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:

<table>
<thead>
<tr>
<th>Physical Model</th>
<th>Mathematical Model</th>
<th>Computational Model</th>
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<tbody>
<tr>
<td>a) Introduce the concept of:</td>
<td>b) Apply the bandstructure tool for calculating the:</td>
<td>c) Validate Bandstructure lab by running different semi-empirical methods</td>
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<tr>
<td>- Electronic Structure (carrier dispersion)</td>
<td>- Bandstructure of Bulk Materials</td>
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<tr>
<td>- Energy Bands and Energy Gaps</td>
<td>- Quasi-2D Electron Gasses</td>
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<tr>
<td>- Effective Masses and Bandgaps at High Symmetry Points</td>
<td>- Nanowires</td>
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Recommended Reading

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

Scientific.


**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?