Band Structure Lab with NEMO5

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Objective:

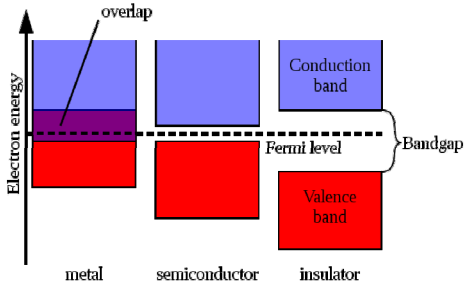
- Understand the basic physics represented in empirical tight binding theory
- Familiarize with previous tool BandStructure Lab tool on nanoHUB and the new engine **N**ano**E**lectronics **MO**deling (NEMO5) for future replacement
- Redesign an initial Rappture framework that computes the electronic structure of various material in the spatial configuration of bulk materials, ultra thin body structures, nanowires, and quantum dot.

Problem:

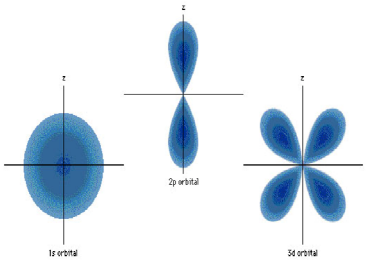
- NEMO5 uses Tight Binding Method to compute the electronic structure and needs different input decks to simulate results
- GUI of the old tool doesn't include some parameters input needed for NEMO5
- Old tool can only computes bands energy along given directions in K space

Theory:

- Any solid has a large number of bands.
- Band structure determines the material's electronic and optical properties.
- Materials can be divided into three groups depend on Band Gaps:
  - Metal
  - Semiconductor
  - Insulator



- Tight Binding Method: An approach to the calculation of electronic band structure using an approximate set of wave functions based upon superposition of wave functions for isolated atoms located at each atomic site
- NEMO5 engine computes band structure by using Tight Binding Theory

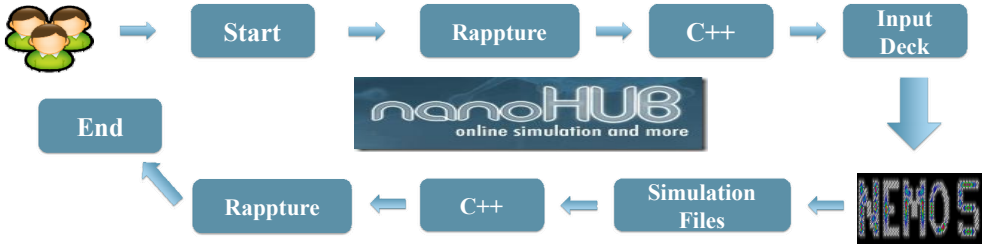


Approach:

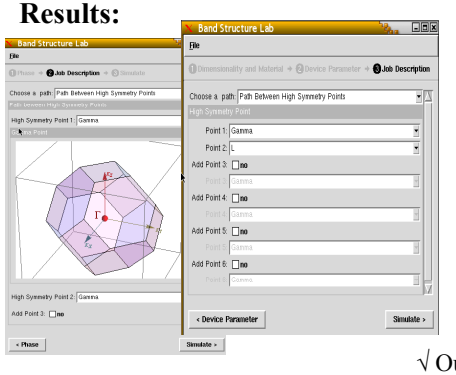
- The project focused on integrating Band Structure Lab tool into **R**apid **App**lication Infrastruc**ture** tool (Rappture) with **N**ano**E**lectronics **MO**deling (NEMO5) engine.

Approach:

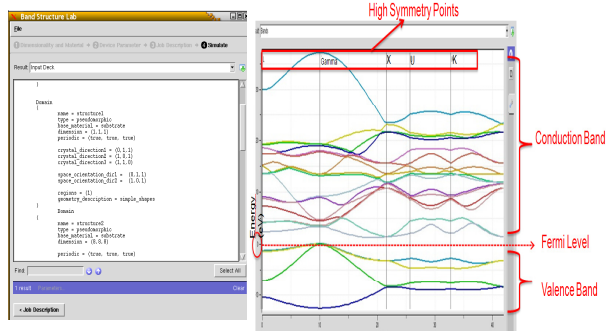
•The communication between Rappture and NEMO5 was achieved by creating a C++ code which creates and manages the information necessary for the communication to exist. The Rappture interface first gathers the information given by the user and creates an input deck which holds the information of different materials along with parameters given by the user. The input deck then runs the NEMO5 simulation and creates several simulation files. Then C++ code analyzes/interprets all these files and properly processes the information required to correctly display the information back to Rapture.



Results:



√ User-defined path between high symmetry points in K space



√ Output NEMO5 input decks for 3D bulk materials (Si, Ge, GaAs, InAs) (with/without strain model applied)

√ Plot E-K diagram for bulk material

Future Work:

- Output NEMO5 input decks for ultra thin body,nanowires, and quantum dot
- Output band gap and band edge information
- Plot unit cell and atomic structure

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