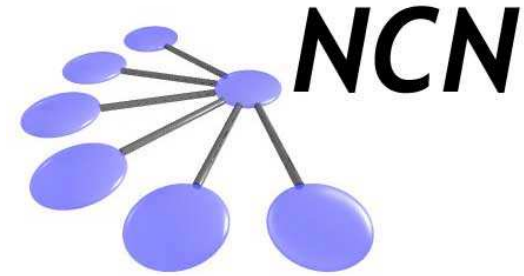
Band Structure Lab



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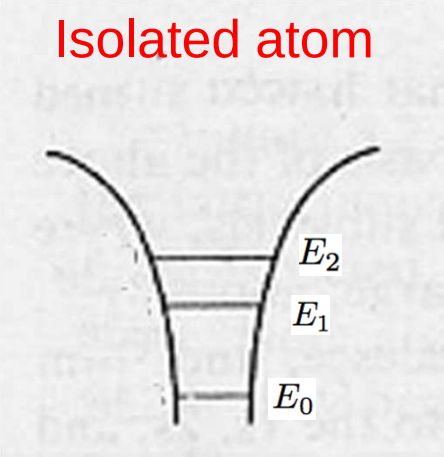
Synopsis

1. What is band structure
2. Calculating band structures
3. Features of “Band Structure Lab”
4. Results
5. Question

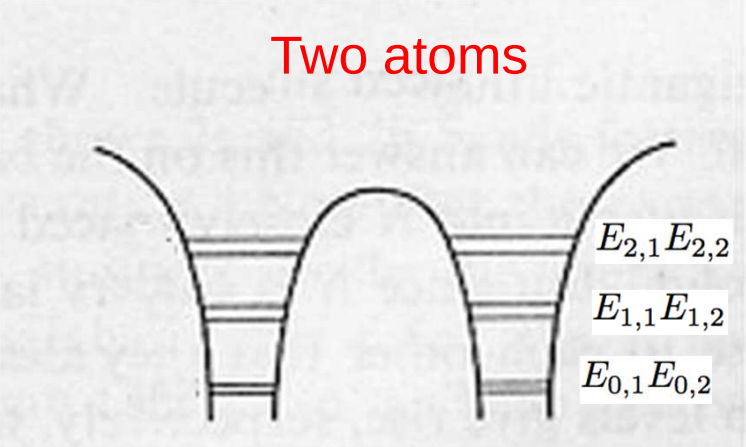
Nature of band structure

Isolated atom



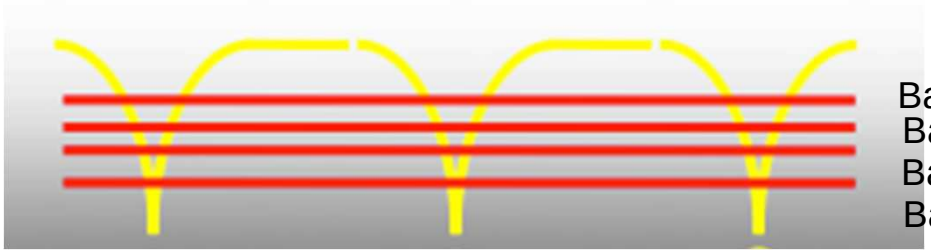
Quantum levels

Two atoms



Splits in two

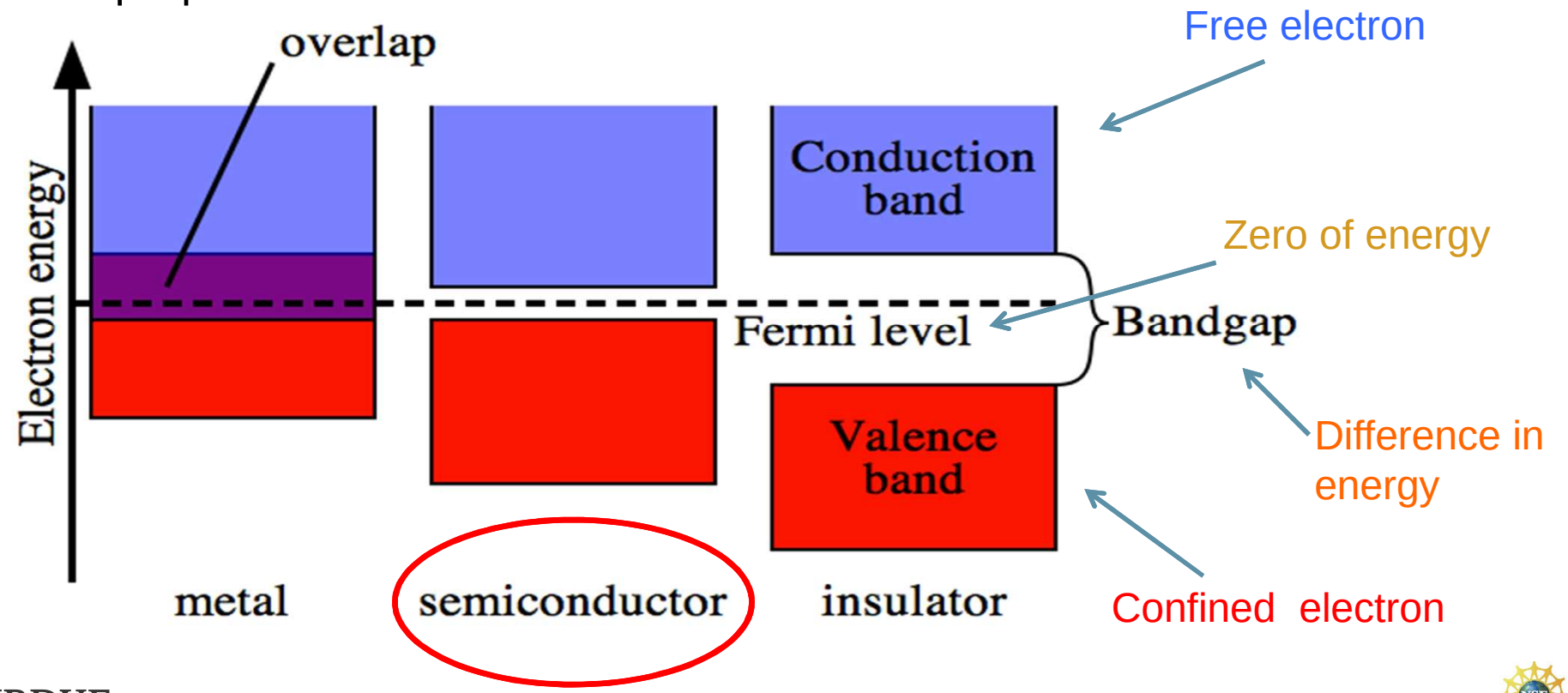
Crystal



Bands of energy

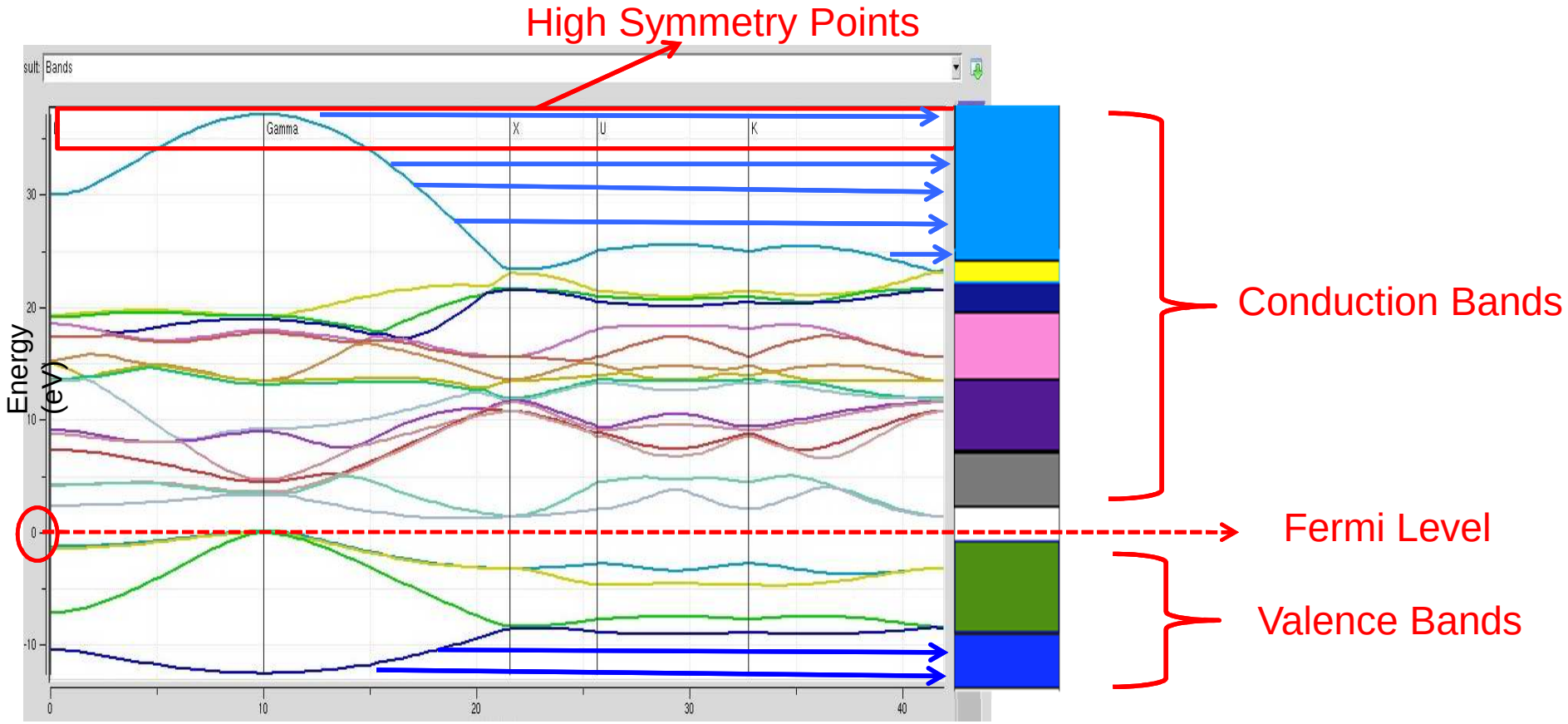
Importance of Band Structure

- Materials can be divided into three groups depending on bandgap
- Band structure determines the material's electronic and optical properties



Band Strucutre

An example:



K (≈ linear momentum)

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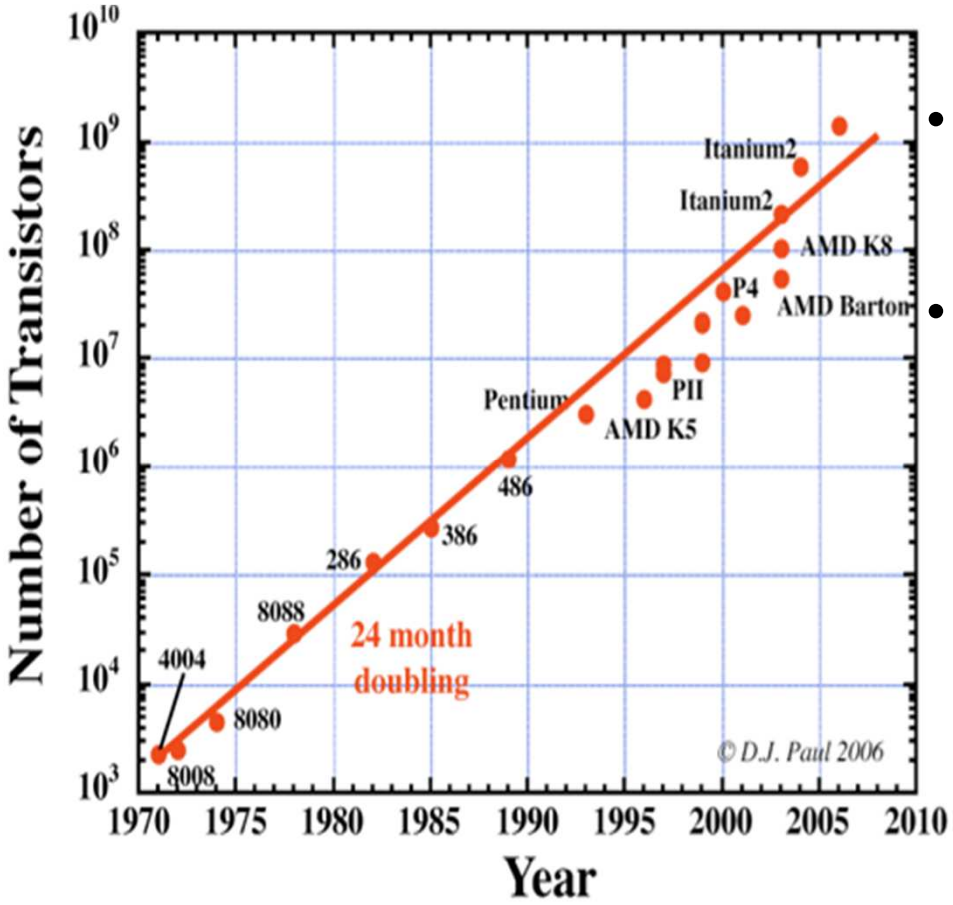
Importance of Band Structure

Moore's Law



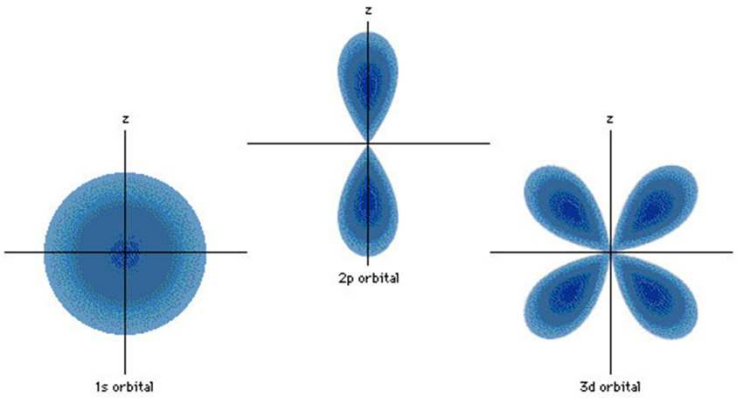
By: http://www.ieee.org/

- Transistor is the most used semiconductor device
- Quantum mechanics plays a central role in systems performance
  - Atom by atom description
  - Wave nature of electron

Methods

Tight Binding Method:

- Approximations
- Based on atomic orbitals
- Different models



By http://www.chemcomp.com/

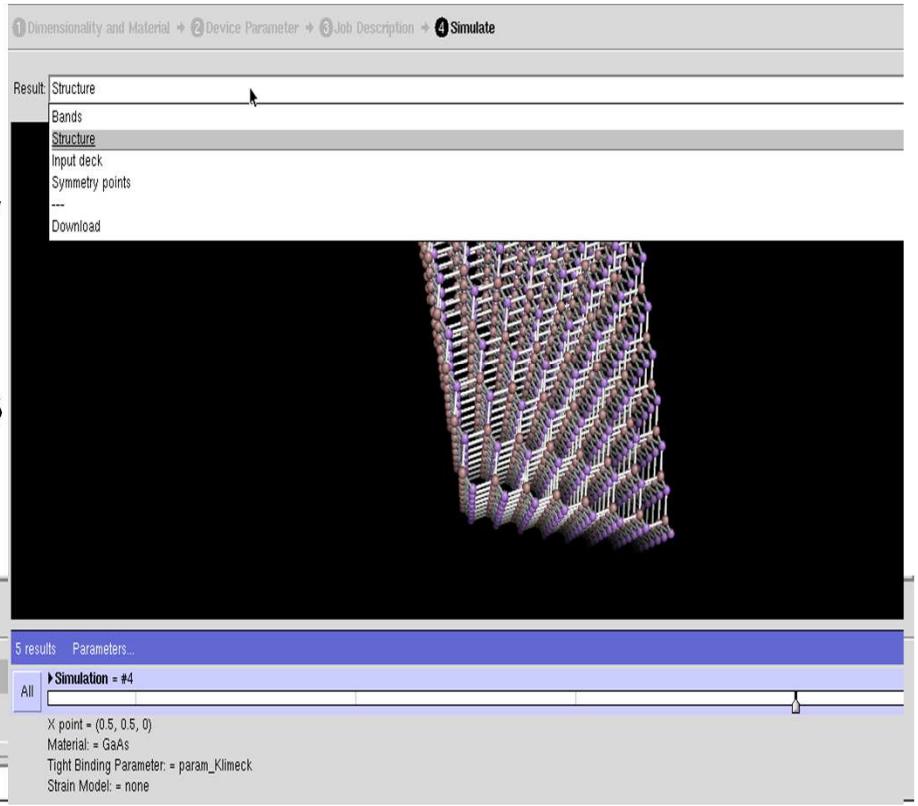
NEMO5:

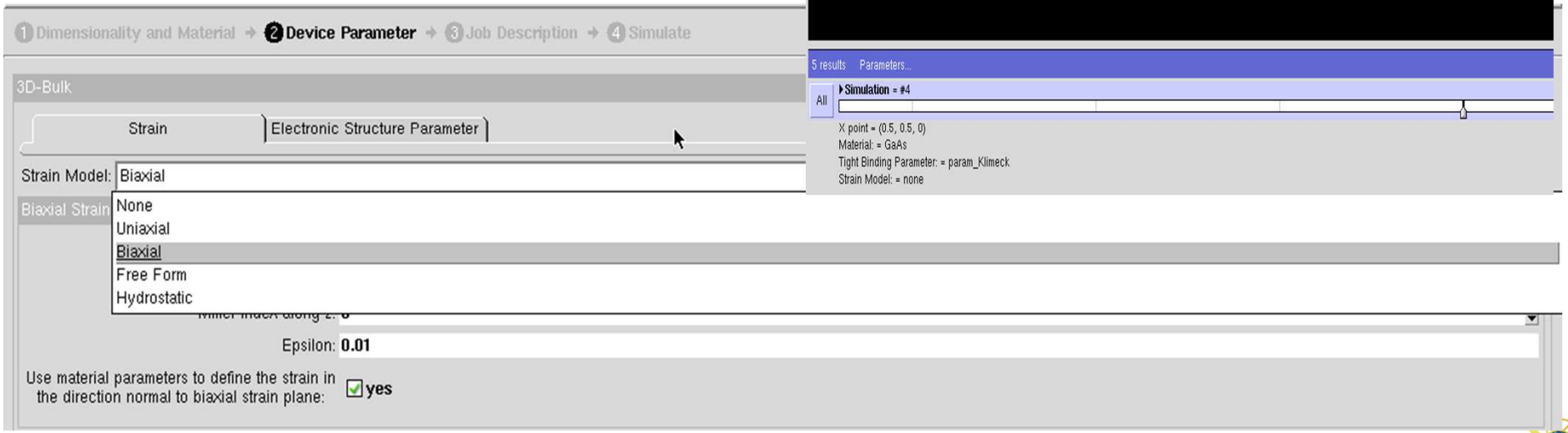
- NanoElectronics MOdeling tool by Prof. Klimeck research group
- Computes band structure using tight binding method
- Atom by atom analysis
- Requires a specific input file

Methods

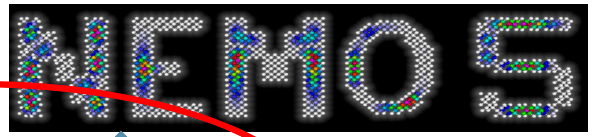
RAPPTURE (Rapid APPlication InfrastucTURE):

- Tool used to easily generate friendly graphical user interface(GUI)
- Allow users to customize simulations and outputs





Inputs



Input Parameters from GUI


```
Structure
{
        Material
        {
                name = GaAs
                tag = substrate
                crystal_structure = zincblende
                regions = (1)
                Bands:TB:sp3d5sstar_SO:param_set = param_Klimeck
                Bands:TB:sp3d5sstar_SO:param_Klimeck:VBO = 0.0
        }

        Domain
        {
                name = structure1
                type = pseudomorphic
                base_material = substrate
                dimension = (1,1,1)
                periodic = (true,true,true)
                crystal_direction1 = (0,1,1)
                crystal_direction2 = (1,0,1)
                crystal_direction3 = (1,1,0)
                space_orientation_dir1 = (0,1,1)
                space_orientation_dir2 = (1,0,1)
                regions =(1)
                geometry_description = simple_shapes
        }

        Domain
        {
                name = structure2
                type = pseudomorphic
                base_material = substrate
```

- Material
- Tight binding model
- Strain
- Points

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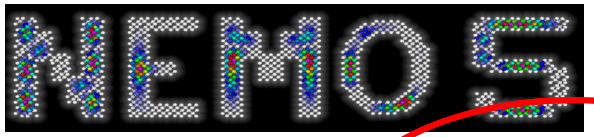
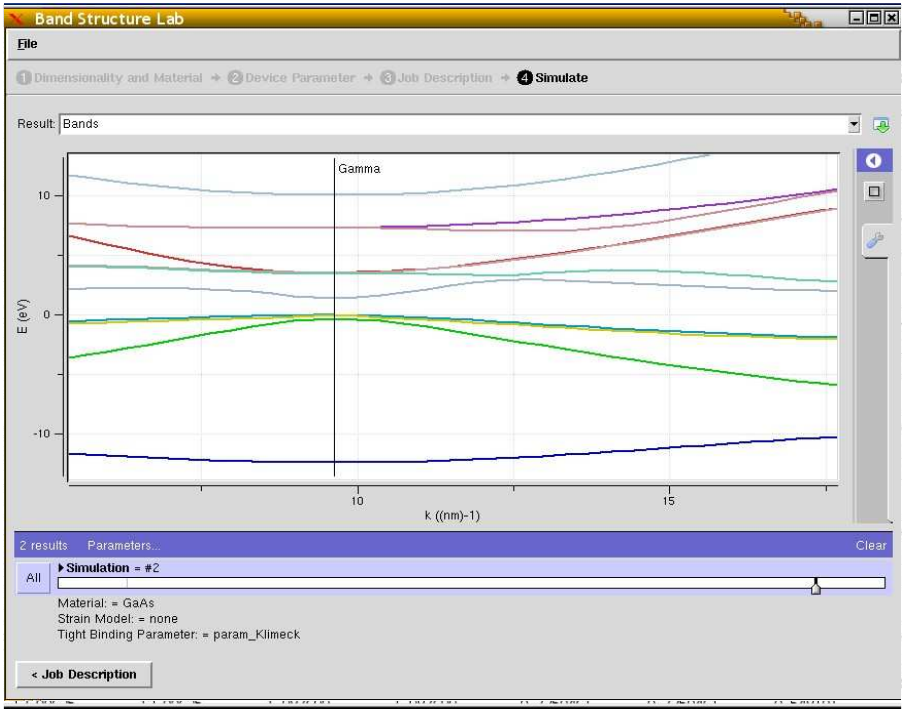
Results



Simulation Results from NEMO 5



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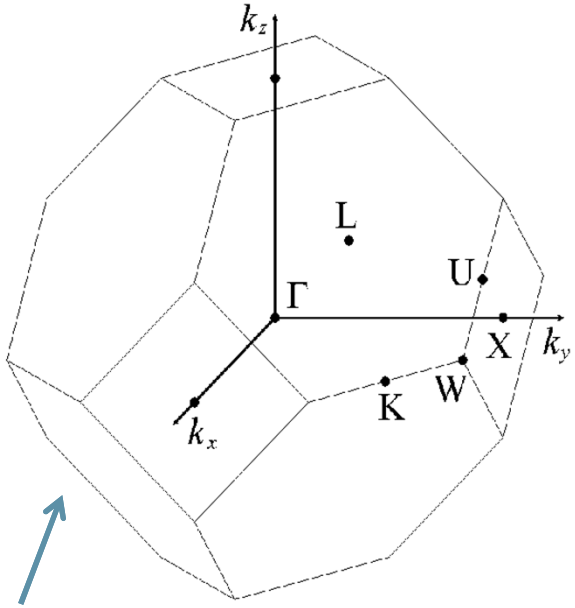
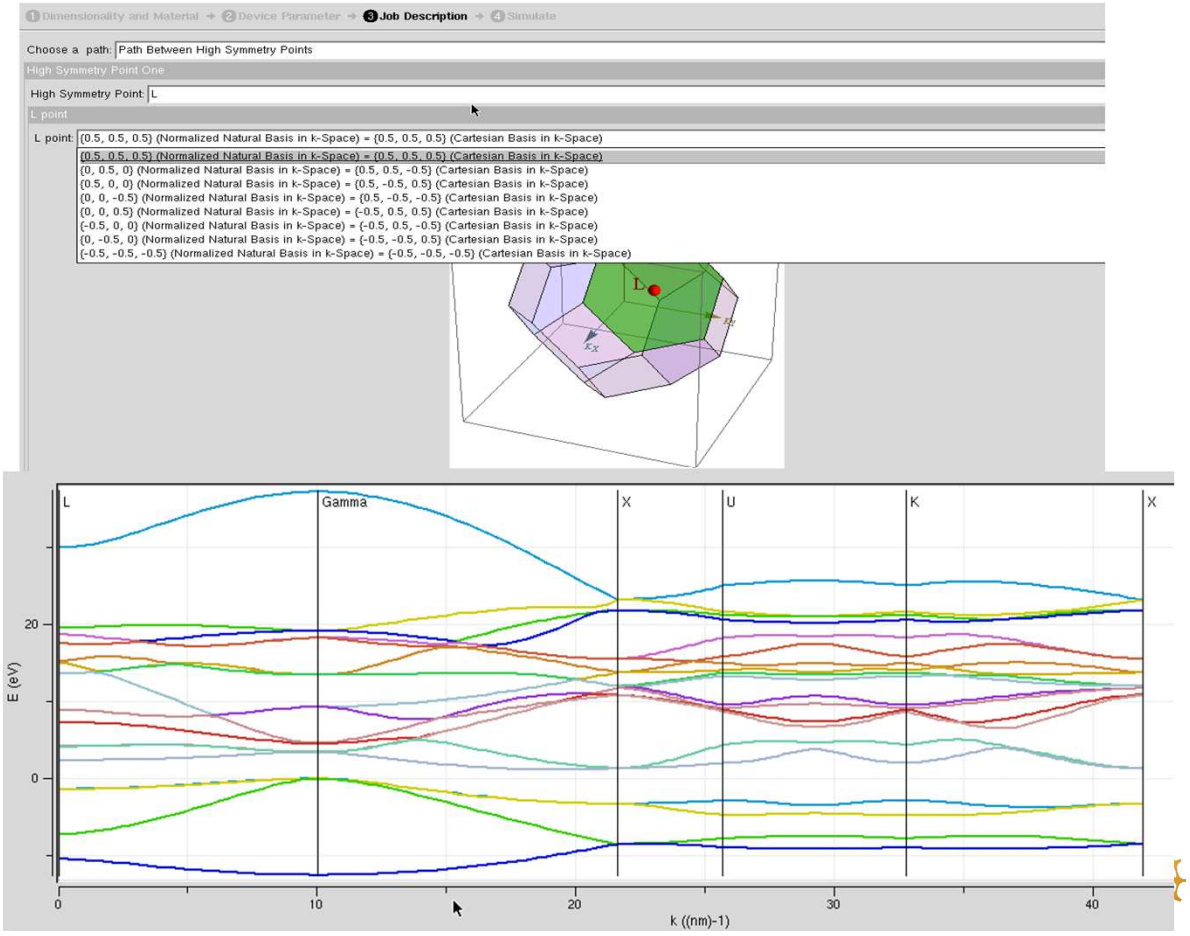
Features

- Intended to scientific and educational environments
- Intuitive input options and output results



Vector and boundaries of the allowed values for **K** (x axis). Is called First Brillouin zone



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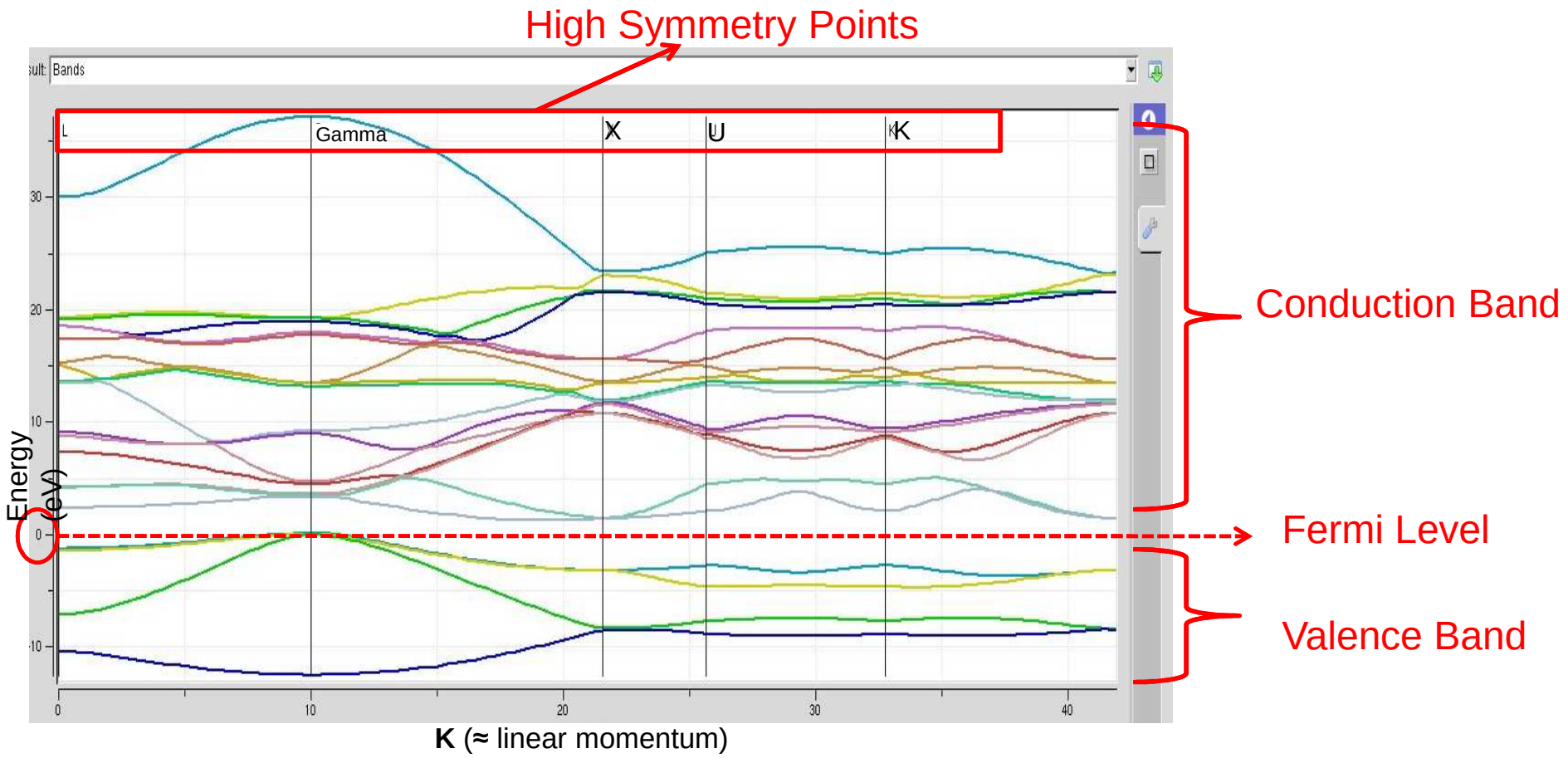
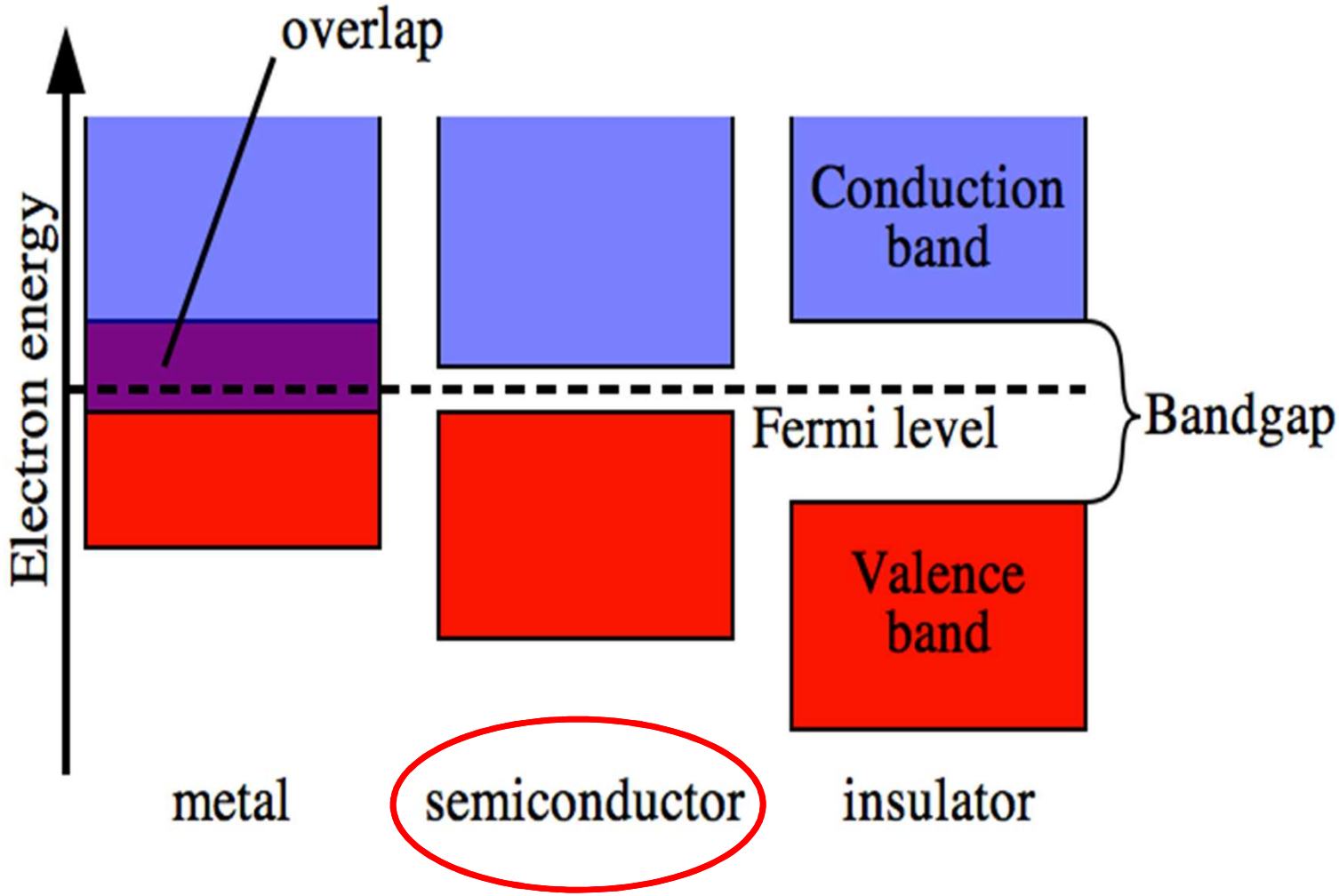
Results - Band Structure



Band Structure



Outputs

1 Dimensionality and Material → 2 Device Parameter → 3 Job Description → 4 Simulate

Result: Input deck

1 Dimensionality and Material → 2 Device Parameter → 3 Job Description → 4 Simulate

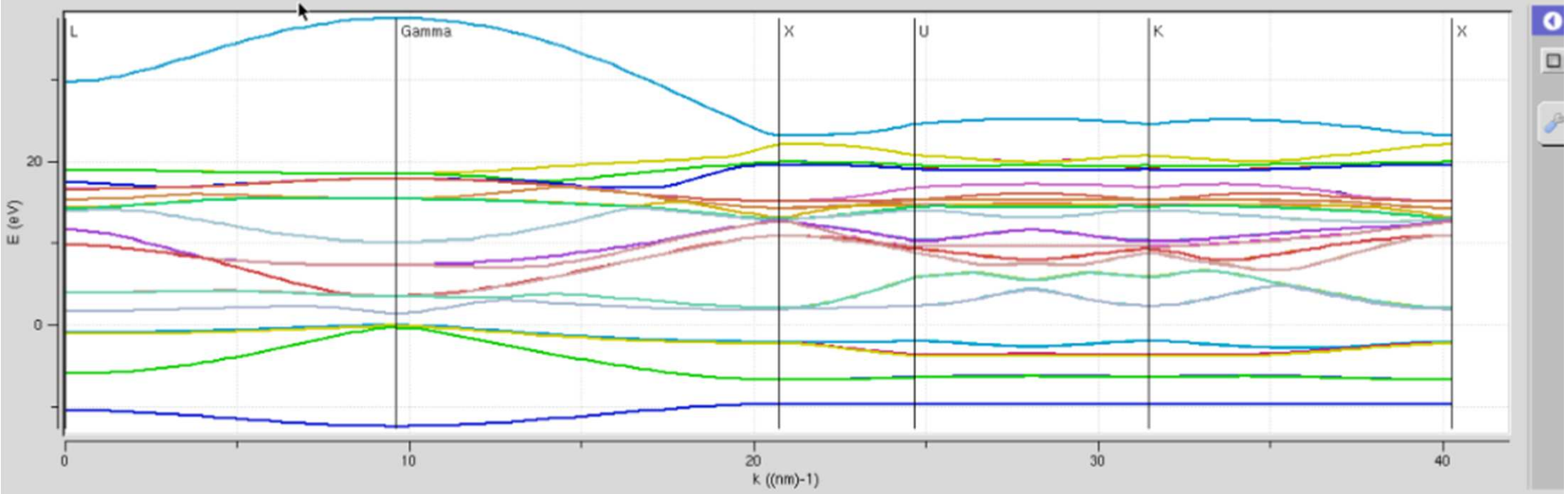
Result: Symmetry points

1 Dimensionality and Material → 2 Device Parameter → 3 Job Description → 4 Simulate

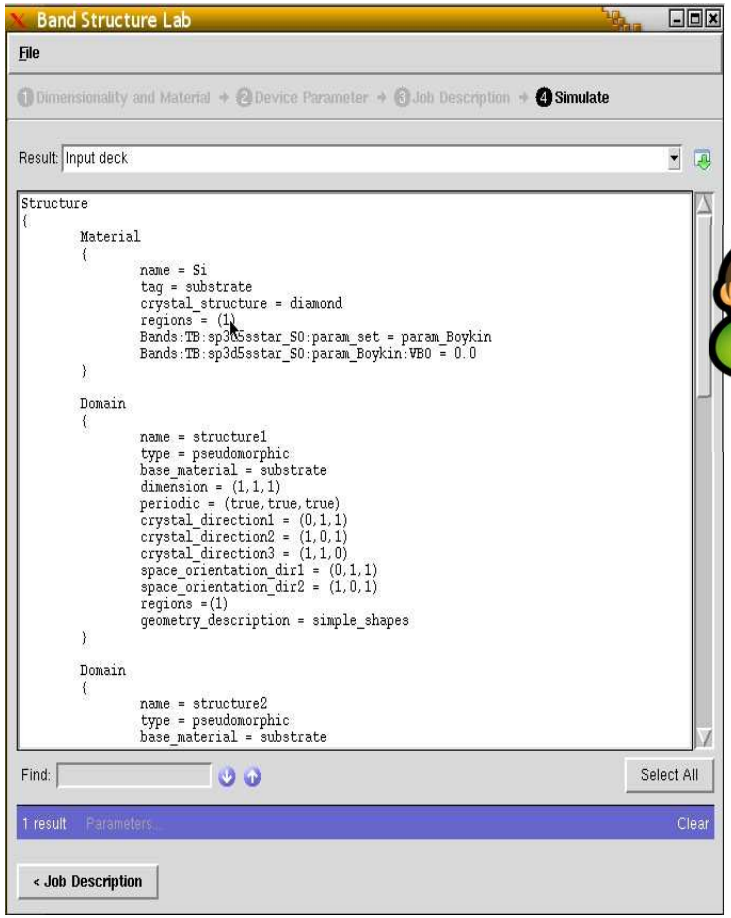
Result: Structure

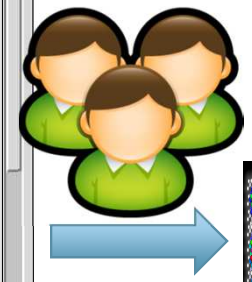
1 Dimensionality and Material → 2 Device Parameter → 3 Job Description → 4 Simulate

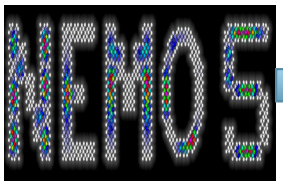
Result: Bands



Results - NEMO5 Input Deck







Band structure

Crystal Structure

Bandgap Info

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Summary

- Band structure
  - Its nature and Importance
- Calculation
  - Tight binding
  - NEMO5
- Band Structure Lab
  - Features and Results

Acknowledgments

- Michael Povolotskyi
- Denis Areshkin
- Prof. Gerhard Klimeck