Learning Module: Bonding and Band Structure in Silicon

The main goal of this learning module is to help students learn about the correlation between atomic structure and electronic properties, and help them develop a more intuitive understanding of the origin of electronic bands in a material via hand-on exploration using online electronic structure calculations at nanoHUB.org.

The module consists of:

- Two introductory lecture slides available online as presentations
  - Overview lecture.pdf (1 MB, uploaded by Ravi Pramod Kumar Vedula 1 decade 3 years ago)
  - Prelab lecture.pdf (1 MB, uploaded by Ravi Pramod Kumar Vedula 1 decade 3 years ago)
- Hands-on lab involving Density Functional Theory (DFT) simulations via nanoHUB.org
  - Lab handout.pdf (115 KB, uploaded by Ravi Pramod Kumar Vedula 1 decade 3 years ago)

Why DFT simulations?

DFT provides an computationally efficient ab initio (first principles) description of the electronic structure and total energy of materials. These simulations produce Kohn Sham energy eigenvalues of a realistic systems and the Kohn Sham band structure. Such a description can help students understand the intimate connection between atomic structure and electronic structure through computational experiments.

Learning Objectives

Upon completion of this learning module most students will be able to:

- Compute Kohn Sham band structures of crystalline structures using online DFT simulations with the DFT calculations with Quantum ESPRESSO
- Understand how bands are formed in real materials
- Identify the how the bands are occupied and calculate the bandgap.
- Identify the type of solid (metallic, semiconducting or insulating)
- Distinguish between direct and indirect band gap materials

Some students are expected to understand:

- How the s and p orbitals interact and their relationship to lattice paramter
- How do the numerical approximations affect the DFT results

Instructors can build on this module to teach hybridization and mixing of the orbitals in Si diamond structure.

Audience

This learning module was designed for advanced undegraduate and graduate students of engineering and science interested in materials and their electronic properties. Students are expected to be familiar with basic quantum mechanics and electronic structure of bonding.

This learning module was originally developed and applied in a technical elective MSE course at Purdue for advanced undergraduate students and graduate students. It is also used as a hand-on activity in a sophomore level course for Purdue MSE students on bonding and crystallography.