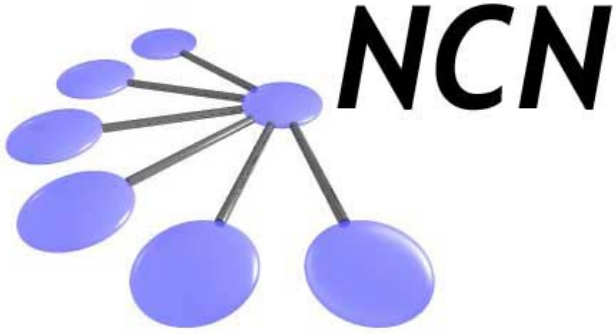
Using NEMO5 to quantitatively predict topological insulator behaviour



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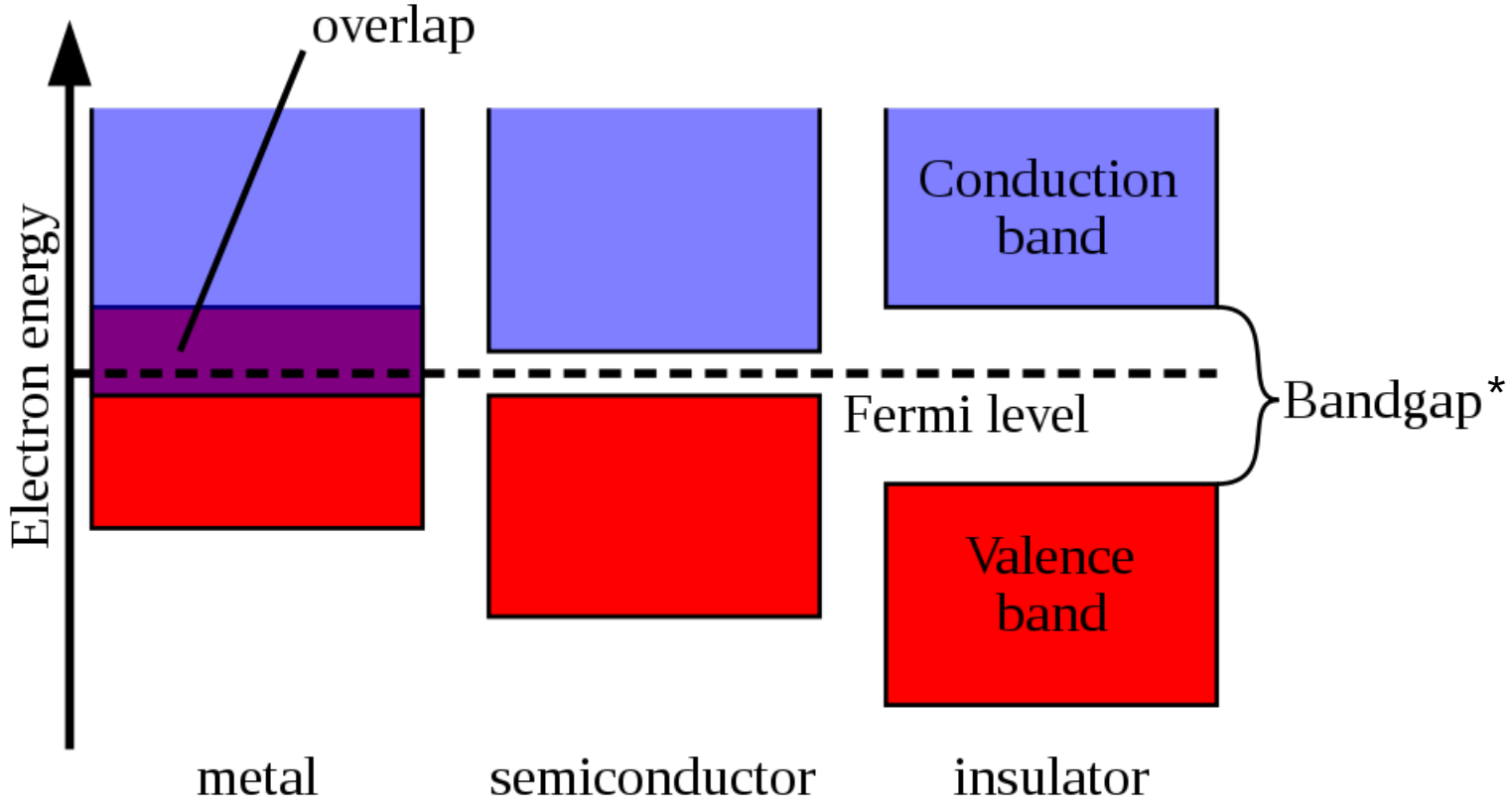
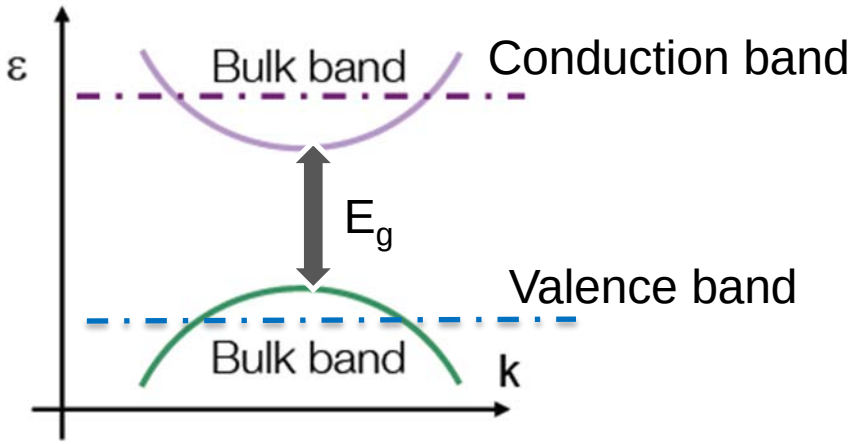
Some commonly known facts



*Wikipedia

A dispersion cartoon



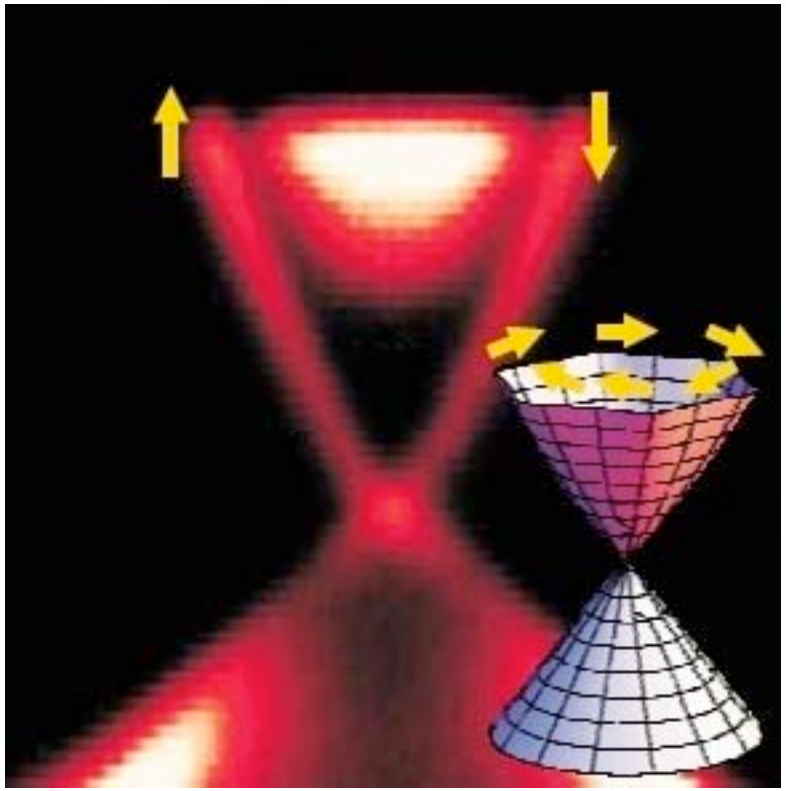
An insulator such as SiO_2, Si_3N_4 with large band-gap

- Conduction and Valence bands describe electrons and holes
- The band gap is zero in a metal

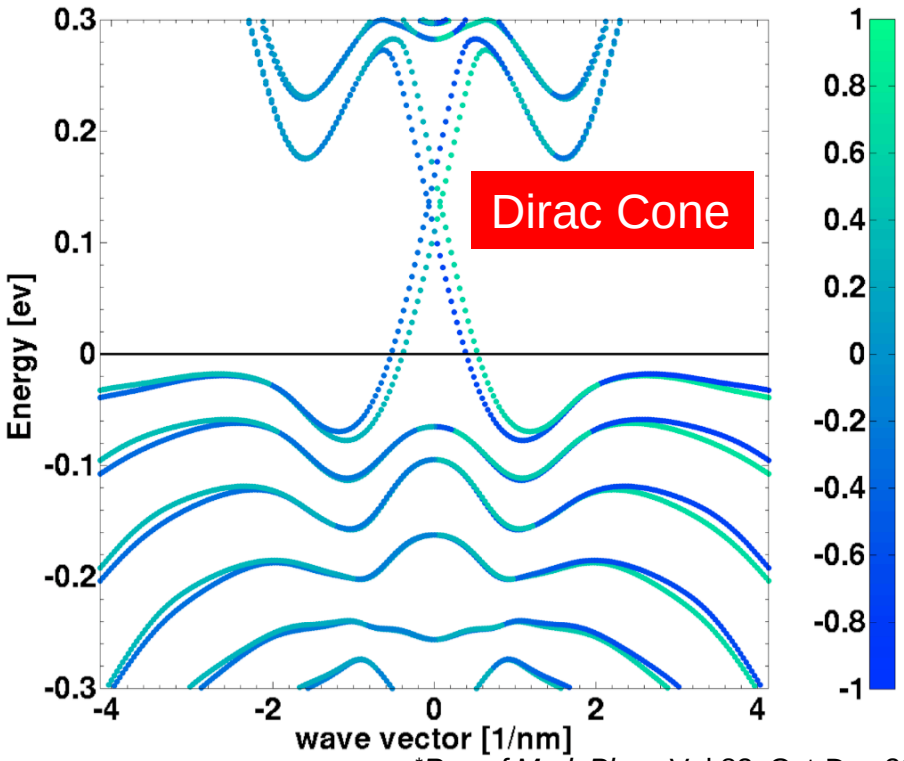
- Some materials possess the dual properties of metals and insulators
- We will use NEMO5 to investigate some of these unique materials

What are these materials?

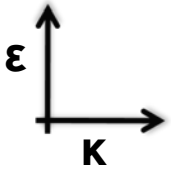
Dispersion obtained through ARPES*



$sp^3d^5s^*$ tight binding calculation



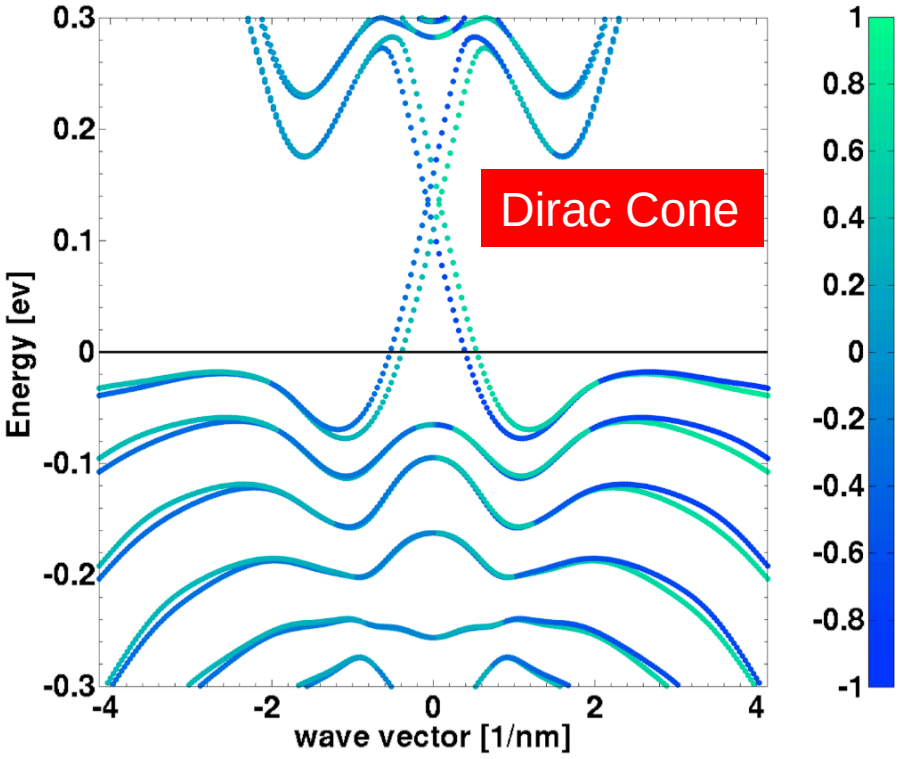
*Rev of Mod. Phys, Vol 82, Oct-Dec 2010



- Primary examples are Bi_2Te_3 , Bi_2Se_3 , Bi_xSb_{1-x} etc…
- They are known as *topological insulators*
- These materials contain bound surface states

Setting up the simulation task

$sp^3d^5s^*$ tight binding calculation



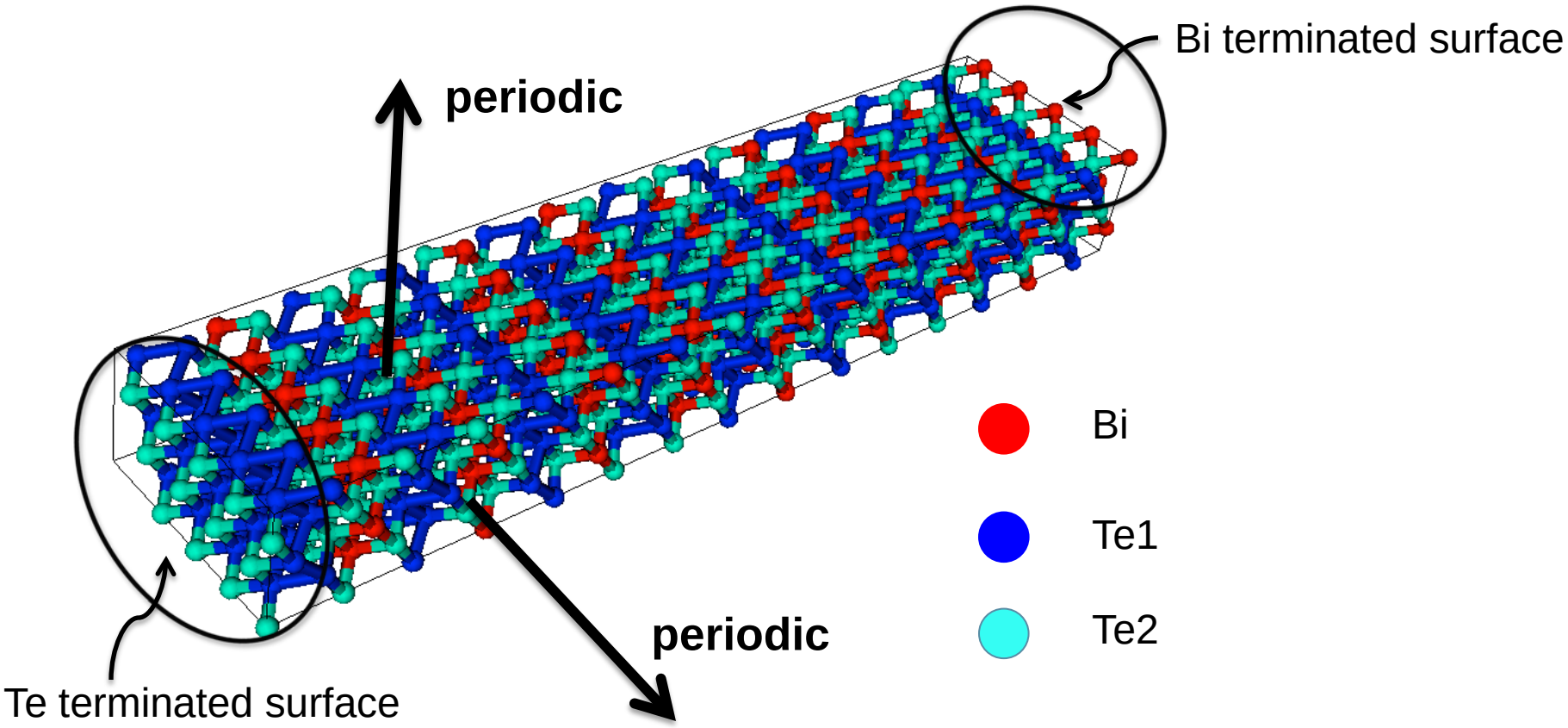
- We will use a $sp^3d^5s^*$ tight binding model
- Bi_2Te_3 is our topological insulator material
- A 9 nm (appx) long quantum well will be the target device
- This will produce a band structure as shown on left

Key feature of this dispersion is a graphene-like linear character (Dirac cone)

Linearity is not due to same reason as in graphene!

Details of the simulation structure

9 nm wide c-axis oriented Bi_2Te_3 thin film



Different surface termination: Surface 1 (2) is Bi (Te2) terminated

The NEMO5 input deck skeleton

There are 3 blocks in the input deck:

```
Structure
{

}
```

→ Defines material and simulation domains

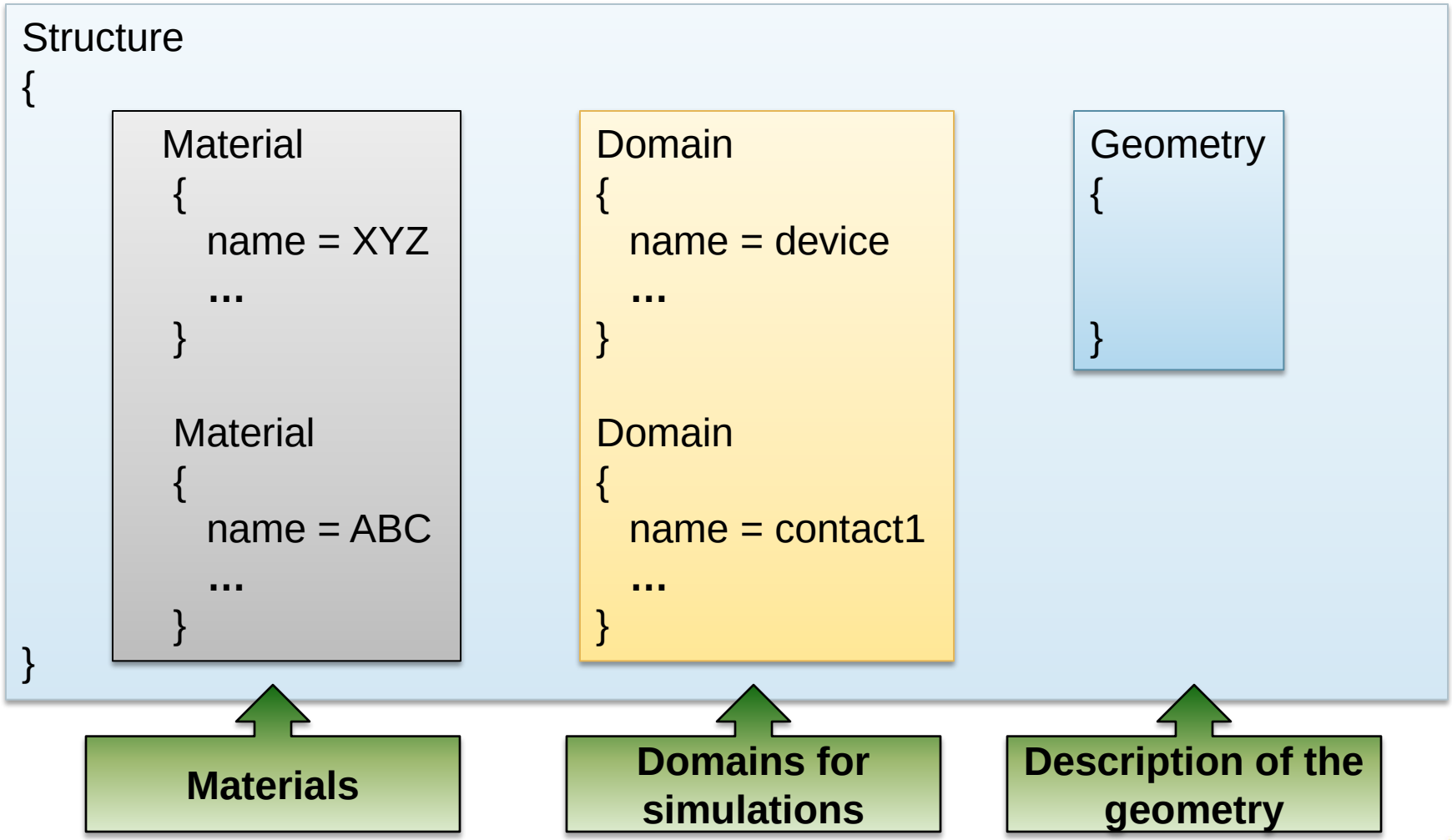
```
Solvers
{

}
```

→ Sets up simulations that has to be solved, e.g. equations, boundary conditions, iterative processes, output, numerical options, etc.

```
Global
{

}
```

→ Defines global variables such as temperature, which database file to use, diagnostic output, etc.

The NEMO5 input deck: The first block “Structure”



Setting the input deck...

```
Structure
{
  Material
  {
   name = Bi2Te3

   tag = shell

   crystal_structure = Bi2Te3

   atom_at_zero = Bi

   regions = (1)
```

- Every input deck begins with the ***Structure*** group
- Each region is identified by a name known as the ***tag***
- The underlying crystal structure of the material needs to be provided
- Each simulation can have multiple ***regions***, NEMO5 needs the exact number of those for correct execution
- The surface atoms can be controlled by asking NEMO5 to place a specific atom when constructing the first unit cell

Defining parameters and the domain

```
Bands:TB:sp3d5sstar_SO:param_Lee_von_Allmen:V_S_S_Sigma_Bi_H    = -10
```

- Any parameter defined in the input deck takes precedence over the corresponding database entry

```
Domain
 {
   name = device

   type = pseudomorphic

   base_material = shell

   dimension = (3,1,1)

   starting_cell_coordinate = (0, 0, 0)

   periodic = (false, true, true)

   passivate = false
```

- ***Dimension*** creates a canvas of unit cells
- Periodicity set as false refers to a confined axis → k is not a good quantum number
- ***Passivate*** options allows inclusion of Hydrogen atoms

Crystal orientation in NEMO5

```
// miller_index_basis = primitive
   crystal_direction1 = ( 0,   0,   1)
   crystal_direction2 = ( 1,   0,   0)
   crystal_direction3 = ( 0,   1,   0)

   space_orientation_dir1 = (0.0, 0.0, 1.0)

   space_orientation_dir2 = (1.0, 0.0, 0.0)

   periodic = (false, true, true)

   regions = (1)
```

space_orientation_dir1 is the z-axis and is confined: the first entry of ***periodic*** option

- Crystal directions set up the coordinate system within the crystal using the basis vectors
- The basis vectors are aligned to the Cartesian axes through the space orientation option
- In this example: crystal_direction1 = (0,0,1) is aligned along space_orientation_dir1 = (0,0,1) or the z-axis.
- You need to specify only 2 directions. N5 computes the third using the crystal structure info.

"*crystal_direction*" & "*space_orientation*": A closer look

```
crystal_direction1 = ( 0,    0,    1)
crystal_direction2 = ( 1,    0,    0)
crystal_direction3 = ( 0,    1,    0)

space_orientation_dir1 = (0.0, 0.0, 1.0)
space_orientation_dir2 = (1.0, 0.0, 0.0)
```

Three vectors in the device_coupling.dat file

1. a = [0 0 3.0487]
2. b = [0.4383 0 0]
3. c = [-0.2191 0.3796 0]

- What NEMO5 internally produces ?
- It produces three basis vectors
- These basis vectors can be obtained by examining the first three lines of the ***device_coupling.dat*** file
- To obtain this file, include ***output = (xyz, coupling)*** in the Domain section. You will see an example of it in your first exercise

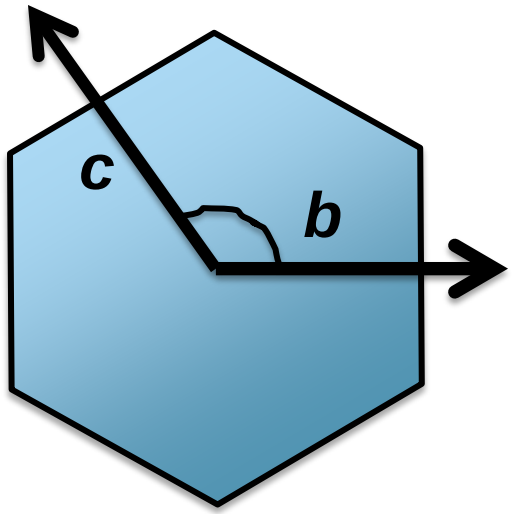
How do you check that these vectors make sense?

All length units are in nm

Reconciling results to known crystal geometry

Our test case here is Bi_2Te_3 which has a hexagonal base

- Each edge of hexagon is 0.4383 nm
- Two hexagons are displaced along z-axis by 3.0487 nm



Three vectors in the ***device_coupling.dat*** file

1. **a** = [0 0 3.0487]
2. **b** = [0.4383 0 0]
3. **c** = [-0.2191 0.3796 0]

Check:

- ✓ Norm of vectors **b** and **c** is equal to 0.4383 nm
- ✓ Norm of vector **a** is equal to 3.0487 nm
- ✓ Angle between **b** and **c** is 120^0 as expected

- Hexagonal base of Bi_2Te_3 quintuple layer
- The vectors **b** and **c** have an 120 degree angle between them

The actual geometry in numbers

```
Geometry
{
    Region
    {
     shape = cuboid

     region_number = 1

     priority = 1

     min = ( -100, -100,  0)
     max = (  100,  100, 10)


    }
}
```

- Shape options allows you to input a geometric shape for your device
- Setting the ***priority*** gives you control over structure creation when dealing with composite geometric shapes.
- ***Higher priority gets constructed first***
- Actual device size is specified through min & max

The NEMO5 input deck skeleton

There are 3 blocks in the input deck:

- ☑ Structure { } → Defines material and simulation domains
- Solvers { } → Sets up simulations that has to be solved, e.g. equations, boundary conditions, iterative processes, output, numerical options, etc.
- Global { } → Defines global variables such as temperature, which database file to use, diagnostic output, etc.

Executing the input deck: The solvers!

```
Solvers
{
  solver
  {
   name        = sim_output

    type       = Structure

    domain     = device

   output_format   = vtk

    structure_file = all_atoms.vtk
```

- Each solver has a name
- The first solver (usually) is the geometry constructor
- The atomic coordinate positions are dumped out in a structure file
- The structure file can have several formats such as vtk, silo, xyz, pdb…

Electronic structure calculation options - I

```
solver
{
    name    = BiTe bands
    type    = Schroedinger
    domain = device

    active_regions = (1)

    job_list = (calculate_band_structure,assemble_H,spin)

    output    = (energies,k-points,spin,eigenfunctions_VTK,orbital_resolved)

    orbital_resolved = true
```

- Electronic structure calculation must set the type to Schroedinger
- ***job_list*** shows what actions N5 must perform
- Setting ***orbital_resolved*** to ***true*** shows the contribution of each orbital to overall band structure

Electronic structure calculation options - II

```
tb_basis = sp3d5sstar_SO

k_space_basis   = reciprocal

k_points = [(0, -0.25), (0.0, 0.25)]

number_of_nodes = (2000)
```

- ***tb_basis*** option lets you choose the band structure calculation model.
- tb_basis can also be set to ***effective mass (em)***
- ***k_space_basis*** can also be set to Cartesian
- Number of nodes → Number of k-points in the chosen k interval

The NEMO5 input deck skeleton

There are 3 blocks in the input deck:

☑ Structure
{
}
→ Defines material and simulation domains

☑ Solvers
{
}
→ Sets up simulations that has to be solved, e.g. equations, boundary conditions, iterative processes, output, numerical options, etc.

Global
{
}
→ Defines global variables such as temperature, which database file to use, diagnostic output, etc.

Putting it all together…

```
Global
{
    solve = (sim_output, BiTe_bands)

    database = ../../../materials/all.mat

    messaging_level = 5
}
```

- The ***global*** section has the command ***solve***: All job names are included under ***solve***
- ***database*** is custom built for N5 and contains all material parameters
- ***messaging level*** indicates ***code progress output*** on screen. Level 5 is verbose

Exercise -I

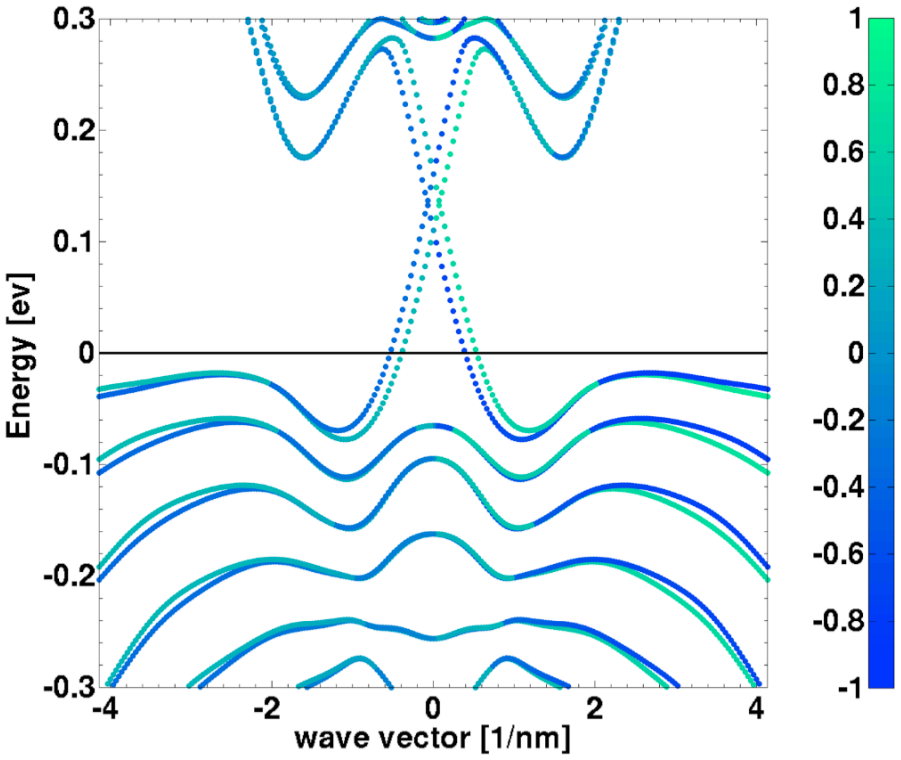
- Log in to your workspace account and create a folder **TI** in your home directory. Navigate to the **TI** folder
  - **mkdir TI**
  - **cd TI**
- Pull the necessary files in your TI folder by typing the following :

  cp ../public_examples/NCN_summer_school_2012/ Topological_Insulators_psengupta/ex*.in .

  cp ../public_examples/NCN_summer_school_2012/ Topological_Insulators_psengupta/spin_analysis_ex*.m .

- **ex1.in** is the input file to calculate the dispersion relationship for a 9.0 (appx) long Bi_2Te_3 quantum well
- Submit a job by typing the command :
  submit -v ncn-hub@coates -i ../all.mat -n 16 -N 8 nemo-r8028 ./ex1.in

What do you expect to see as a solution?



Band structure for a 9.0 nm long Bi_2Te_3 quantum well

- NEMO5 will produce four files (SS12_TI_ex1_*.dat)
- Start MATLAB on your workspace
- Your folder has a MATLAB file called **spin_analysis_ex1.m**
- Execute the MATLAB script by typing **spin_analysis_ex1** at the command prompt
- You will have the figure on your left!

To run Matlab:
$ use matlab-7.12
$ matlab

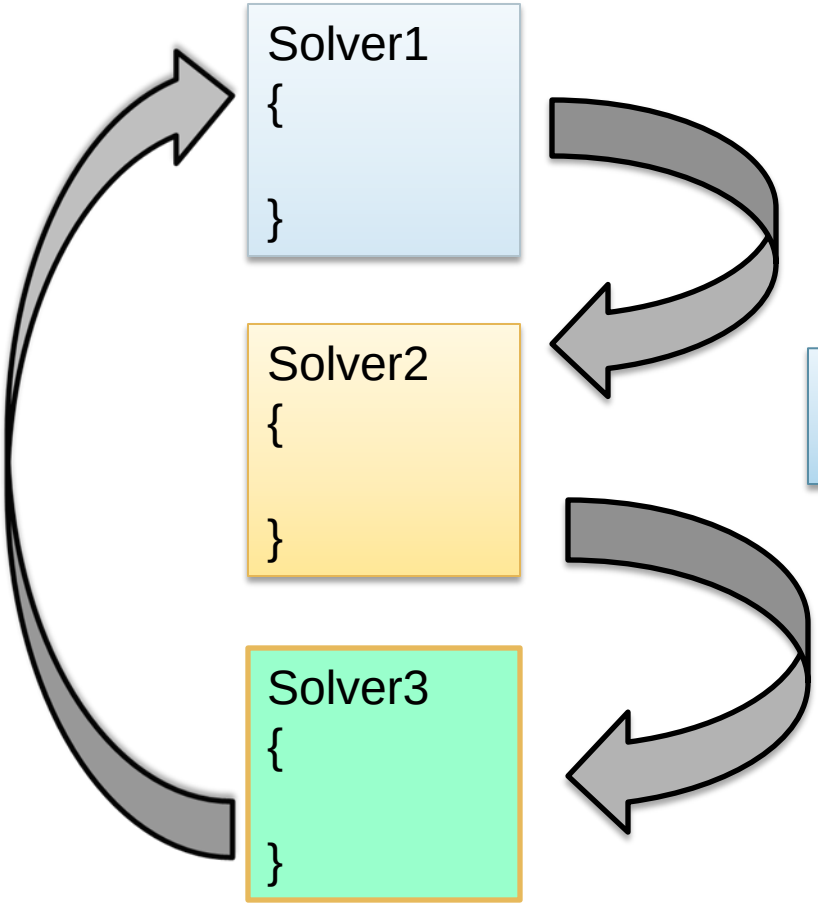
Exercise –I contd…

Pre-computed results are stored in folder /public_examples/NCN_summer_school_2012/Topological_Insulators_psengupta

- Supplementary exercise :
- Change line 20 of the spin_analysis_ex1.m file from the preset
  - ***n = [1 0 0]*** to ***n = [0 0 1]*** and ***n = [0 1 0]***
  - Run Matlab
- The three different spin-polarized plots that you obtain highlight a fundamental theory of TIs

Inter-linking solvers in NEMO5

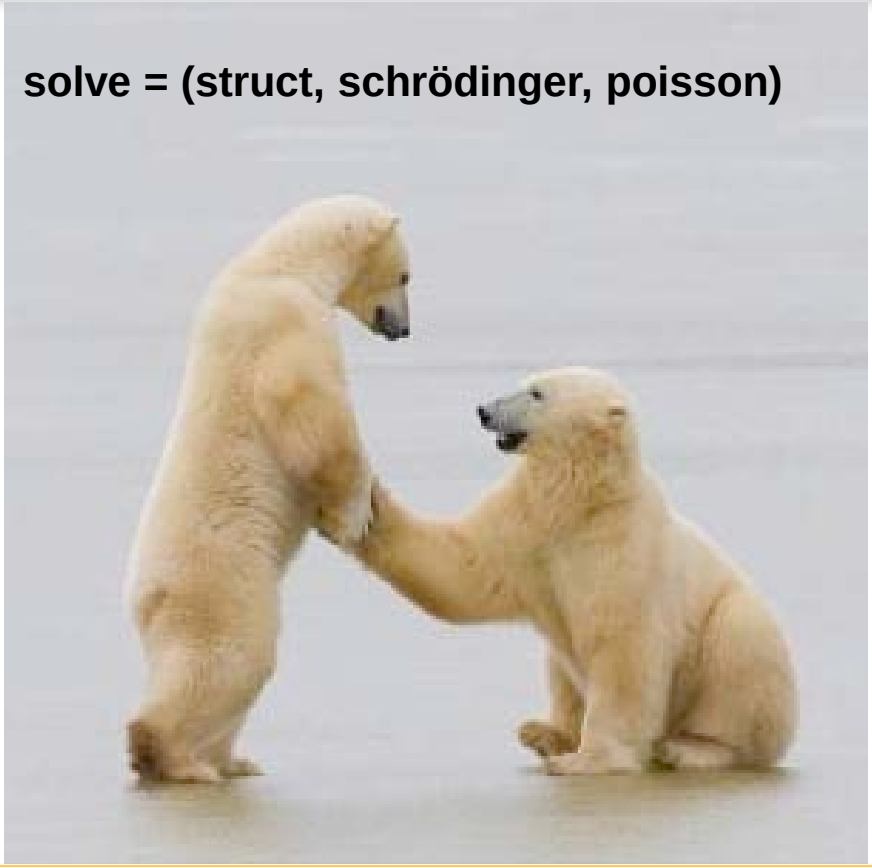
Several solvers defined in the Solver block can be inter-linked:

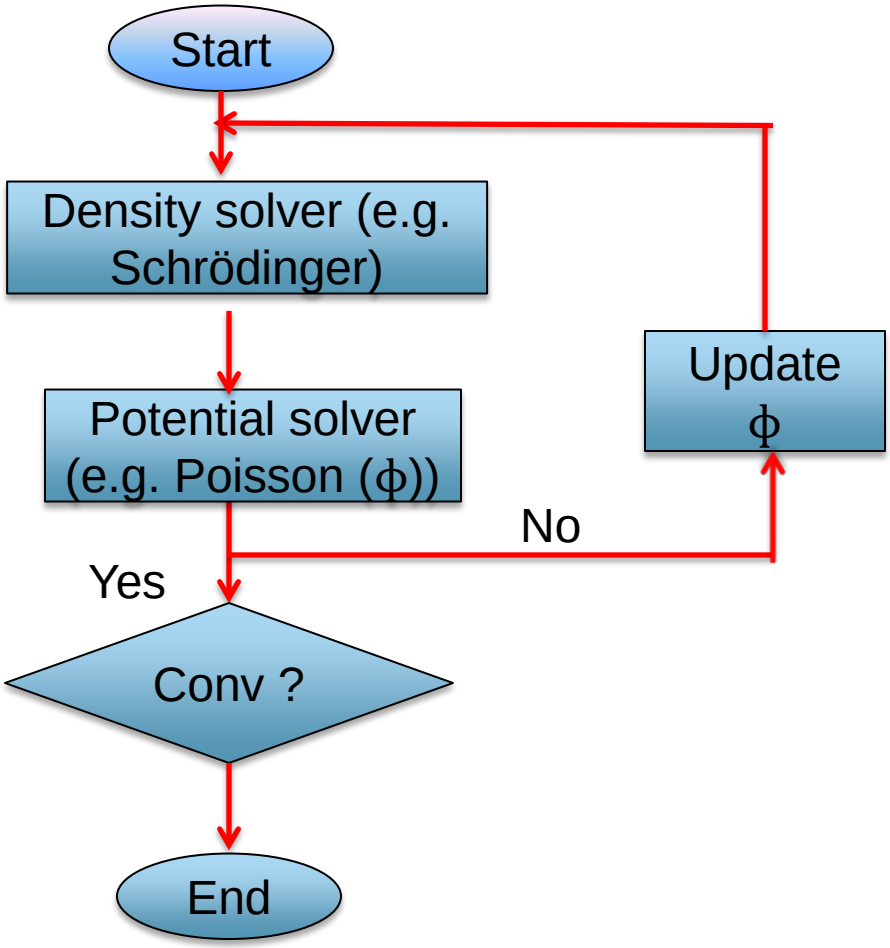


We will see a specific example of this coupling of solvers in the next part of the tutorial

NEMO5 is a toolbox….

solve = (struct, schrödinger, poisson)





Solvers can also speak to one another
- e.g. A self-consistent charge calculation

Setting up the Poisson…

```
solver
{
  name = my_poisson

  type = NonlinearPoisson

  domain = continuum

  ksp_type = gmres
  pc_type = ilu

  atomistic_output = (potential, charge)
  one_dim_output = (potential, charge)
  one_dim_output_average = false
```

- A ***name is assigned to the Poisson solver*** (similar to previous slides)
- A ***non-linear Poisson*** will be solved
- A ***continuum domain*** is constructed
- Linear solver settings
- Electrostatic output option

Linking Poisson to Schroedinger…

```
charge_model = electron_core

rel_tolerance = 1e-6
max_nonlinear_step = 500

density_solver = BiTe_density
}
solver
{
   name    = BiTe_density
   type    = Schroedinger
   domain  = device

job_list = (electron_density,derivative_electron_density_over_potential)
output   = (electron_density_VTK)
```

- Specific model applicable to topological insulators
- Convergence criterion
- The simple linking step done through ***inserting name of desired solver***

- ***job_list*** tells NEMO5 to compute specific physical quantities
- For a self-consistent calculation ***electron density*** is computed

A few options in the density solver

```
charge_model = electron_core
tb_basis = sp3d5sstar_SO
number_of_eigenvalues = 100
```

```
k_space_basis = reciprocal
threshold_energy  = -20
```

```
chem_pot = 0.0
number_of_k_points = 30
potential_solver = my_poisson
```

Inter-linking solvers : ***my_poisson*** and ***BiTe_density***

- First two blocks of input statements are identical to normal eigen value calculations done earlier
- ***threshold_energy*** lets you choose eigen states beginning with energy as set in the option
- ***chem_pot*** is the Fermi level to start calculations
- Schrodinger receives the potential from the ***my_poisson potential solver***

More advanced calculations can use boundary condition options

Implementing boundary conditions

```
boundary_condition
{
  type = NormalField

  type = ElectrostaticContact

  boundary_regions = (1)
  potential = 0.0

  E_field = 7.2e+07
}
```

- Boundary conditions can be of two forms in NEMO5.

1) Dirchlet (potential (ϕ) = constant)

2) Neumann ($\partial\phi$ = constant)

- The input deck statements shown on left can be included multiple times at all possible external boundaries
- The right boundary region number must be specified
- ***E_field*** allows to apply an electric field of certain magnitude to device structure. It is in units of V/cm

Updating Schrödinger for eigen states calculation

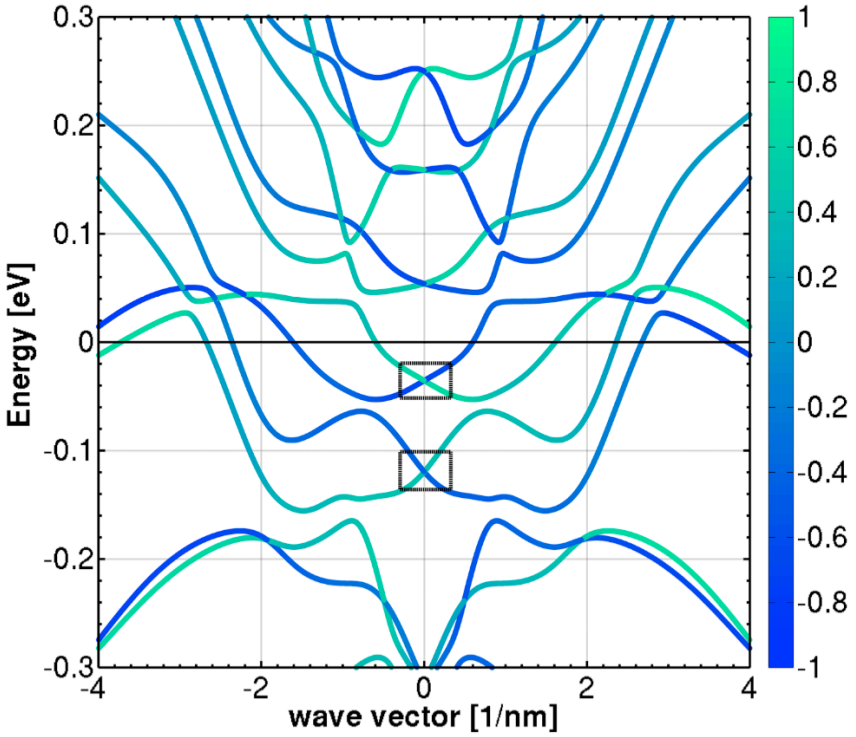
```
tb_basis = sp3d5sstar_SO

k_space_basis   = reciprocal

k_points = [(0, -0.25), (0.0, 0.25)]

number_of_nodes = (2000)

potential_solver = my_poisson
```

- Exactly same format as in Exercise 1
- ***Potential solver*** is added which supplies potential to the ***tight - binding Hamiltonian***

Exercise -II

- **ex2.in** is the input file to calculate charge self-consistent dispersion relationship for a 9.0 (appx) long Bi_2Te_3 quantum well
- This task will produce a dispersion relationship, potential landscape, and the charge profile in the device
- Submit the job by typing the command :
  submit -v ncn-hub@coates -i ../all.mat -n 16 -N 8 nemo-r8028 ./ex2.in

What do you expect to see as a solution?



Self-consistent band structure for a 9.0 nm long Bi_2Te_3 quantum well

- NEMO5 will produce four .dat files (SS12_TI_ex2_*.dat) and a .xy file (poisson_ex2.xy)
- Start MATLAB on your workspace
- Your folder has a MATLAB file called **spin_analysis_ex2.m**
- Execute the MATLAB script by typing **spin_analysis_ex2** at the command prompt
- You will have the figure on your left!

Electrostatic calculations

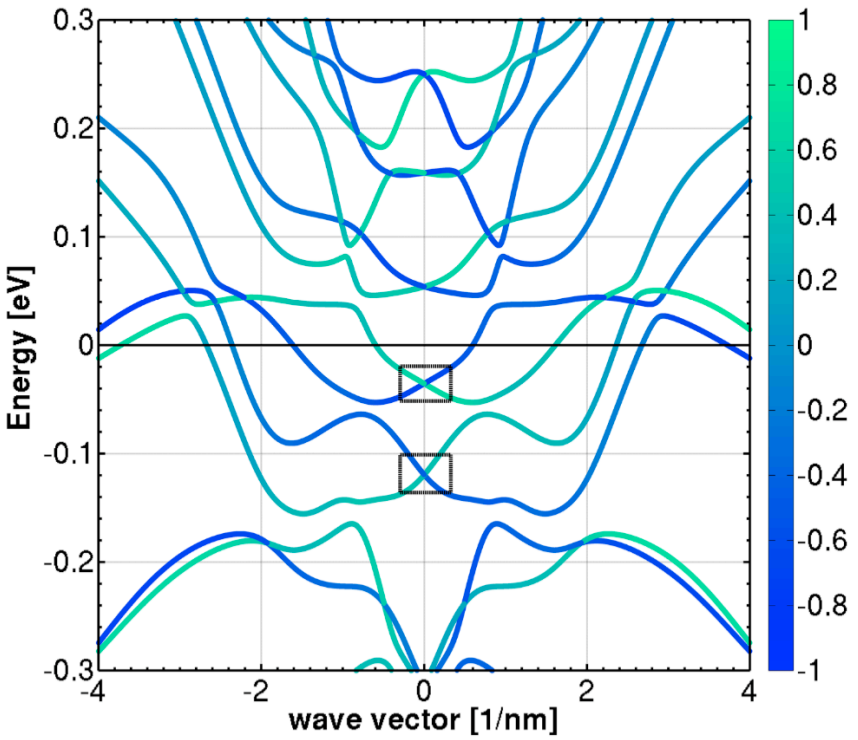
- Use the **poisson_ex2.xy file** (three column file) in your folder to plot the charge and potential profile
- Start MATLAB on your workspace
- Type the following for the charge & potential plot :

```
cp = load('poisson_ex2.xy');

% potential plot
figure(1)
plot(cp(:,1), cp(:,2))

% charge plot
figure(2)
plot(cp(:,1), cp(:,3))
```

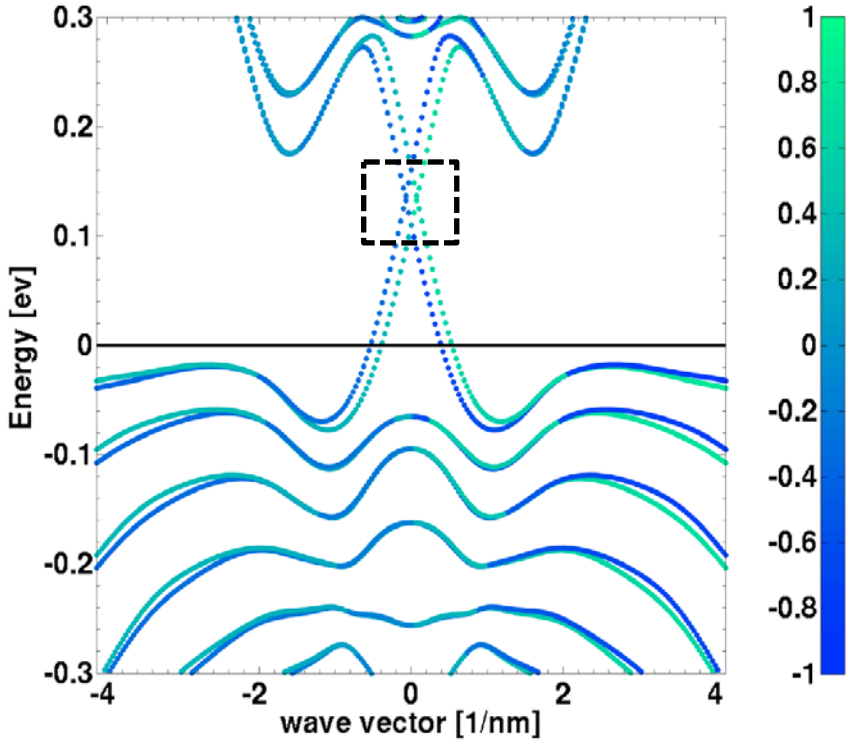
You can also use any plotting software :
Please remember : Column 1 is device coordinate followed by potential and charge data on columns 2 and 3

How do the results from Exercise I and II look like?

Self-consistent electronic structure



Schrödinger 20 band tight binding

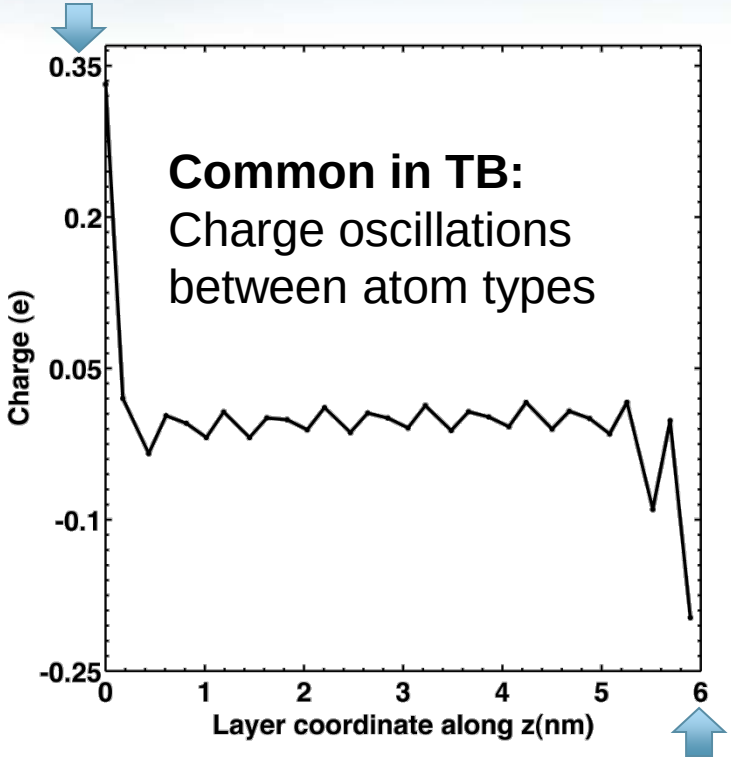


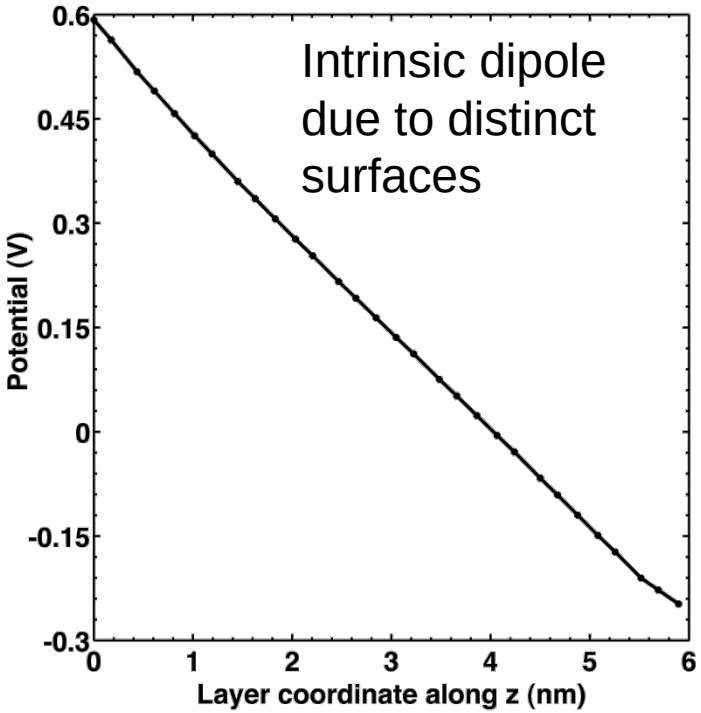
Poisson calculation has large impact:

- Energy separation between Dirac cones gets enhanced
- Fermi velocity of Dirac states changes (mobility)
- Dirac points move below the Fermi level, into the bulk DOS

Self-consistent electrostatic calculations

Bi terminated surf.





Te terminated surf.

- Smooth perturbative potential
- Oscillations in the potential between anion/cation covered by bulk parameters
- Change of charge polarity at two surfaces due to different atomic termination

Conclusion

- Band structure calculations
  - Can handle the newest materials like *topological insulators*
- Charge self-consistent band structure calculation
  - For accurate device prediction
- Use of solvers to accomplish modular tasks
  - *As many solvers* as needed can be added
- Solvers can be inter-linked
  - Simple process accomplished by *inserting appropriate solver name*

Thank you.