2025 Fall Computational Physics II

Lecture 1

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Instructor

- **Prof. Young Woo Choi**
  - Computational condensed matter physics
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  - Office: F303C
  - If you need any assistance, feel free to send an email.

Tell me about your experience

- We have 15 undergraduates.

- I want to adjust the level of the course to make it appropriate for the majority of students.

- Let’s gauge your your experience with:
  - Programming (python, others)
  - Physics
  - AI tools (ChatGPT, Grok, Copilot, etc.)

Course Overview

- Using computers to get numerical solutions for physics problems too complex to solve analytically
- Goal: **understand physics**, not just code

Computational

Numerical methods:
calculus, ODE/PDEs, linear algebra, Monte Carlo, …

Programming (AI-assisted):
Python, fortran, C++
OpenMP(multi-thread), MPI(multi-process), GPU

Physics

Schrödinger’s equation
Band structure calculation
Density functional theory (DFT)
Quantum many-body problem, …

Course Format

- Not a one-way lecture.

- We **code together in class.**

- I will introduce the problem of the day, and we solve it step by step through coding.

AI-Assisted Tools in Computational Physics

- **Good Things:**
  - Use AI tools to speed up coding and debugging
  - Great for learning syntax and trying new approaches

- **Be Careful**:
  - AI may generate **incorrect or non-physical code**
  - Do not rely blindly, you must **understand your source code**
  - Always verify results against physical principles

Useful References

- We will not follow a specific textbook.

- Computational Physics
  - Lots of course materials are available online
  - Rutgers
    - Undergraduate: https://www.physics.rutgers.edu/~haule/488/
    - Graduate: https://www.physics.rutgers.edu/~haule/509/
  - Univ. of Houston: https://vovchenko.net/computational-physics/intro.html
  - https://compphysics.github.io/ComputationalPhysics/doc/web/course
  - https://compphysics.github.io/ComputationalPhysics2/doc/LectureNotes/_build/html/intro.html#

Useful References

- Programming
  - VSCode: https://code.visualstudio.com/
  - Python, numpy, scipy, matplotlib, jupyter

- AI tools
  - GitHub Education Pack (Copilot Pro): https://education.github.com/pack
  - Google Gemini Pro for Students: https://gemini.google/students/ (1-year free, offer ends Oct 6, 2025)

- **AI-assisted programming (ChatGPT, Copilot, etc.) is strongly encouraged, but I will uphold a higher standard for assignments and projects.**

Course Evaluation

- **In-class Presentations (90%)**
  - 1st presentation: 10-minute presentation in class on 10/10, 10/17, or 10/31.
  - 2nd presentation: 10-minute presentation in class on 11/7, 11/21, or 11/28.
  - Final presentation: 10-minute presentation in class on 12/19.

- **Participation (10%)**

- **No midterm/final exam (but, the final presentation is scheduled during the final exam week)**

Presentation Guidelines

- Topics
  - Concepts covered in class or independent computational physics projects with code demonstrations.
  - Your job is **to find a good problem** and solve it.

- Format
  - 10-minute presentation (in-class)

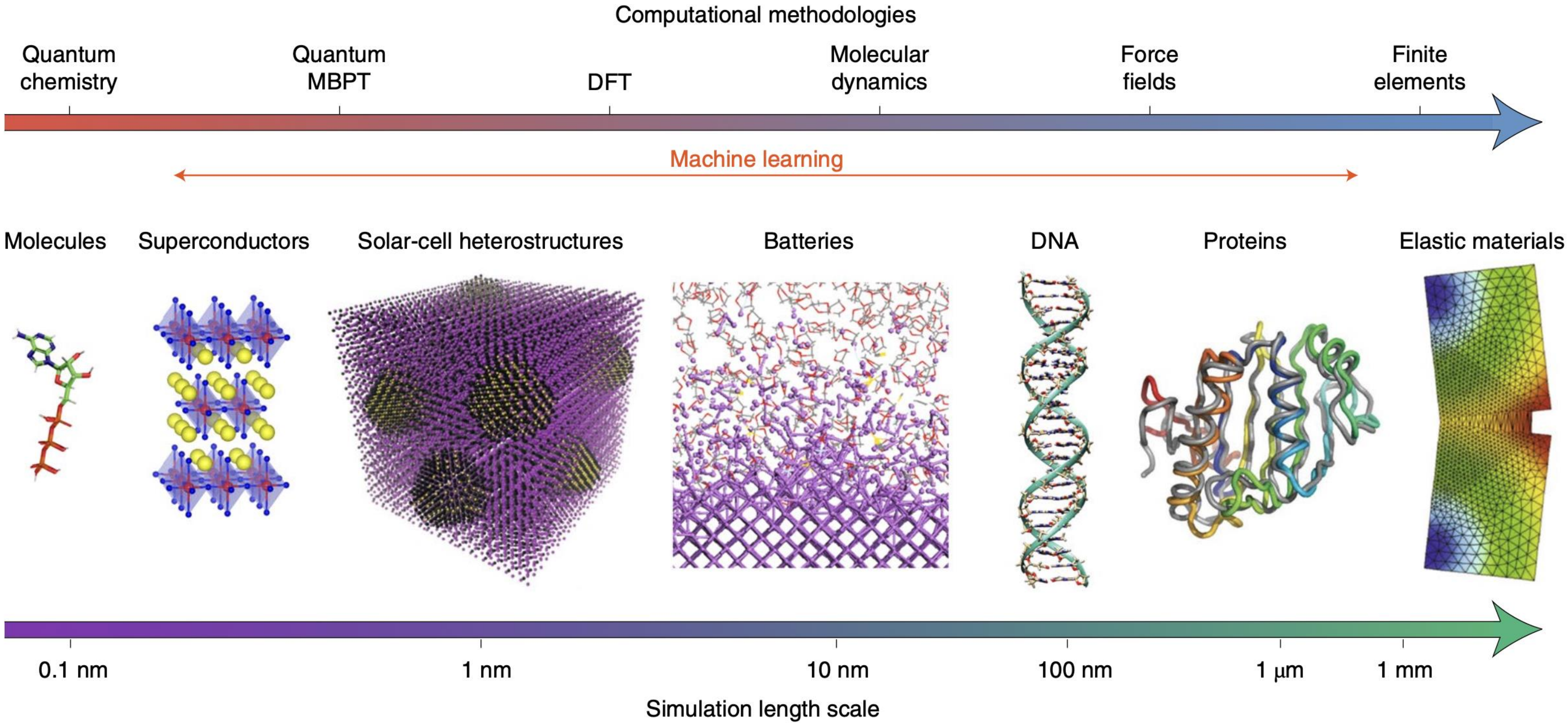
- For each presentation, the output includes
  - Presentation slides
  - Source code
  - (Final project only) Term paper

Course Schedule

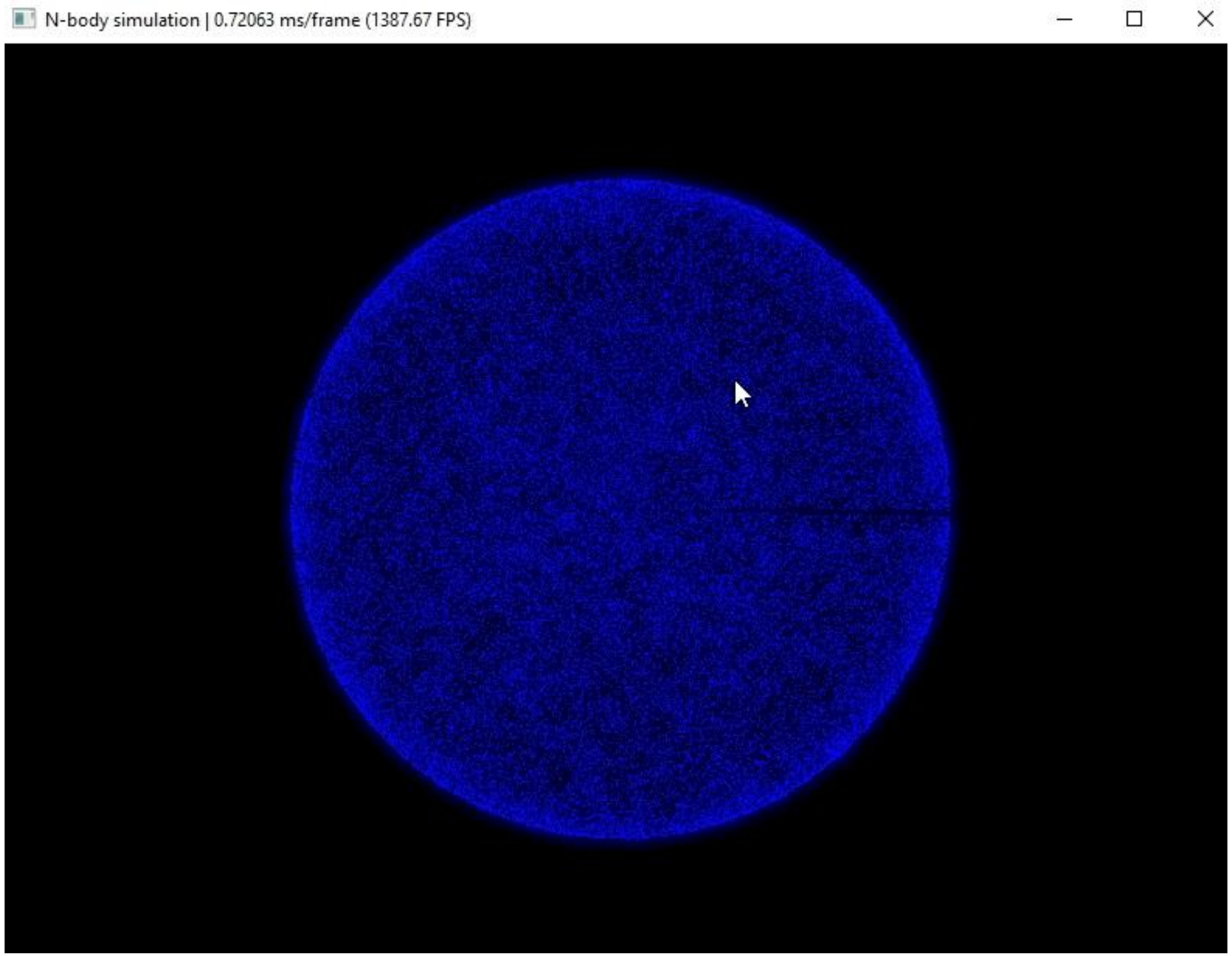
- Sep (9/5, 9/12, 9/19, 9/26)
  - Python basic, Numerical Schrödinger's equation
- Oct (10/10, 10/17, 10/31) ※ No class on 10/3
  - 1st presentation: 5 students per week
  - Band structure, density functional theory (DFT)
- Nov (11/7, 11/21, or 11/28) ※ No class on 11/14
  - 2nd presentation: 5 students per week
  - DFT, Monte Carlo, spin systems
- Dec (12/5, 12/12, 12/19)
  - 12/5 Special Seminar (1): Diana Qiu (Yale University)
  - 12/12 Special Seminar (2): Steven G. Louie (UC Berkeley)
  - 12/19 Final Presentation

Introduction

Computational Methods at Different Scales

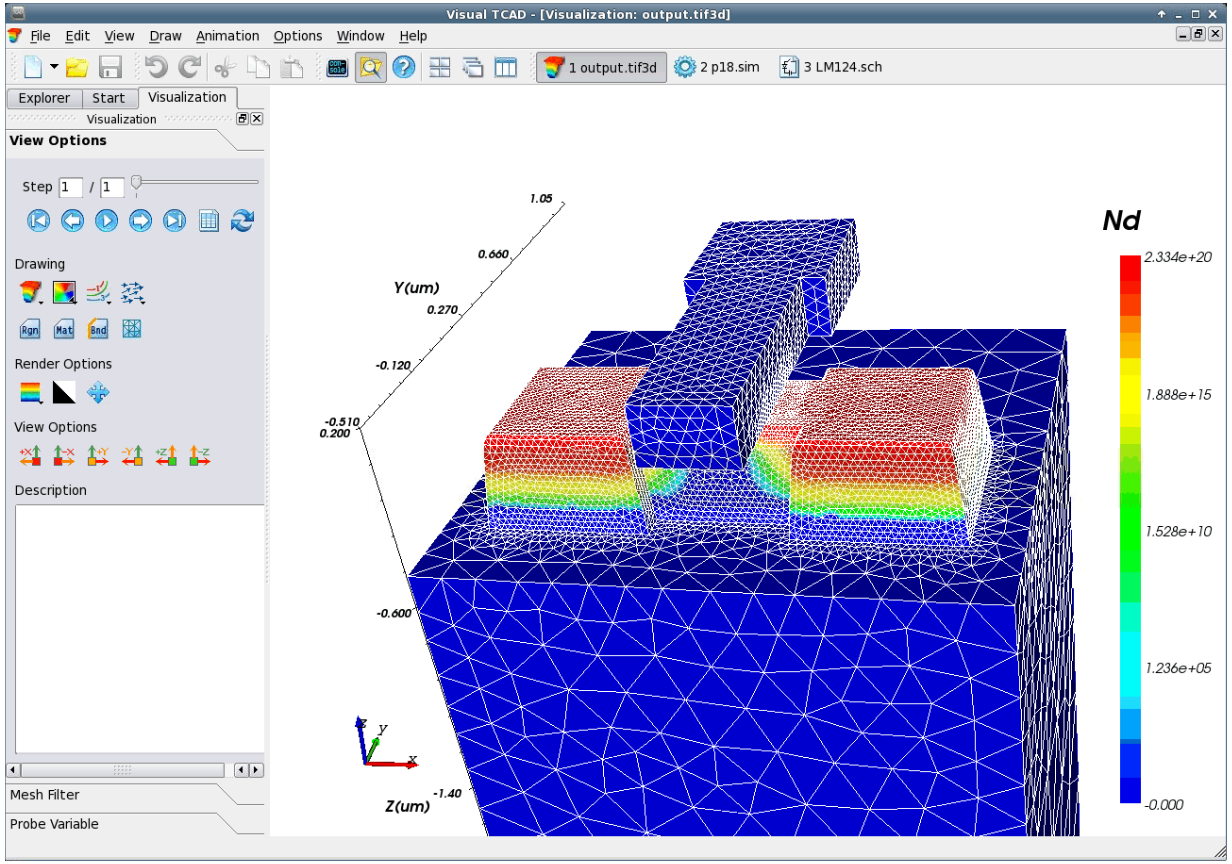


Example 1: N-body simulation



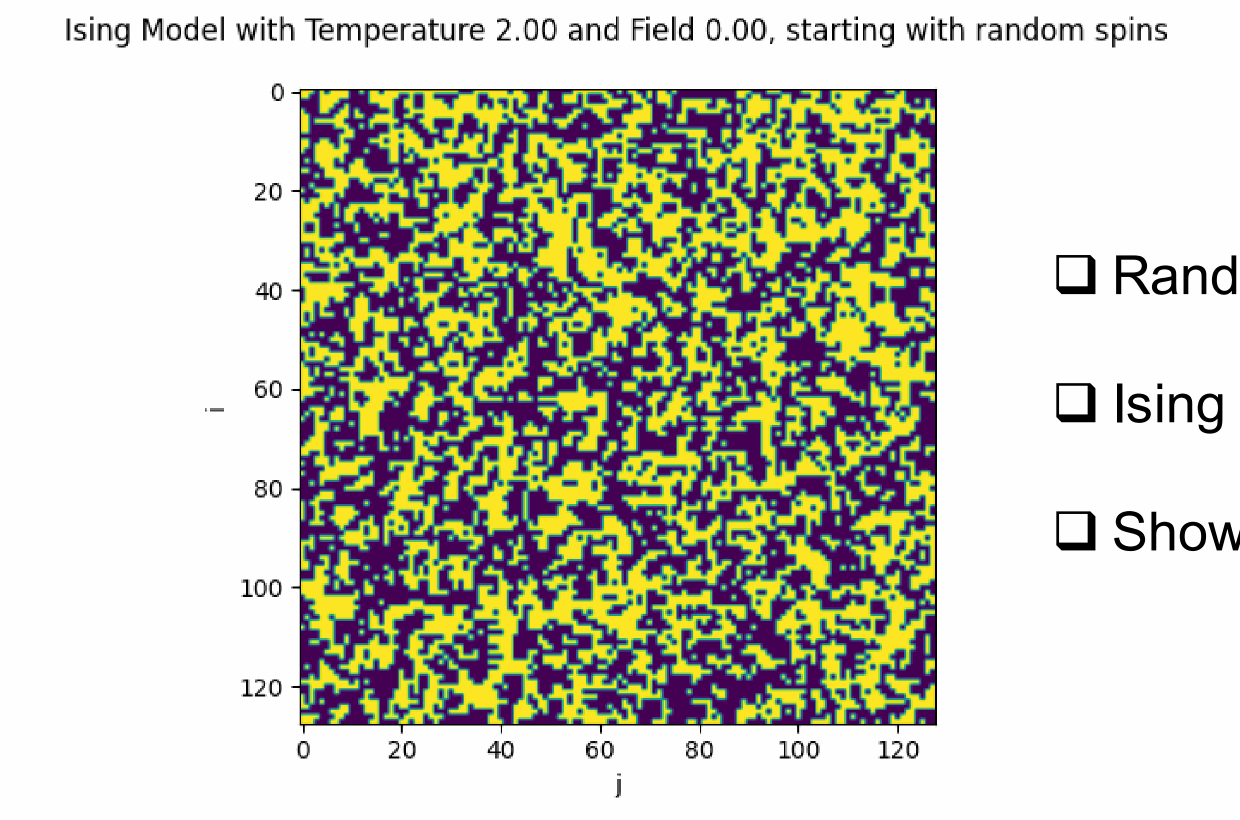
- **Astrophysics at scale**: planets, galaxies, even the universe
- Governed by **large-scale classical mechanics**
- Core tool: **Newton's equations of motion**
- Solved via **numerical PDEs**
- Specialized methods: tree algorithms, particle–mesh, magnetohydrodynamics (MHD), etc.

Example 2: Electromagnetics



- ❑ TCAD (Technology Computer-Aided Design)
  - **Physics-based simulation** of semiconductor devices
  - Predicts doping profiles, electric fields, and device performance
  - Reduces cost and time by testing designs **before fabrication**

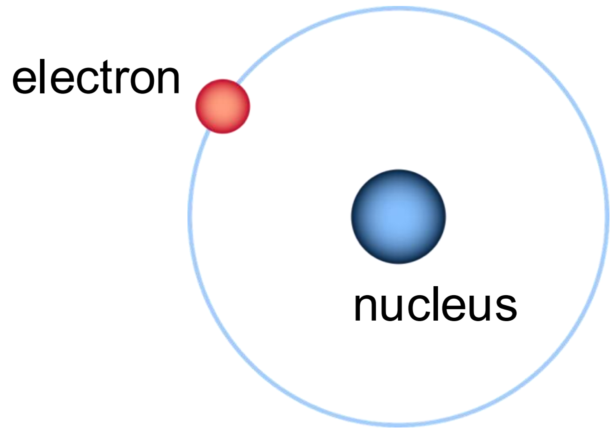
Example 3: Monte Carlo Simulation



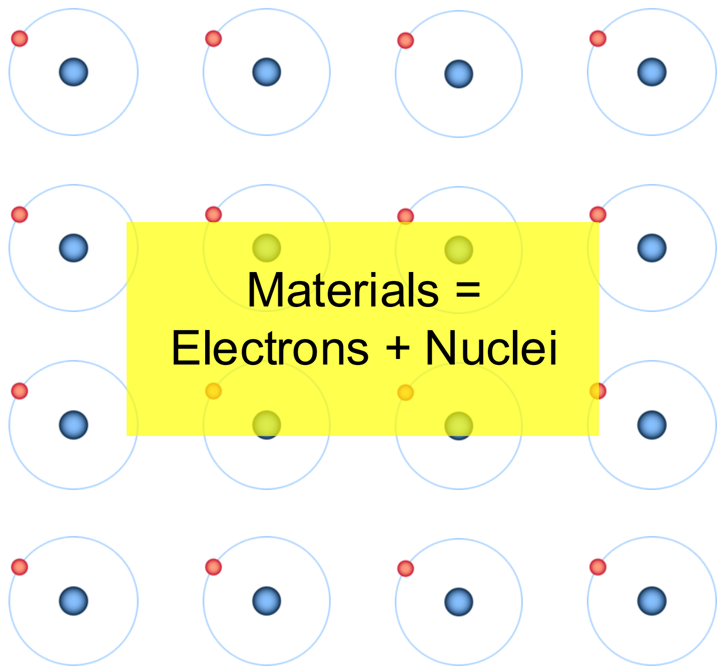
- ❑ Random sampling to solve physics problems
- ❑ Ising model: study magnetism & phase transitions
- ❑ Shows how order emerges from randomness

Example 4: Quantum mechanics

Schrödinger's equation for the H atom



$$-\frac{\hbar^2}{2m_e}\nabla^2\psi - \frac{e^2}{4\pi\epsilon_0\left|\mathbf{r}\right|}\psi = E\psi$$

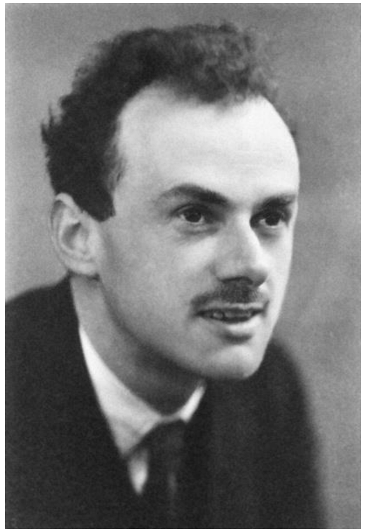


$$\left[-\sum_i \frac{\hbar^2}{2m_e}\nabla_i^2 - \sum_I \frac{\hbar^2}{2M_I}\nabla_I^2 + \frac{1}{2}\sum_{i\neq j}\frac{e^2}{4\pi\epsilon_0}\frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} + \frac{1}{2}\sum_{I\neq J}\frac{e^2}{4\pi\epsilon_0}\frac{Z_I Z_J}{|\mathbf{R}_I - \mathbf{R}_J|} - \sum_{i,I}\frac{e^2}{4\pi\epsilon_0}\frac{Z_I}{|\mathbf{r}_i - \mathbf{R}_I|}\right]\Psi = E_{\mathrm{tot}}\Psi$$

P. A. M. Dirac (1929)

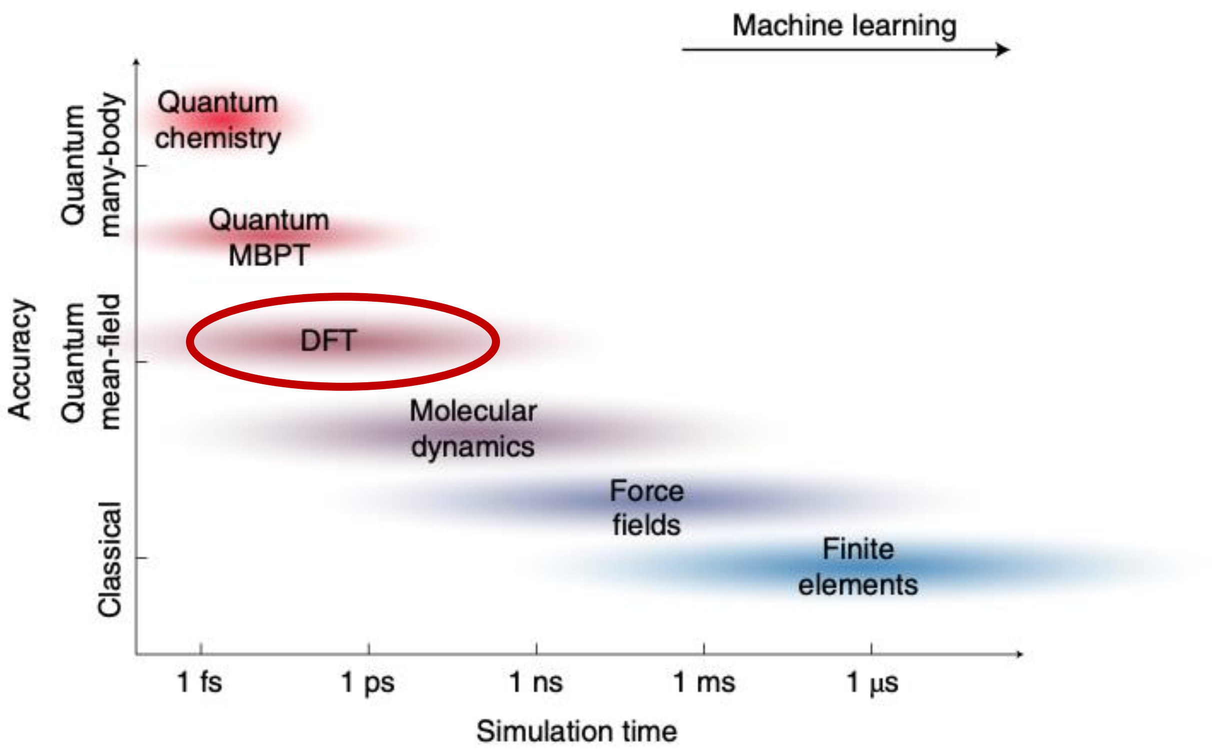
"The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble."

Proc. Roy. Soc. (London) A **123**, 714 (1929).

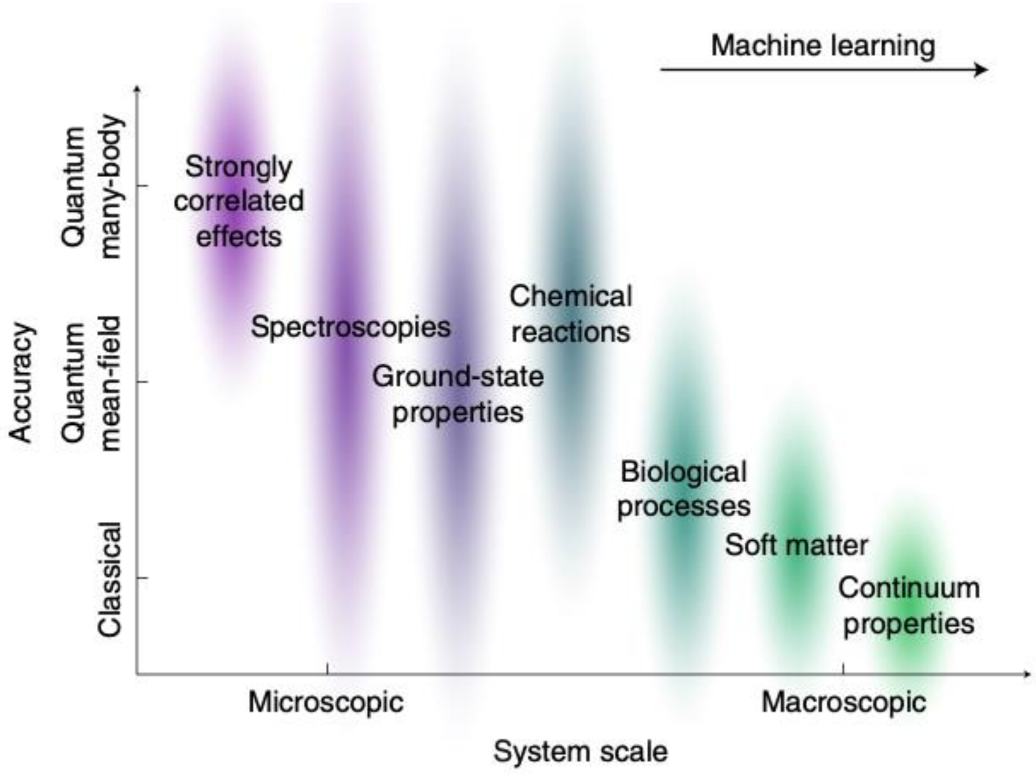


Discovering and understanding materials through computations

Required accuracy vs simulation time scale



Different phenomena at different scales



S. G. Louie *et al.*, Nat. Mater. **20**, 728 (2021), Perspective article

Density Functional Theory (DFT) and Kohn-Sham equations

$$-\frac{\hbar^2}{2m_e}\nabla^2\psi_n + V_{\mathrm{SCF}}\,\psi_n = E_n\,\psi_n$$

$$n(\mathbf{r}) = \sum_{n\in\mathrm{occ}} |\psi_n(\mathbf{r})|^2$$

Ground-state electron density

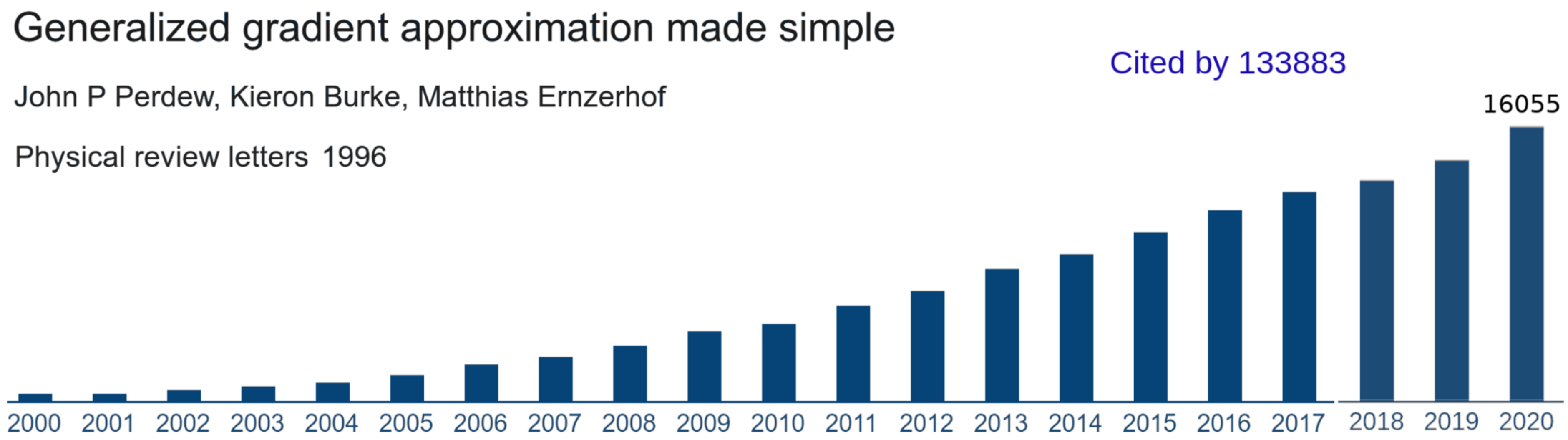
$$V_{\mathrm{SCF}}(\mathbf{r}) = -\frac{e^2}{4\pi\epsilon_0}\left[\sum_I \frac{Z_I}{|\mathbf{r}-\mathbf{R}_I|} - \int \frac{n(\mathbf{r}')d\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|}\right] + \boxed{V_{xc}\left[n(\mathbf{r})\right]}$$

Ionic potential

Hartree potential

Exchange-correlation potential

Impact of DFT

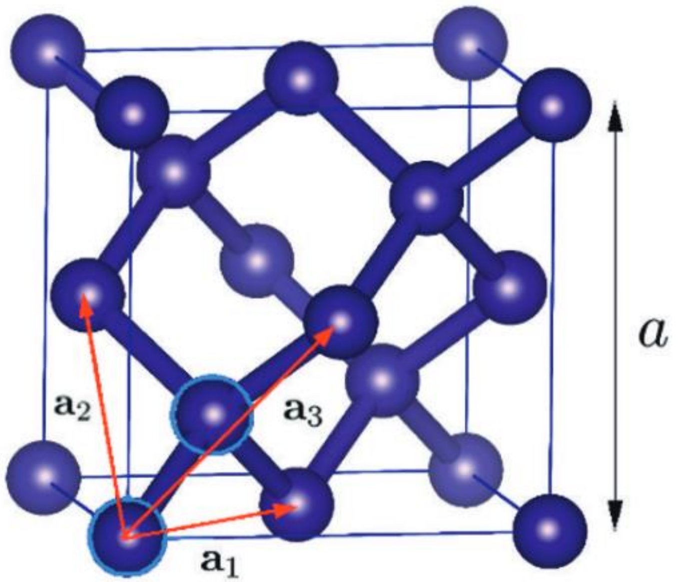


Approx. 1 paper every 30min based on this work

First-principles electronic structure calculations using DFT

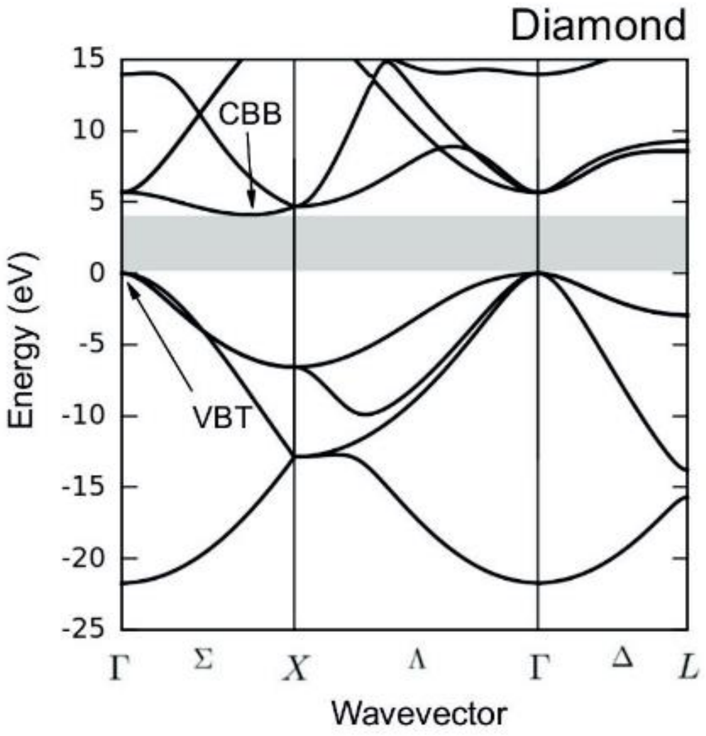
Physical Inputs

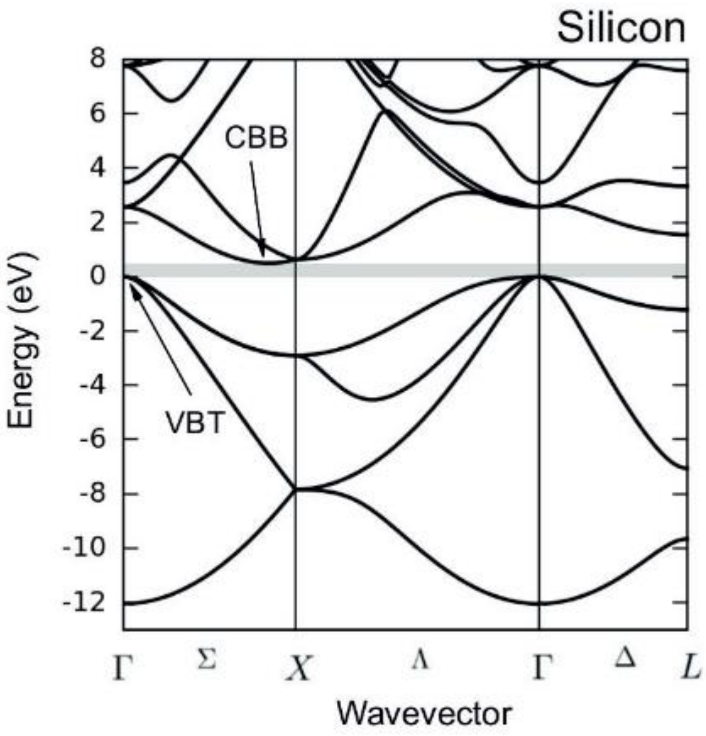
- ❑ Atomic composition
- ❑ Atomic positions



Realistic description of electronic structure of materials

Electronic structure is fundamental for understanding spectroscopic, optical, and transport properties in materials.

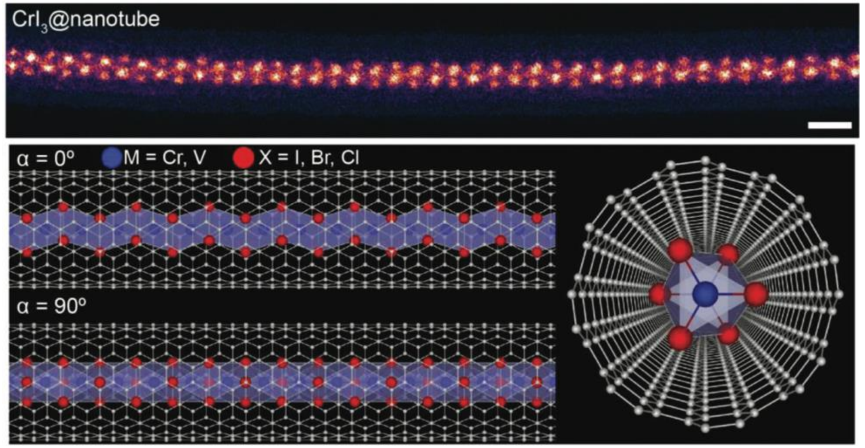




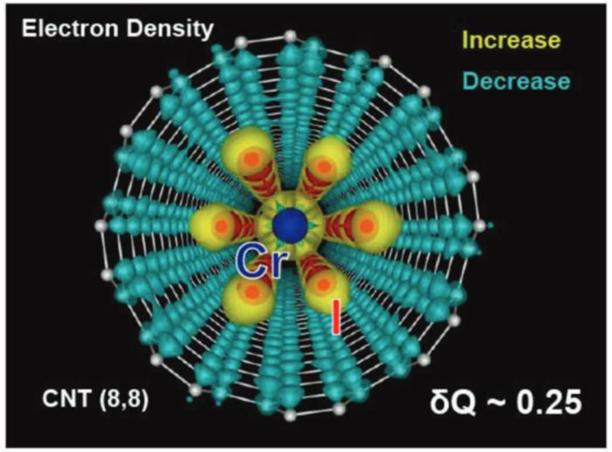
Collaboration of experiments and calculations

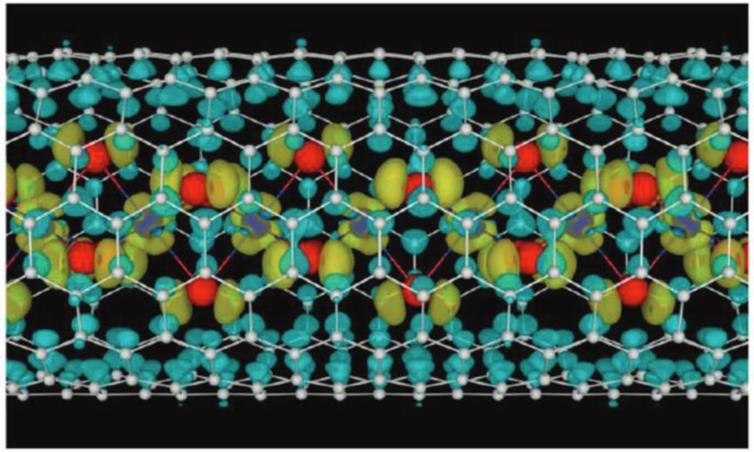
1D CrI_3 Single Chain in Carbon Nanotube

Experimental STEM Imaging



Calculated electron density distribution



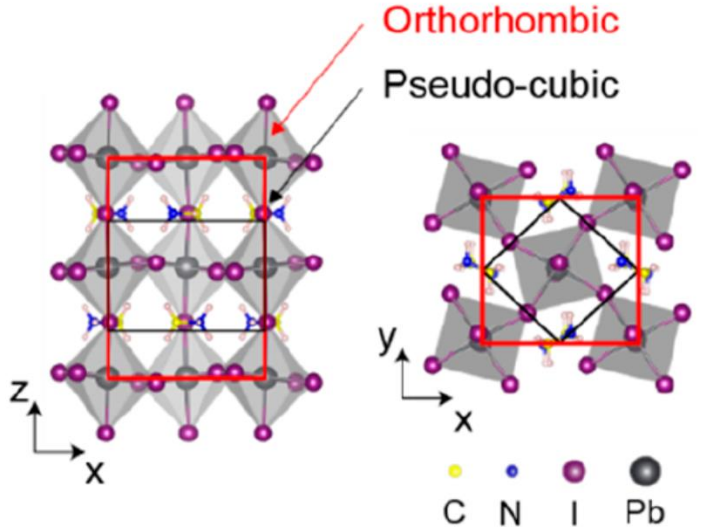


Our DFT calculations revealed the role of electron transfer on the stability and magnetism of CrI_3 single chains

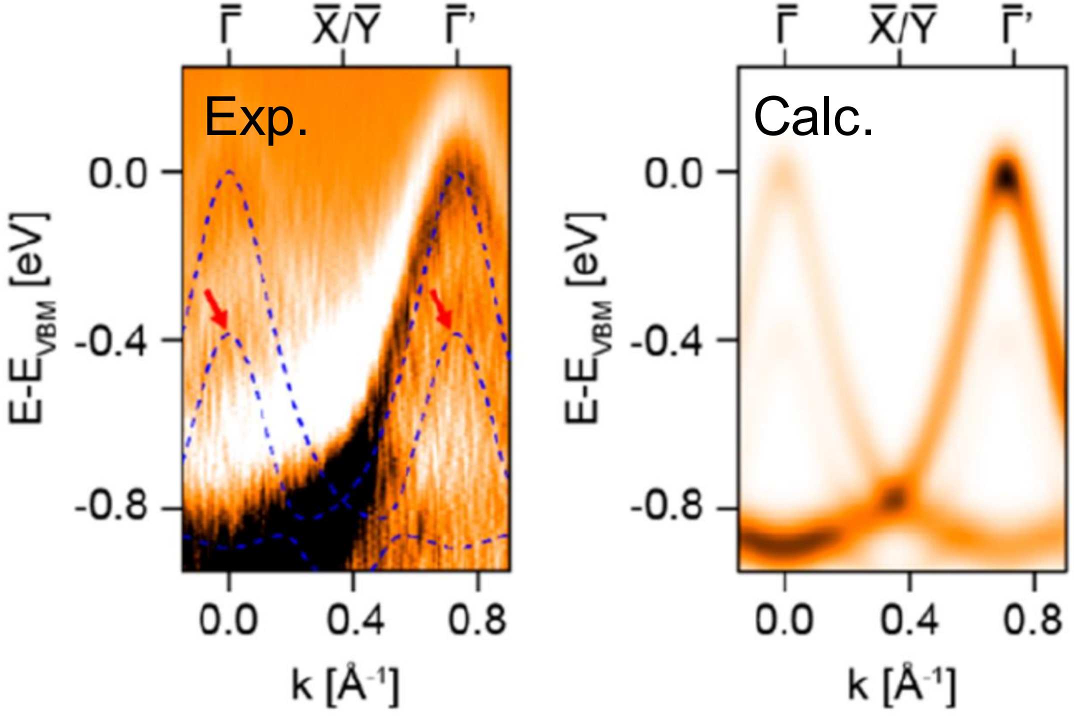
YL†, **YWC**† *et al.*, Adv. Mater. 2307942 (2023).

Collaboration of experiments and calculations

$CH_3NH_3PbI_3$ (MAPI)
Perovskite solar cell material



Band folding effect due to orthorhombic distortion

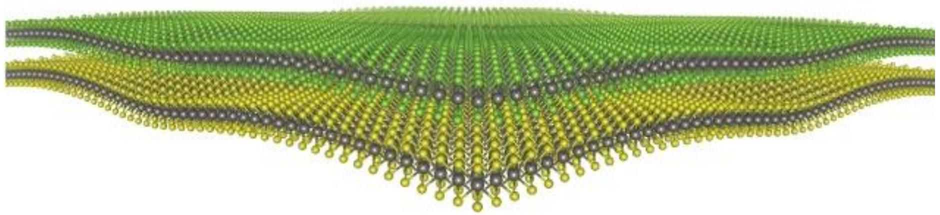


Angle-resolved photoemission

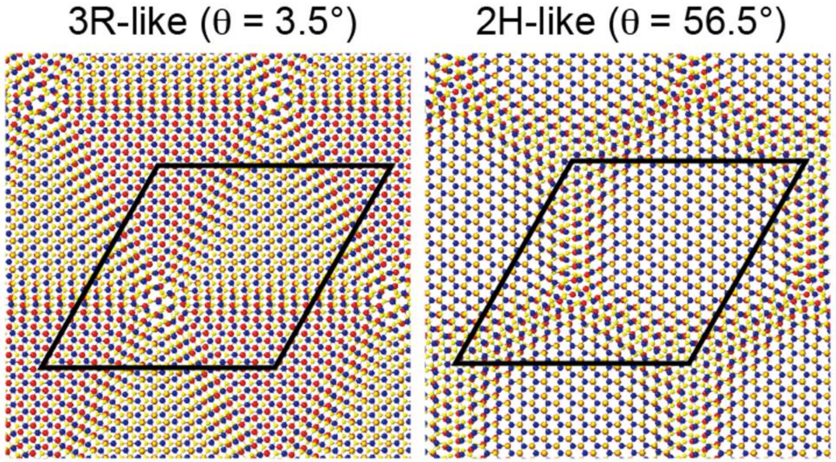
JP†, SH†, **YWC**† *et al.*, ACS Nano **18**, 13938 (2024).

Collaboration of experiments and calculations

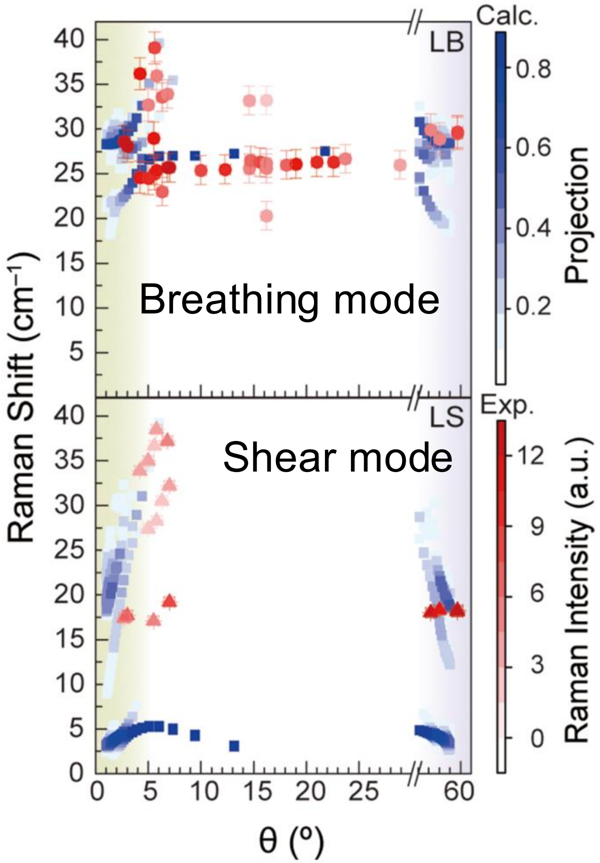
Twisted $MoSe_2/WSe_2$
Heterobilayer moiré material



Calculated moiré-scale atomic reconstructions



Moiré Phonon Raman Exp. & Calc.



Our calculations captures evolution of moiré phonons in experiments

S. Y. Lim†, H.-G. Kim†, **Y. W. Choi**†, T. Taniguchi, K. Watanabe, H. J. Choi, and H. Cheong, ACS Nano **17**, 13938 (2023).

Let’s setup dev-env

Installations

GitHub Education Pack (Copilot Pro)

VSCode https://code.visualstudio.com/

Miniconda https://www.anaconda.com/docs/getting-started/miniconda/main

VSCode Extensions
- GitHub Copilot / Copilot Chat
    - VScode GitHub login
- Python
- Jupyter