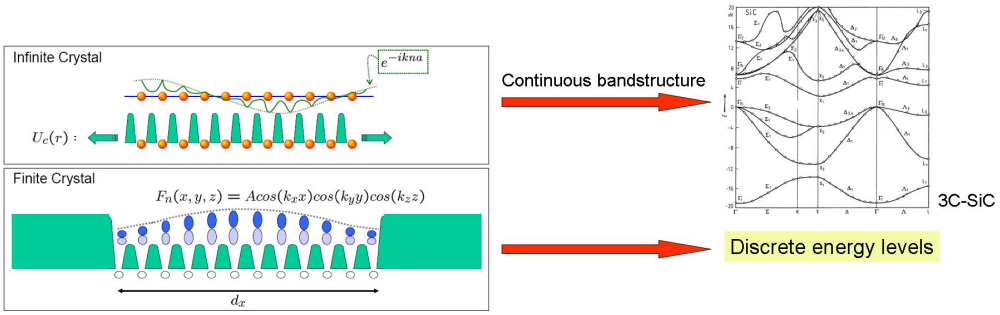
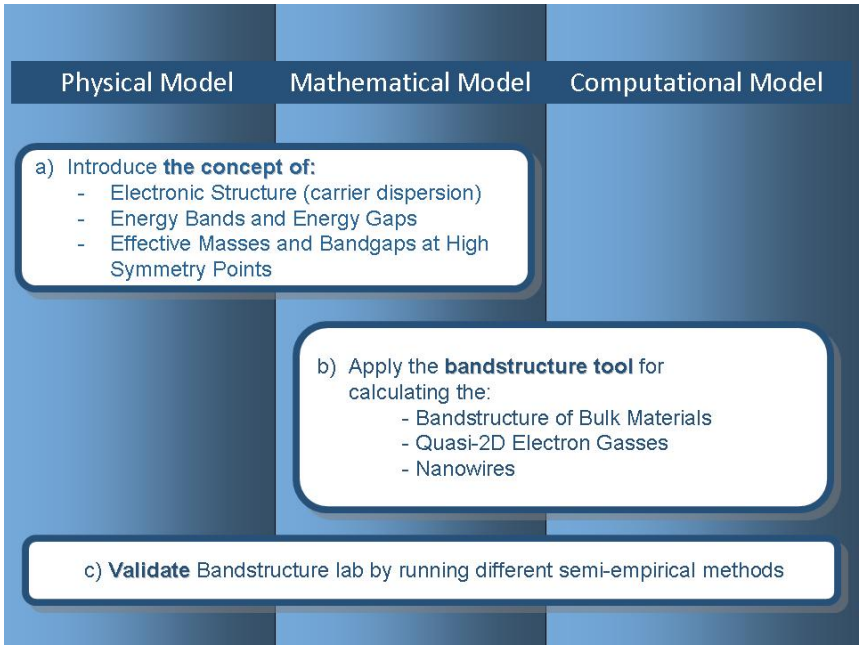
Band Structure Lab Learning Materials



By completing the Bandstructure Lab in [ABACUS - Assembly of Basic Applications for Coordinated Understanding of Semiconductors], users will be able to understand a) the concept of carriers dispersion in a solid, b) the concept of effective masses and energy gaps, and c) the bandstructure in low-dimensional systems.

The specific objectives of the Banstructure Lab are:



Recommended Reading

Users who are new to the concept of bandstructure and how to calculate it should consult the following resources:

1. Walter Harrison. (2004). *Elementary Electronic Structure*. Rev. ed. Singapore: World

Scientific.

2. Peter Y. Yu and Manuel Cardona. (2010). *Fundamentals of Semiconductors: Physics and Material Properties*. 4th ed. Heidelberg: Springer.

3. Dragica Vasileska, Stephen M. Goodnick and G. Klimeck. (2010). *Computational Electronics: Semiclassical and Quantum Device Modeling and Simulation*. Boca Raton, LA: CRC Press. (See especially Appendix A)

Demo

Band Structure Lab: First-Time User Guide

Band Structure Lab Demonstration: Bulk Strain

Theoretical Descriptions

* Band Structure Calculation: General Considerations

* Empirical Pseudopotential Method Description

* Tutorial on Semi-empirical Band Structure Methods

* Description of the K.P Method for Band Structure Calculation

* Tight-Binding Band Structure Calculation Method

* Empirical Pseudopotential Method: Theory and Implementation

Tool Verification

Verification of the Validity of Bulk Bandstructure Lab

Examples

Verification of the Validity of Bulk Bandstructure Lab

Exercises and Homework Assignments

1. Bulk Band Structure: a Simulation Exercise

2. Computational Electronics HW - Bandstructure Calculation

3. Energy Bands as a Function of the Geometry of the n-Well Potential: an Exercise

4. Band Structure Lab Exercise

5. ABACUS Exercise: Bandstructure – Kronig-Penney Model and Tight-Binding Exercise

Solutions to Exercises

Solutions are provided only to instructors!

Evaluation

This test will assess the users conceptual understanding of the physical, mathematical, and computational knowledge related to the formation of bandstructures in crystals, as well as the concepts of energy bands and energy gaps.

ABACUS: Test for Bandstructure Lab

Challenge

Users are challenged to integrate their knowledge about the calculation of bandstructure in bulk as well as in low-dimensional systems such as nanowires.

Can we define unique effective masses in Si nanowires?