation

Kinetic energy Potential energy Wave function

$$\left[-\frac{\hbar^2}{2m}\nabla^2+V(\mathbf{r})\right]\psi(\mathbf{r})=E\psi(\mathbf{r})$$

: Eigenvalue problem

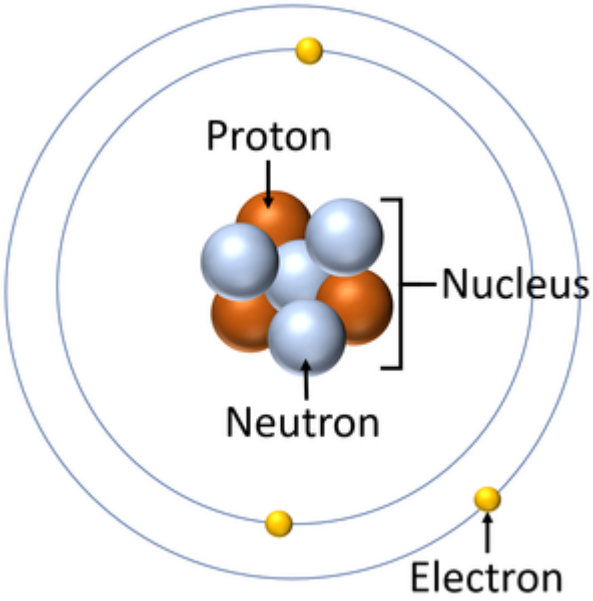
Energy

$$V(\mathbf{r})=V_{ion}(\mathbf{r})+V_H(\mathbf{r})+V_{xc}(\mathbf{r})$$

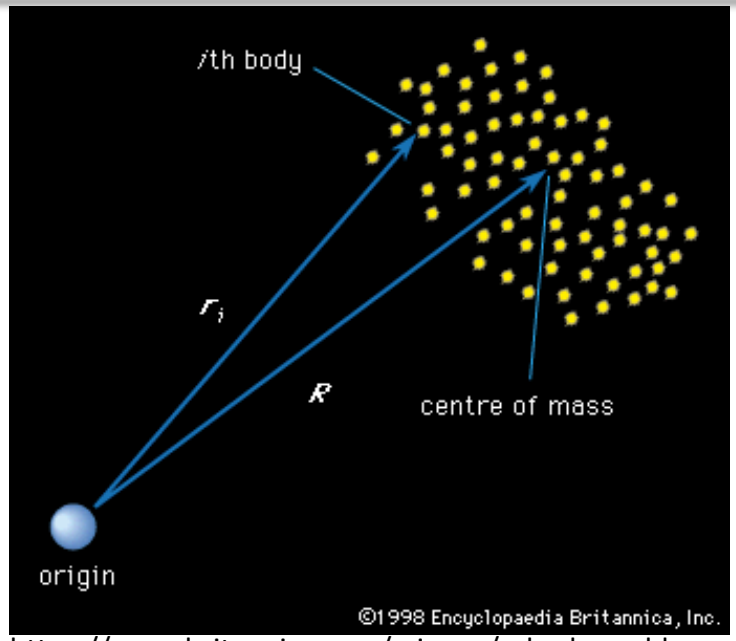
V_{ion} = Coulomb interaction between nucleus and electrons (~1/r)
V_H : Coulomb interaction between electrons
V_{xc} : exchange-correlation potential (quantum effects)

- DFT : Density Functional Theory
- A way to understand the interaction between atoms and electrons.
- Three-body problem : no general closed-form solution exists.
- Hydrogen – 1 proton and 1 electron (two body problem) for 1 single atom

DFT



https://keystagewiki.com/index.php/Electron



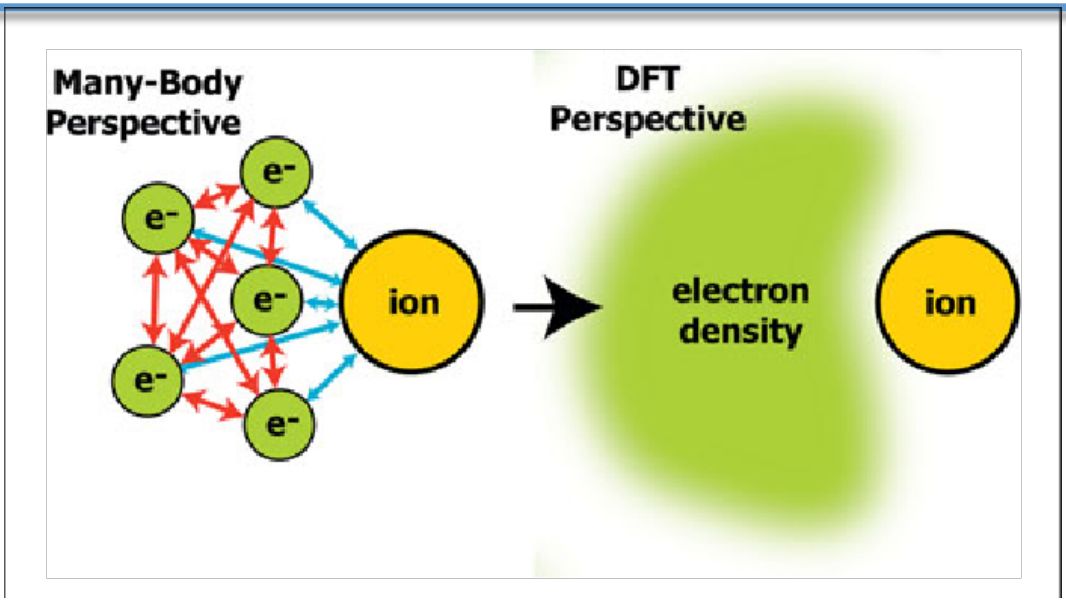
https://www.britannica.com/science/n-body-problem

- 1 mole of H? 1 mole of He? cannot be solved.

- N-body problem – wave function contains 3N degrees of freedom

-> solving Schrodinger equations becomes very difficult.

DFT



Lusk, M.T., Mattsson, A.E. High-performance computing for materials design to advance energy science. *MRS Bulletin* **36,** 169–174 (2011).

- Key concepts of DFT : consider many electrons as electron density.
- Using electron density ρ(r) instead of wave function are attractive.
- By this method, we can understand the properties of a system.

MD

- MD : molecular dynamics
- Numerical method for studying many-particle systems such as molecules, clusters.
- Basic idea of molecular dynamics : solution of Newton's equations of motion for individual particles (atoms, ions, …)
- Interaction between atoms and molecules results from electronic structure – requires quantum physics
- Two different types of MD – classical MD and ab-initio MD

MD

	Classical MD	Ab-initio MD
Accuracy	Low	High
Speed	Fast (time scale : ~ns)	Slow (time scale : ~ps, fs)
Computational cost	Low	High
System size	Large particle numbers	Small particle numbers

- Both methods have pros and cons.

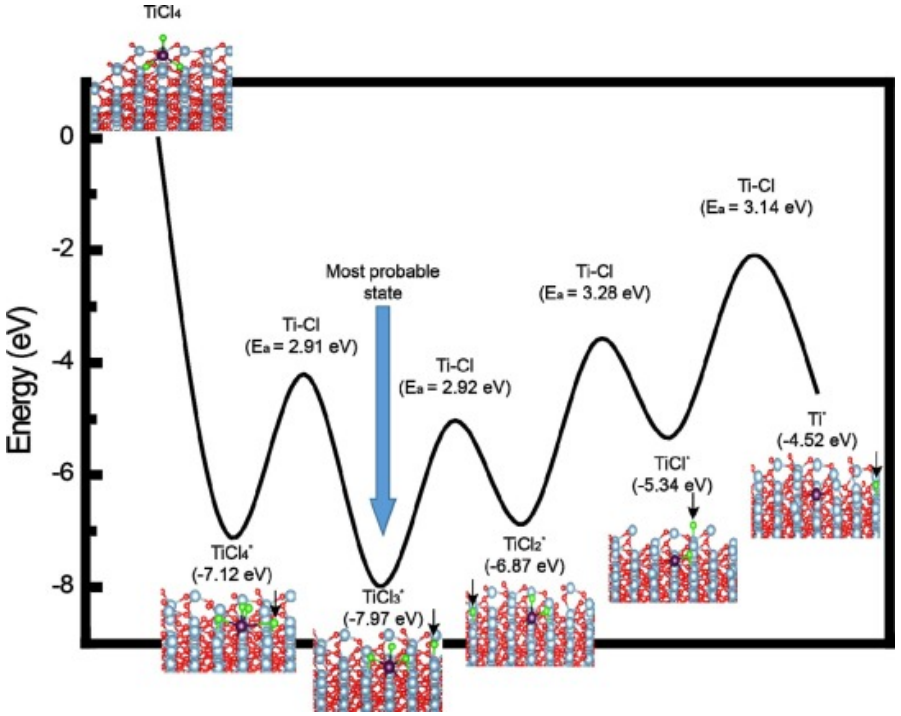
- Some ways to get the advantages of both methods are ongoing.

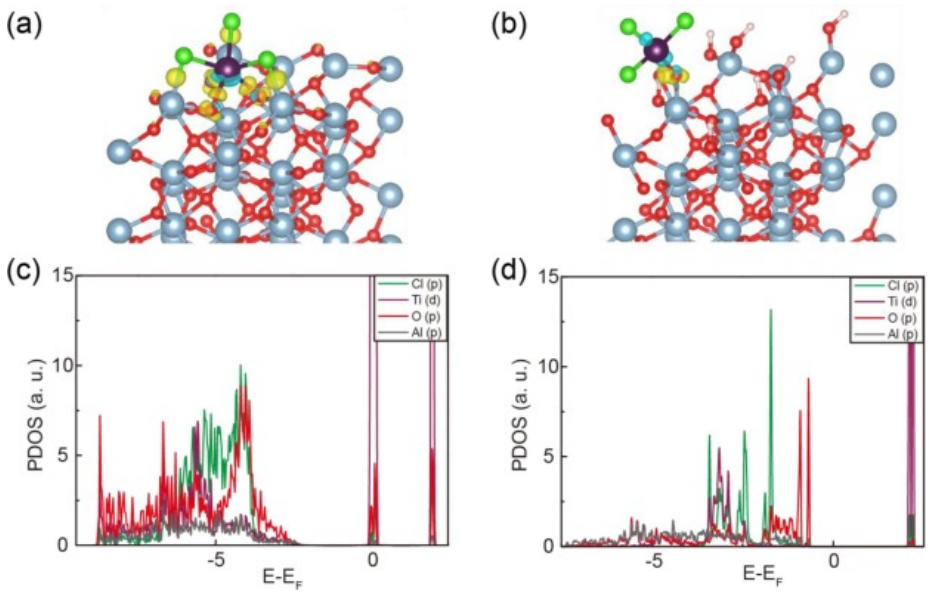
Ex) developing classical potentials that precisely describe the simulation (Reactive force field, etc).

Apply

Apply

- Describe stable state – can expect whether this state is stable or not.
- Can calculate energy – surface energy, defect formation energy, binding energy, activation energy, …
- Can see charge density, density of state (DOS).

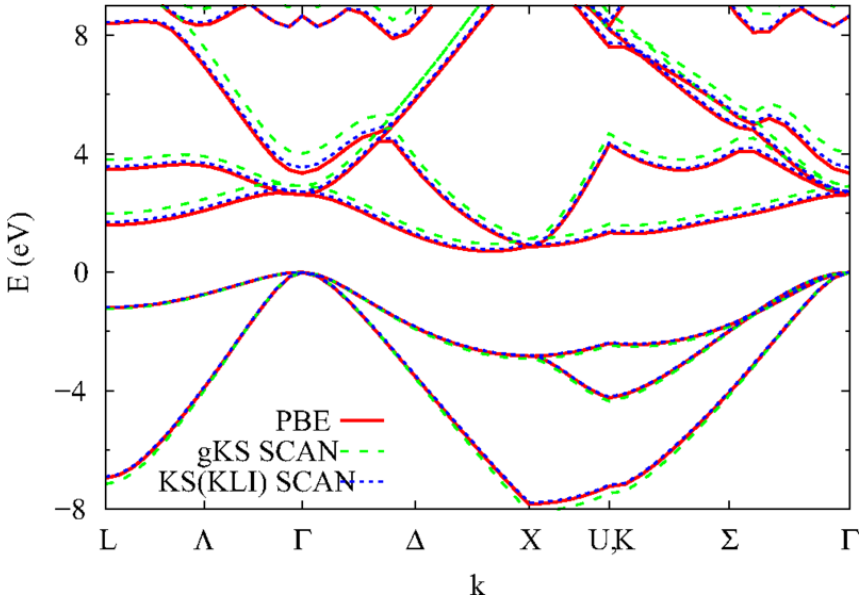




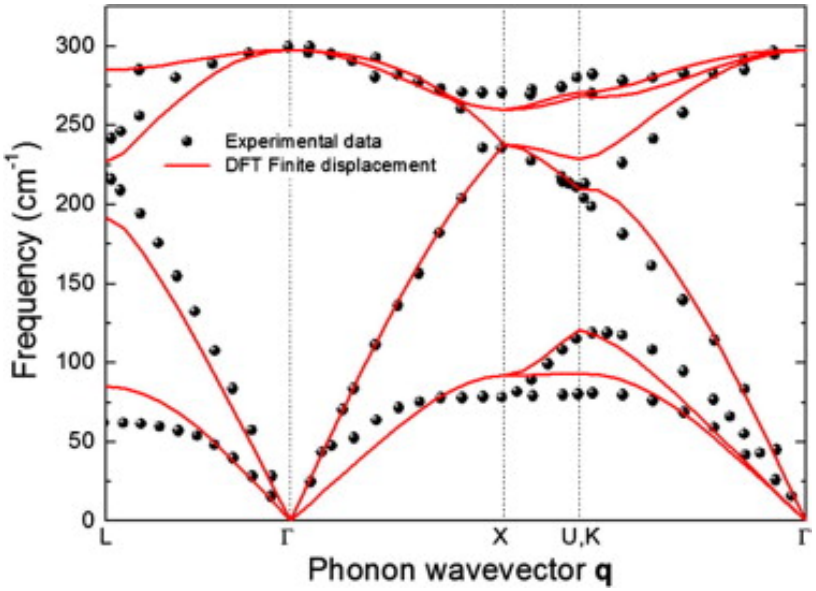
Woojin Choi et al., Applied Surface Science, 551, 149391 (2021)

Apply

- Calculate band structure – electronic band of a material.
- Calculate phonon (can be experimentally observed by Raman)



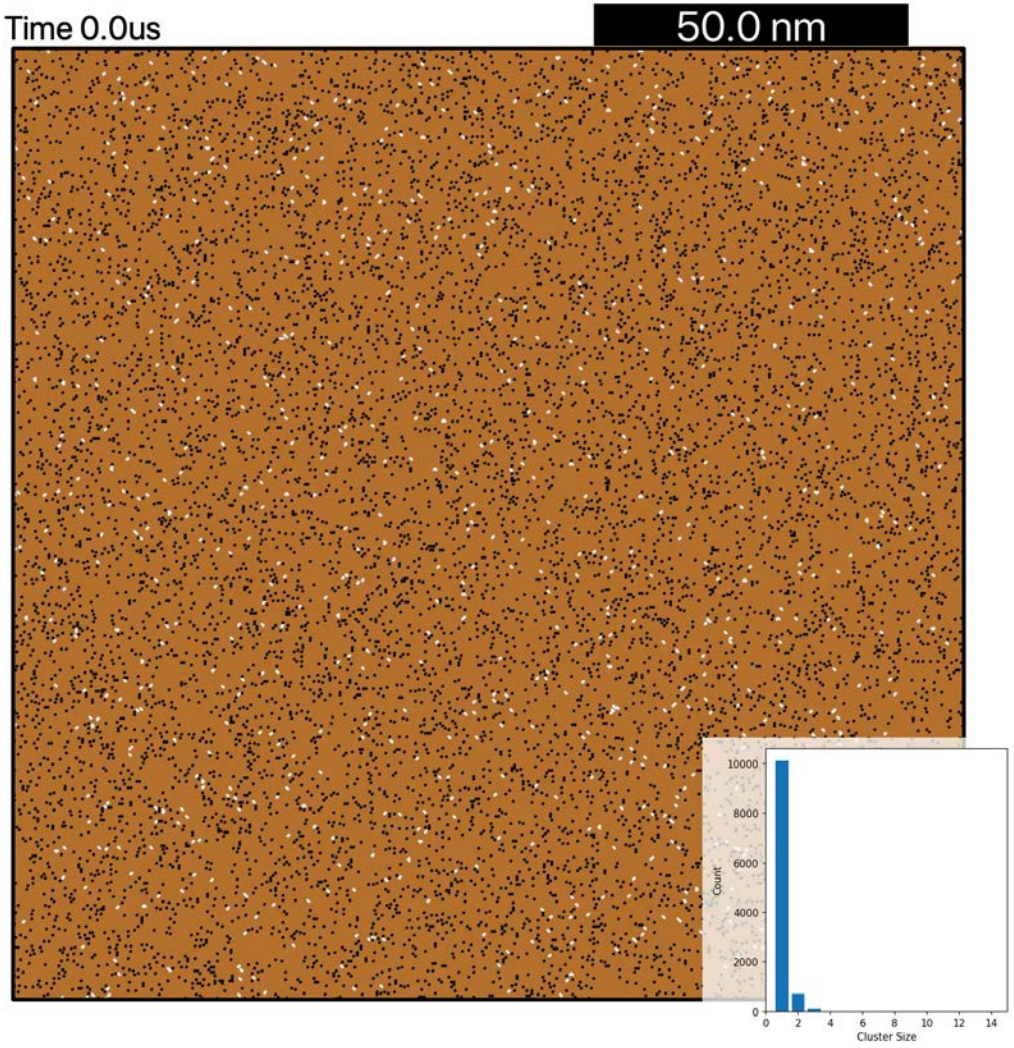
Zeng-hui Yang, Haowei Peng, Jianwei Sun, and John P. Perdew, Phys. Rev. B **93**, 205205 (2016)



A. Trejo et al., Microelectronic Engineering, 90, 141-144 (2012)

Apply

- See what happen to the atoms!



https://lammps.sandia.gov/movies.html#hyperdynamics

Limitations

- Computational cost – needs clusters to calculate
- Limitation of size and time scale – up to μm and ns scale(differs with simulation techniques)
- Classical MD – fast and can calculate large cell, but not precise and need to develop potentials that fit with specific material.
- Ab initio MD – precise but slow, need high computational cost, timescale is small(to calculate ns, you may need 10^6 or more steps)
- DFT tends to underestimate bandgap – some techniques need to be added to accurately calculate bandgap.
- There are many fields that are still unknown by using DFT and MD (ex calculating activation energy of a process with proton and electron is not yet developed - $H^+ + e^-$).

Summary

- ✓ DFT and MD – computational simulation techniques to understand what happens under nanometer scale.
- ✓ DFT – using electron density to easily solve N-body problem.
- ✓ MD – solving Newton's equations of motion.
- ✓ Can calculate energetics, band structure, phonon, DOS, …
- ✓ Computational simulations is a powerful tool, but also has limitations.

Thank you for listening