First Principles Workshop

An introduction and hands-on tutorial with the Quantum ESPRESSO

Welcome to The Workshop

R. Saito group

What is DFT?

- An approach to calculate the (ground state) properties of many-electron systems from *first-principles*

- Features:
  - *Ab initio* / *first-principles* / no empirical information
  - Quantum mechanical
  - Numerical

Quantum ESPRESSO is one of the **most-popular** and **open-source** DFT packages

Nice things about DFT

- Predictive capability
- Very accurate for most materials (errors typically < few %)
- Can calculate lots of properties of scientific / technological interest
- Many DFT packages are just a kind of **black boxes** (user-friendly)

Walter Kohn, 1998

Today's Schedule and Goal

- **10:15 – 10:45 = Introduction to Computer System and DFT package**
  Participants can **run** basic Quantum Espresso program.
- **10:15 – 12:00 = Hands-on tutorial #1**
  Participants can show **total energy** and **lattice constant** of Si and Graphene.
- **12:00 – 13:30 = Lunch break**
- **13:30 – 14:30 = Hands-on tutorial #2**
  Participants can show **charge density**, **energy bands**, **DOS** of Si and Graphene.
- **14:30 – 14:45 = Extra Tutorial**
  Participants obtain extra information (practice it at home)
- **14:45 – 15:00 = Closing**

Let's enjoy Quantum ESPRESSO!