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!