# Fundamentals of Density functional theory (DFT) and it's applications to 2D materials

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## Abstract

The study of two-dimensional (2D) materials is new and vibrant research field of interest. Electronic, mechanical and optical properties of such materials are significantly different, compared to their respective three-dimensional allotropes due to the reduction of their dimensions, from bulk down to the atomic thickness. Because of such exciting properties, these materials hold a great potential for use in various fields of electronics.

In this seminar, I will explain the steps that Density functional theory (DFT) uses to approximate solution of many-body system Schrodinger equation and consider it's application to 2D materials. Following, will present how to configure Quantum Espresso DFT software, and use it to do calculations and extract materials' properties this way.

Keywords: 2D materials, DFT, Density functional theory, Quantum Espresso