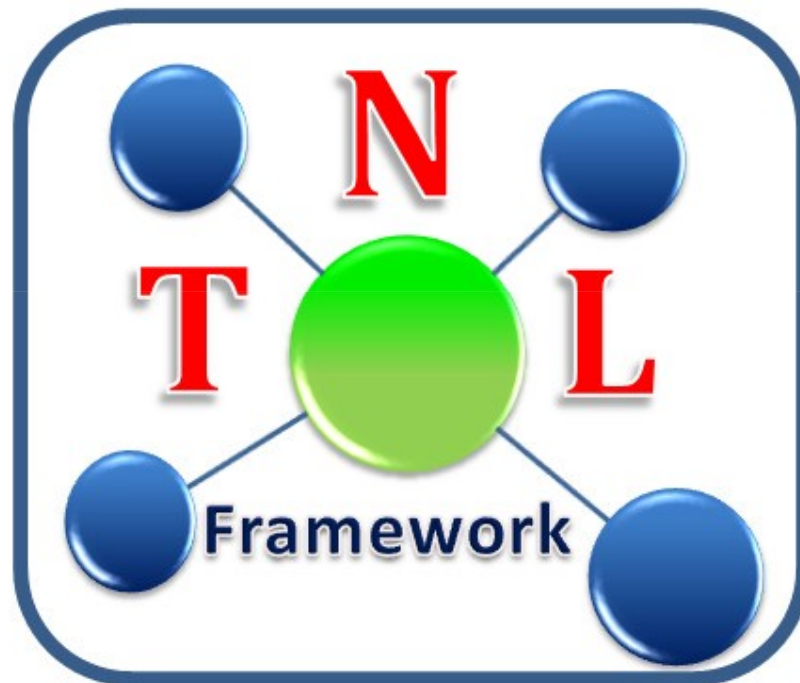




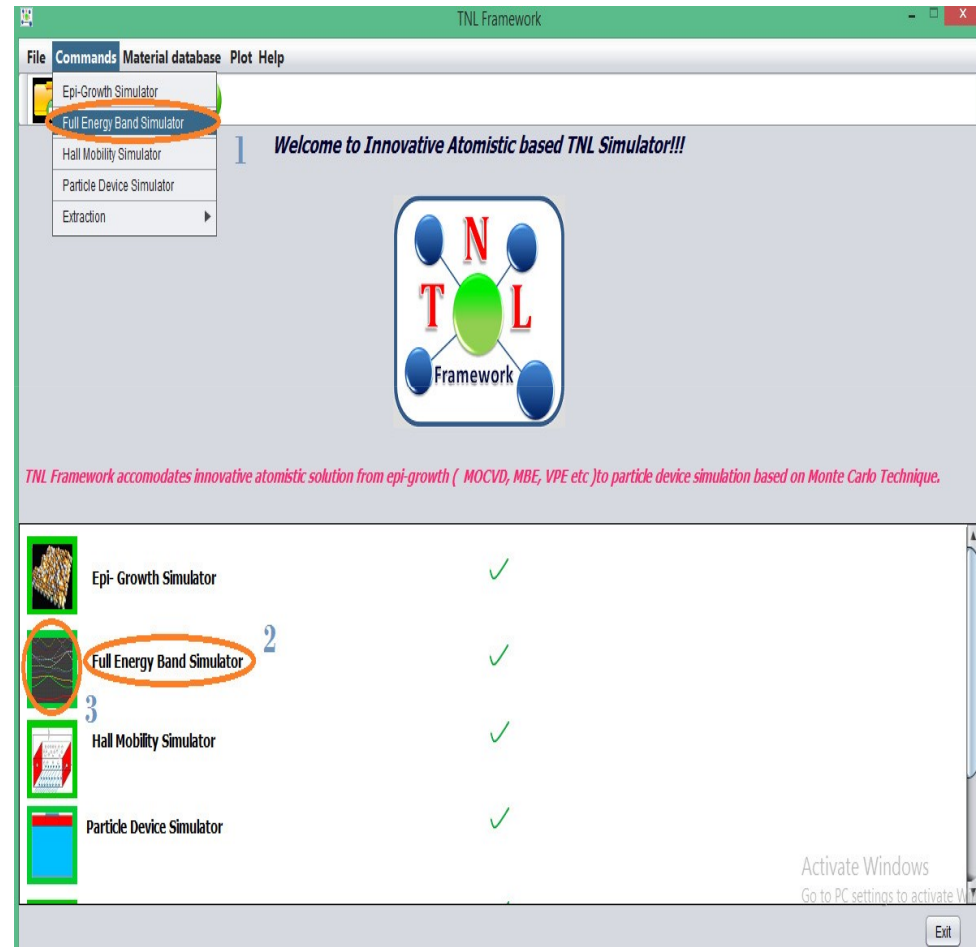
Welcome to TNL Era



FULLBAND Simulator

For invoking FULLBAND Simulator, user has three option.

- Using Menu, choose option 1.
- Using Simulator Yard, user can choose option 2.
- Using Simulator yard user can choose option 3.



FULLBAND Simulator

Fullband simulator consist two type materials.

1. Zincblende
2. Wurtzite

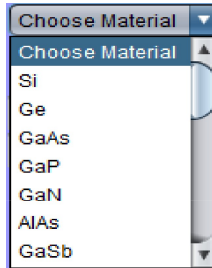
For both case user has to first choose material.

With the help of Load button, load all required data.

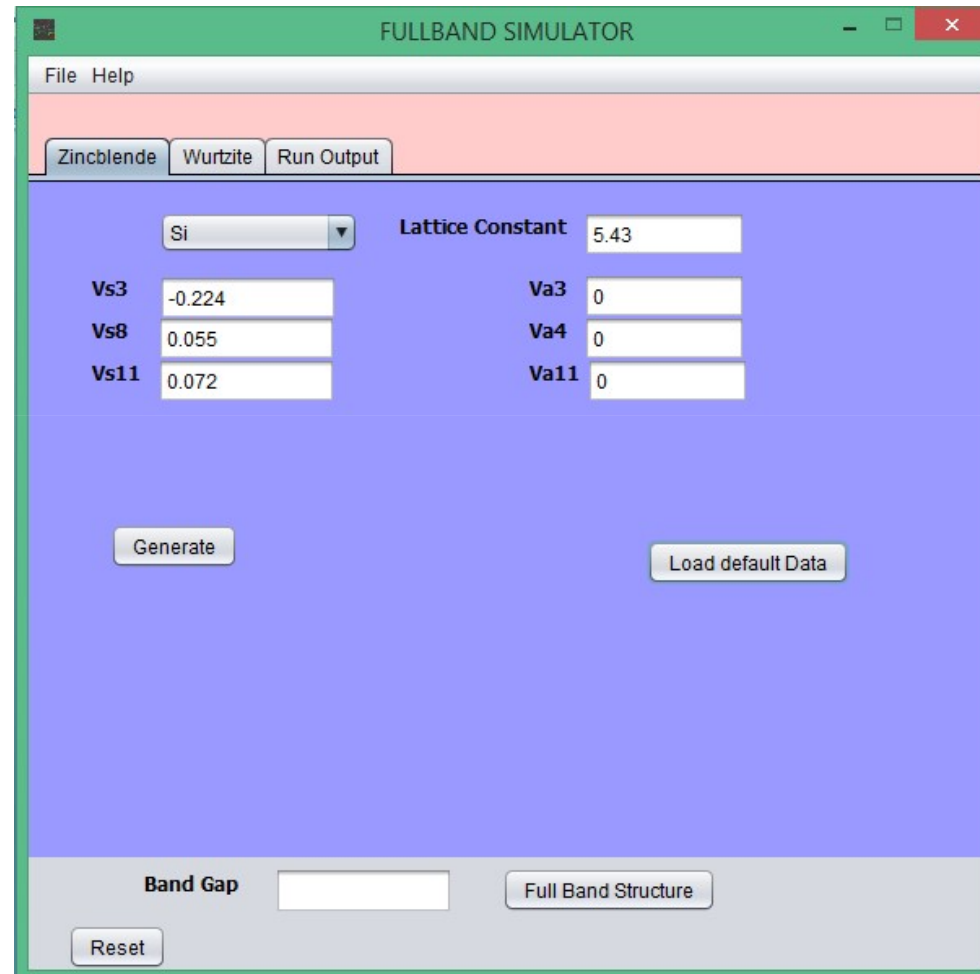
The screenshot shows the FULLBAND SIMULATOR software interface. The window title is "FULLBAND SIMULATOR". The menu bar includes "File" and "Help". Below the menu bar, there are three buttons: "Zincblende", "Wurtzite", and "Run Output". The main area is divided into two columns of input fields. The left column has a "Choose Material" dropdown menu and three input fields labeled "Vs3", "Vs8", and "Vs11", each with a "Default Value" placeholder. The right column has a "Lattice Constant" label and three input fields labeled "Va3", "Va4", and "Va11", each with a "Default Value" placeholder. At the bottom of the main area, there are two buttons: "Generate" and "Load default Data". The bottom bar contains a "Band Gap" input field, a "Full Band Structure" button, and a "Reset" button.

FULLBAND Simulator

- In this tutorial, Select material “Si”(Silicon).



- Click “Load default Data” Button.
- Click “Generate” Button.



FULLBAND Simulator

- In this tutorial, Select material “Si”(Silicon).
- Try with edit Lattice Constant, Form factors values (Vs3,Vs8,Vs11, Va3,Va4 and Va11)
- Click “Generate” Button.
- Get the results.

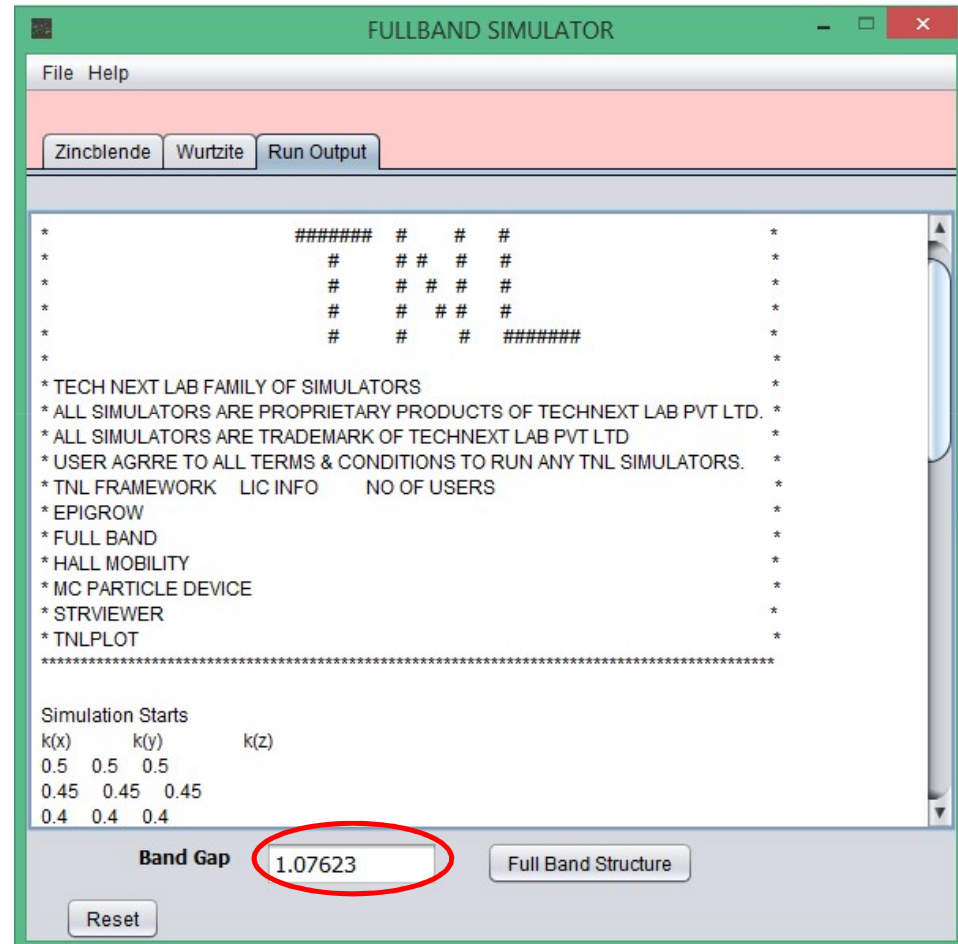
The screenshot shows the FULLBAND SIMULATOR interface. At the top, there is a menu bar with 'File' and 'Help'. Below the menu bar, there are three tabs: 'Zincblende', 'Wurtzite', and 'Run Output'. The main area is divided into two columns of input fields. The left column has a dropdown menu set to 'Si', and three input fields for 'Vs3' (-0.224), 'Vs8' (0.055), and 'Vs11' (0.072). The right column has a 'Lattice Constant' input field set to 5.43, and three input fields for 'Va3' (0), 'Va4' (0), and 'Va11' (0). Below these fields are two buttons: 'Generate' and 'Load default Data'. At the bottom, there is a 'Band Gap' input field, a 'Full Band Structure' button, and a 'Reset' button.

FULLBAND Simulator

Using “Run Output” Tab watch the Simulation output.

Once Simulation completed Successfully.

The Bandgap is “1.07623”.

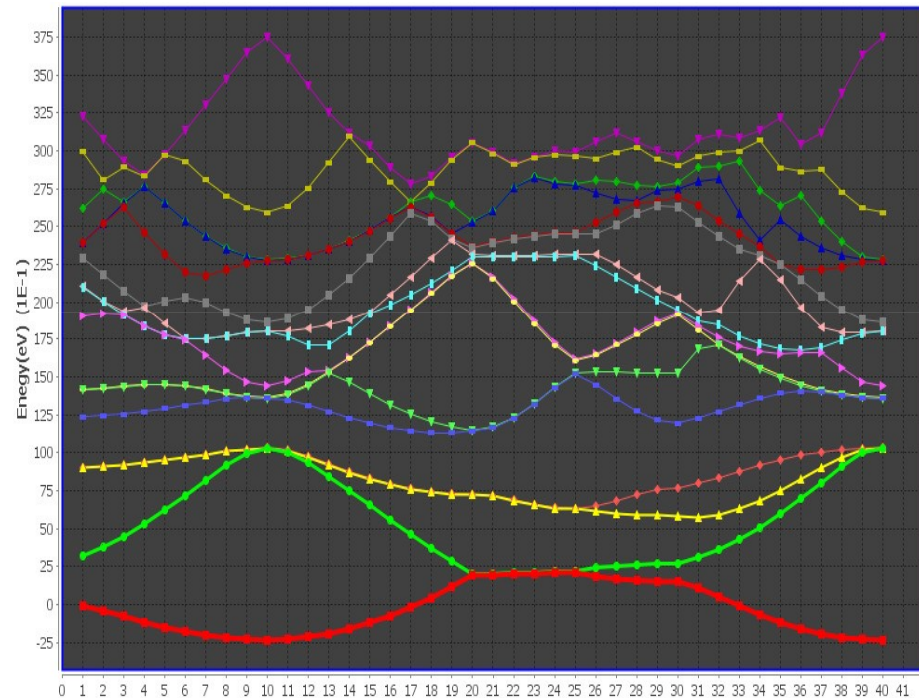


FULLBAND Simulator

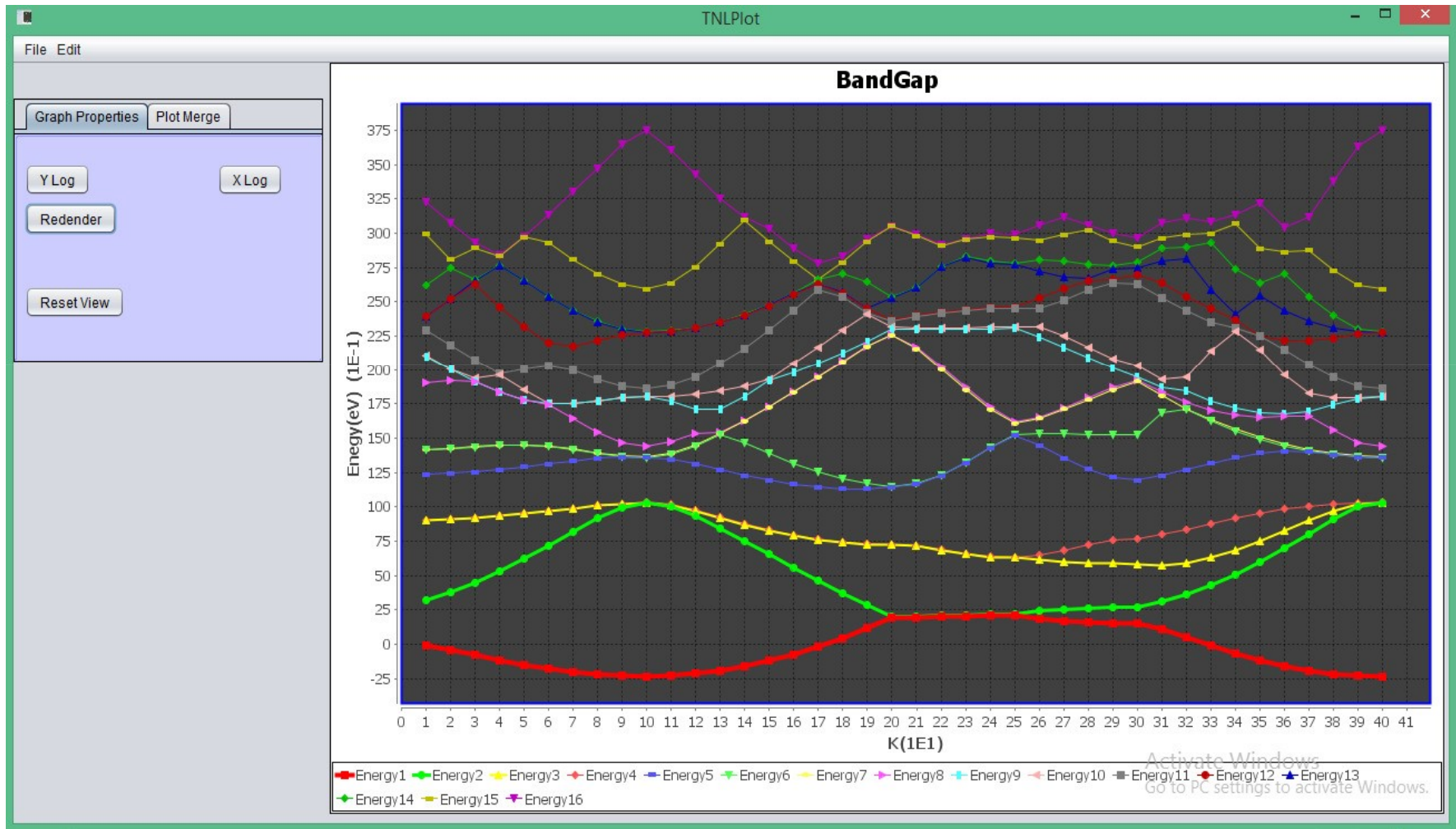
For View full band Structure open “**TNLVIEW**”.

In **TNLVIEW**, open ‘plot’ file, which is generate in same Directory where we save our project before generate.

X Axis shows value of k and Y Axis Shows Energy in eV.

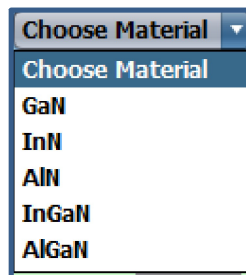


FULLBAND Simulator

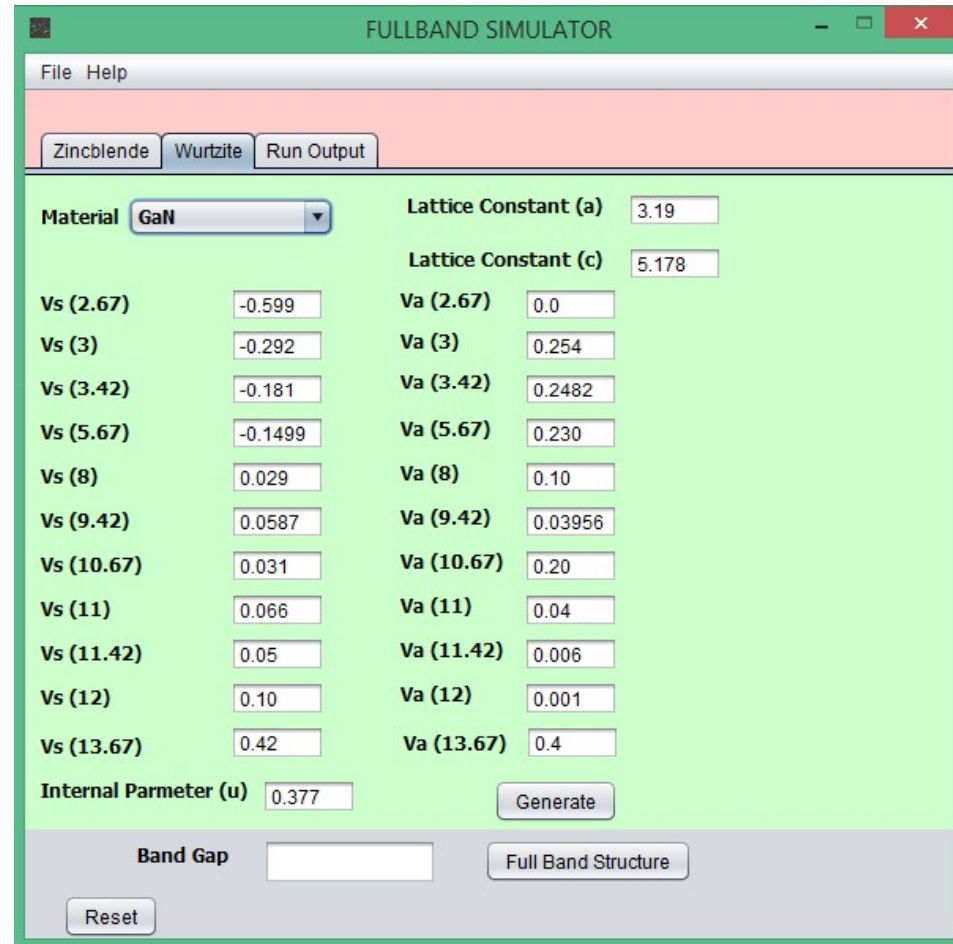


FULLBAND Simulator

- In this tutorial, Select material “GaN”(Gallium Nitride).



- Click “Generate” Button.



FULLBAND Simulator

- In this tutorial, Select material **“GaN”**(Gallium Nitride).
- Try with edit Lattice Constant, Form factors values (Symmetric and Asymmetric)
- Click **“Generate”** Button.

File Help

Zincblende Wurtzite Run Output

Material **GaN** Lattice Constant (a) 3.19 Lattice Constant (c) 5.178

| | | | |
|------------|---------|------------|---------|
| Vs (2.67) | -0.599 | Va (2.67) | 0.0 |
| Vs (3) | -0.292 | Va (3) | 0.254 |
| Vs (3.42) | -0.181 | Va (3.42) | 0.2482 |
| Vs (5.67) | -0.1499 | Va (5.67) | 0.230 |
| Vs (8) | 0.029 | Va (8) | 0.10 |
| Vs (9.42) | 0.0587 | Va (9.42) | 0.03956 |
| Vs (10.67) | 0.031 | Va (10.67) | 0.20 |
| Vs (11) | 0.066 | Va (11) | 0.04 |
| Vs (11.42) | 0.05 | Va (11.42) | 0.006 |
| Vs (12) | 0.10 | Va (12) | 0.001 |
| Vs (13.67) | 0.42 | Va (13.67) | 0.4 |

Internal Parameter (u) 0.377 **Generate**

Band Gap **Full Band Structure**

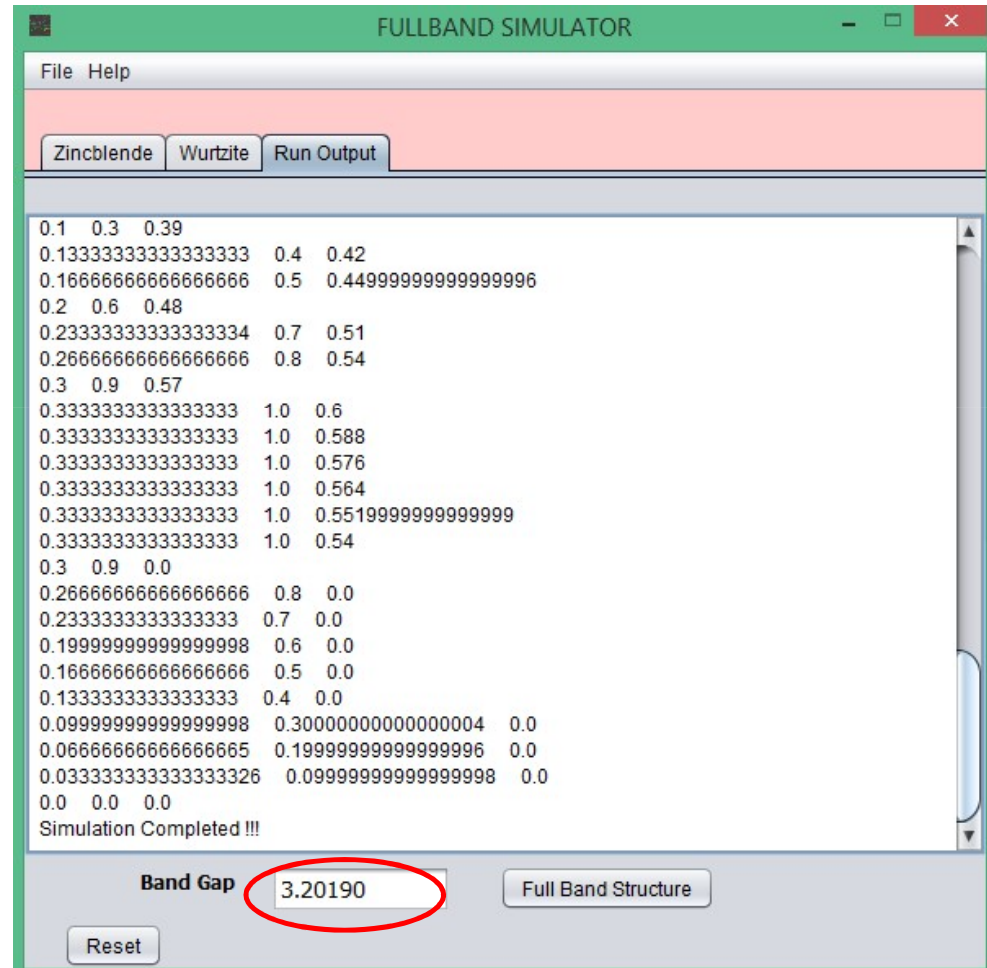
Reset

FULLBAND Simulator

Using “Run Output” Tab watch the Simulation output.

Once Simulation completed Successfully.

The Bandgap is “3.20190”.

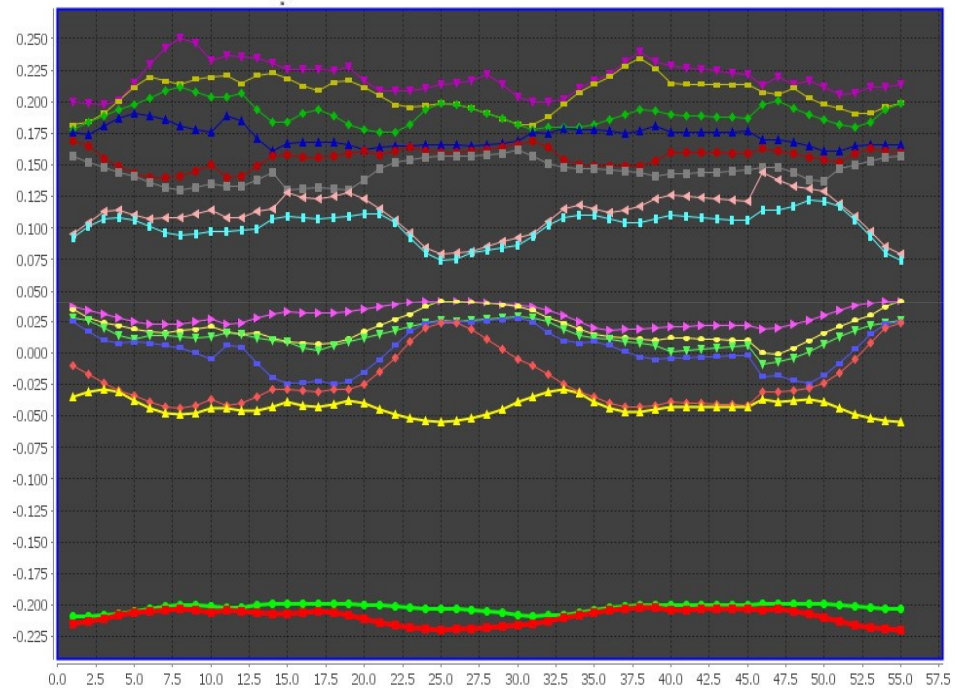


FULLBAND Simulator

For View full band Structure open “**TNLVIEW**”.

In **TNLVIEW**, open ‘.plot’ file, which is generate in same Directory where we save our project before generate.

X Axis shows value of k and Y Axis Shows Energy in eV.



FULLBAND Simulator

