Workshop - Material Modeling with DFT using QE (beginner level)

This workshop is focused on the application of Density Functional Theory (DFT) through a code called Quantum ESPRESSO (QE). This workshop is intended for beginners in DFT-based simulations. There will not be any rigorous introduction to the theoretical aspects of DFT. We will get introduced to the working principle, some conceptual basics and hands-on sessions where we will do simple DFT calculations.
The choice of the software is QE since it is free, open-source and easy to use. Installation and troubleshooting will be covered in the workshop. Note that if you need to work with other codes such as VASP, CASTEP, ORCA etc., you are still encouraged to attend since once you get the basics, switching code is not a big barrier. You just need to switch the syntax, the working principle remains more-or-less the same. However, please do not attend if you know how to use one of these codes, or have experience with DFT-based simulation.
The workshop will be conducted primarily in Bangla. Below I provided a tentative schedule. This schedule is flexible, i.e., if there is some consensus among attendees on the timing, I can adjust the schedule up to certain extent. If you cannot attend SOLELY due to timing, let me know. Also, depending on how much interactive the sessions are, we might have to shuffle some of the topics due to time constraint.
There will be only a few seats since this workshop is intended to be personalized. So to make sure that only the interested ones register, there are some ground rules and you must commit to these rules:

- You must be familiar with quantum mechanics at the level of any modern physics textbook covers. Such familiarity should include Schrodinger's equation, the particle in a box system, and familiarity to the solution of Hydrogen atom and simple harmonic oscillator. I guess at minimum, this corresponds to the sophomore level physics, chemistry or material science curriculum. If you are unsure whether you have the prerequisite, send an email.

- You have a computer with good internet connection
- You already have/will have installed Discord in your computer
- You will not miss any lecture/hands-on sessions and will submit assignments (if given) even if incomplete
- Since this will be an online workshop, response from your side is expected to keep the sessions interactive. I will not enforce camera-on rules due to privacy and security purpose, but please be attentive and responsive.
- You will download and prepare the files before the workshop starts. Detailed instruction will be sent once you are registered.
- This is an online workshop and a FREE one! There will be no certificate, no recognition. So please do not register if you do not need DFT in your research work.

Tentative schedule:

Day 0: (will be done through Discord before the workshop starts)

- Installation of QE, setting up computational environments
- Downloading all the files to be used in the hand-on session

Day 1:

- 06:30 PM - 07:20 PM (Lecture sessions)
    - An absolute beginner's guide to DFT - 20 minutes
        - DFT as a black-box
    - Approaches of doing DFT - 30 minutes
        - Approximations used in DFT
        - Born-Oppenheimer approximation (frozen core)
        - Pseudopotential
        - an introduction to QE and comparison with other codes
- 07:30 PM - 08:20 PM (Lecture sessions)
    - Structural and electronic properties of solids - 50 minutes
        - Brillouin zone integration
        - smearing methods
        - basis set

        - supercell
        - electronic structure (band, DOS)
        - metallicity of solids
- 08:30 PM - 09:20 PM (Hands-on sessions)
    - Introduction to Linux environments and basic commands - 10 minutes
    - DFT calculation of Si semiconductors using QE - 40 minutes
        - self-consistent field calculation
        - non self-consistent field calculation
        - band structure calculation
        - density of states calculation
        - plotting

Day 2:

- 06:30 PM - 07:20 PM (Lecture sessions)
    - A review of Day 1 - 10 minutes
        - Structure optimization, and others - 40 minutes
        - XC functional
            - Hellman-Feynman theorem
            - Ionic vs cell relaxation
            - PWTK
- 07:30 PM - 08:20 PM (Hands-on sessions)
    - Structural properties - 30 minutes
        - lattice parameters
            - relaxation
            - variable-cell relaxation
            - hexagonal cells
    - Convergence testing - 20 minutes
        - kinetic energy cutoff
        - k-points
        - broadening
        - supercell sizes, charge density,
- 08:30 PM - 09:20 PM (Hands-on sessions)

- DFT in molecules - 20 minutes
    - bond length, angle, and dihedrals
    - quantum dots
    - Improvement of some property - 30 minutes
        - LDA to GGA
        - band gap

Day 3:

- 06:30 PM - 07:20 PM (Lecture sessions)
    - Magnetism 0 40 minutes
        - origin of magnetism in materials
        - spin-polarized DFT
        - Hubbard calculation: DFT+U - 10 minutes
- 07:30 PM - 08:20 PM (Hands-on sessions)
    - spin-polarized calculation
        - density of states
        - exchange splitting
    - DFT+U calculation
- 08:30 PM - 09:20 PM (Review sessions)
    - Kahoot
        - Review
        - Next plan

To register: https://forms.gle/ANE2jsFrqo38kBNRA
Contact: muhaymin.ph@gmail.com