

# **TECH NEXT LAB**

To reduce the technology development cost, time and manpower consumption & to cater semiconductor material industry needs, TNL Material characterization CAD tools are useful and provide flexibilities to do hit & trail on computer.



#### Introduction

Full Energy Band simulator depends upon lattice parameters extracted from the epitaxially grown thin film over TNL-EpiGrow simulator or XRD obtained. Emperical pseudopotential method (EPM) is implemented in TNL-FB simulator. The EPM method involves the fitting of the atomic form factors symmetric Vs(G) and asymmetric Va(G) potentials with the experiment. The main feature of Full Energy Band simulator is to accurately predict the electronic band structures of zincblende and wurtzite materials. Users have flexibilities to adjust the form factors to reproduce the most important band features. Relevant energy spacing's as well as direct and indirect band gaps nature is also be derived from the band structures. The electron effective masses, DOS at high symmetry points are obtain from TNL-FB simulator. The calculated parameters are calibrated and tested against reported existing experimental data and successfully use for interpretation of experiments and for numerical simulation purposes. TNL-FB



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simulator provides flexibility to users to chose lattice constant and analyze the full electronic band structures over computer.

### **Features**

- Electronic structure of the group IV, III-V and II-VI binary compounds
- Lattice constants of binary materials have been used to determine the lattice constant of the ternary alloy through interpolation
- Virtual crystal approximation (VCA) included
- Semi-empirical disorder contribution included
- Different energy valleys
- Local atomic pseudopotentials
- Band structures, reflectivity spectra, electronic densities of states, and valence charge densities

#### Benefits can be realized

- Binary (GaN, GaAs etc.) and ternary (AlGaN, InGaAs etc.)
- Users input lattice constant
- Full Electronic Energy Band
- Extraction of Velocity of carriers in different energy states
- Extraction of Effective Mass of carriers
- Parabolic & Nonparabolic bands effects
- Density of state (DOS) calculation
- Ability to deal with different cubic, Zincblende & Wurtzite alloys
- Carrier's position & energy on different Energy levels in full band