



EURO²

Density Functional Theory with Quantum Espresso
Hande Toffoli, Middle East Technical University
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Welcome to the Course

Meet the Instructor

Hande Toffoli

- BSc in Physics from Middle East Technical University (METU), 1999
- PhD in Computational Condensed Matter Physics, Cornell U, 2005
- Postdoc at SISSA, 2006-2007
- Faculty of the Department of Physics at METU, 2007-present
- Research lines
 - Computational surface science
 - Computational heterogeneous catalysis
 - Materials for Energy Applications
 - ML-Aided Spectroscopy of Molecules

Prerequisite(s)

- Familiarity with basic quantum mechanics
- Familiarity with basic Linux commands
- Basic understanding of usage of HPC systems

Learning Objectives

At the end of this course, you will

- have a basic understanding of density functional theory,
- be introduced to the basic capabilities of the open-source code suite Quantum Espresso (QE),
- have a basic understanding of the input/output structure of the QE code,
- and see how QE is run on an HPC system, specifically TRUBA.

Course Overview

The outline of this course is as follows:

Lesson 1: Basics of density functional theory, Part 1

Lesson 2: Basics of density functional theory, Part 2

Lesson 3: Practicalities, Part 1

Lesson 4: Practicalities, Part 2

Lesson 5: I/O Structure of Quantum Espresso, Part 1

Lesson 6: I/O Structure of Quantum Espresso, Part 2

Lesson 7: Hands-on Exercise 1

Lesson 8: Hands-on Exercise 2

What this course is

This course is

- a concise introduction to the basics of DFT,
- an overview of practicalities associated with a typical DFT calculation,
- a guide to the basic functions of Quantum Espresso,
- and a few practical exercises.

What this course isn't

This course is not

- a complete and rigorous introduction to density functional theory
- a complete manual for Quantum Espresso
- a guide for running QE on an arbitrary HPC system

Preparation

To follow along the hands-on exercises in this course, you will need

1. An installation of Quantum Espresso, which can be provided free-of-charge from <https://www.quantum-espresso.org/>
2. An installation of XCrysDen, which works directly for the input and output files of QE: <http://www.xcrysden.org/>

End of Introduction

Next: Introduction to DFT, Part 1



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