

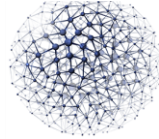


First Principles Workshop

An introduction and hands-on tutorial with the
Quantum ESPRESSO



Yambo[©]



AFLOW
Automatic - FLOW for Materials Discovery



TOHOKU
UNIVERSITY

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!