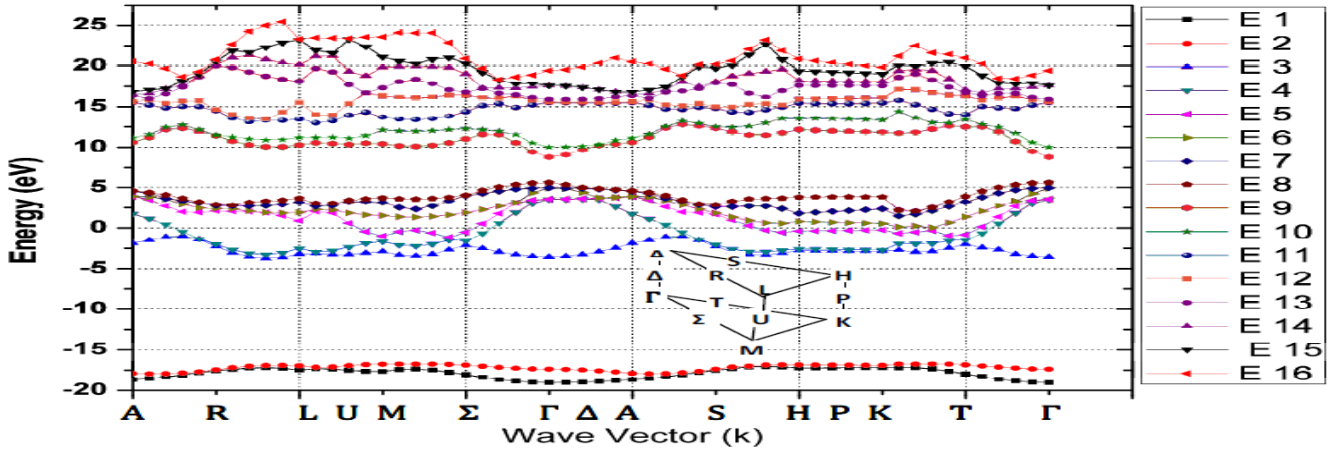
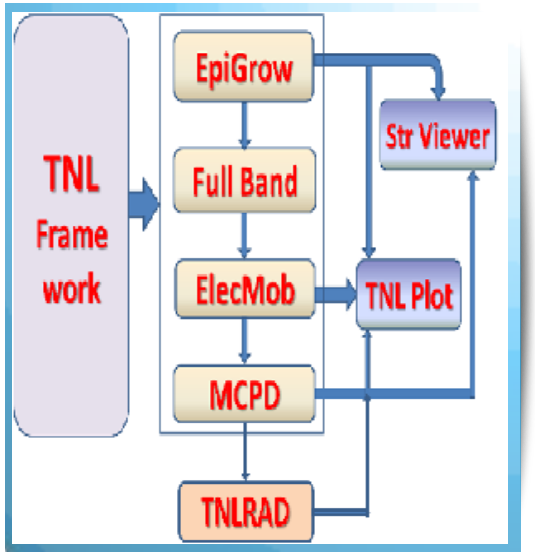
An Atomistic Solution: TNL FullBand (FBS) Simulator

Technology of Next Level
driven through innovation



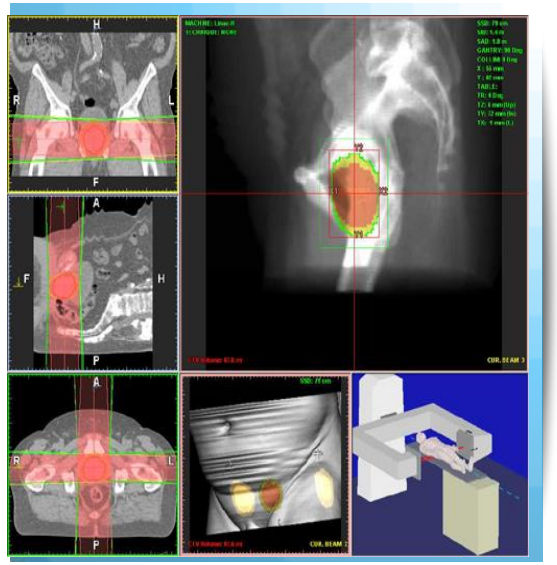
Company Overview



Atomistic TCAD Full Flow

Radiation Monitoring System

Night Vision & Border Surveillance



Medical Radiation Dosimetry

Company Overview

Development Offices

1. Lucknow, UP, India
2. IISC Bangalore, India
3. Hyderabad, India

Sales & Support Offices

1. Delhi
2. Lucknow
3. Hyderabad

Customers

1. Indian Defence Labs
2. Indian Space Labs
3. Universities
4. R & D labs (Europe)
5. Teledyne e2v (USA)

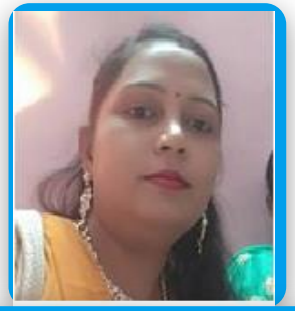
Core Team Members

TCAD Expert
Experience 15 years

Praveen Saxena
Founder & CEO

Material Scientist
Experience 10+ years

Pankaj Srivastava
CPO



Software Engineering
7+ years

Anshu Saxena
Cofounder & Director

Nuclear Scientist
3+ years

Anshika Srivastava
Manager

Device Expert
3+ years

Fanish Gupta
Manager

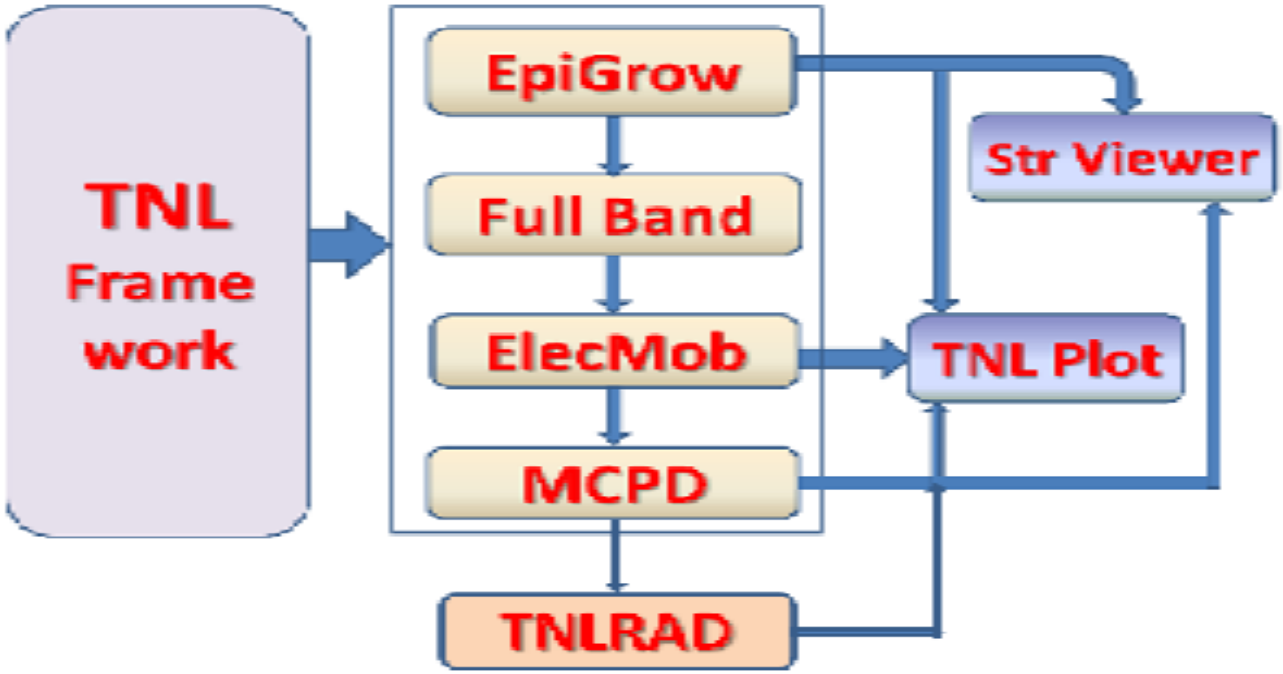
ADVANCE LICENSING & PRICE VALUE

TNL's tools support advanced and unique licensing models tailored for unique customer needs.

➢ ADVANCED LICENSING OPTIONS:

- Term-Based
- Perpetual
- TCAD Academic Suite
- 24x7 Technical Support for **Academic Institutions**

ATOMISTIC TCAD TOOLS



- ❑ Epitaxial Growth Process
- ❑ Material Characterization
- ❑ Material Characterization
- ❑ Particle based Device
- ❑ Impact of Radiation / High Frequency EM waves (under Development)

TNL-FBS SIMULATOR

Free Electrons

- ❑ **Most transport descriptions in semiconductors treat electrons as quasi-free particles**
- ❑ **For free particles, the electron wave function is the solution to the time-independent Schrödinger equation:**

$$\left(\frac{\hbar^2}{2m}\nabla^2 + E\right)\emptyset(r) = 0$$

- ❑ **The solutions form the basis of plane waves:** $\emptyset_k(r) = C_k e^{ik.r}$

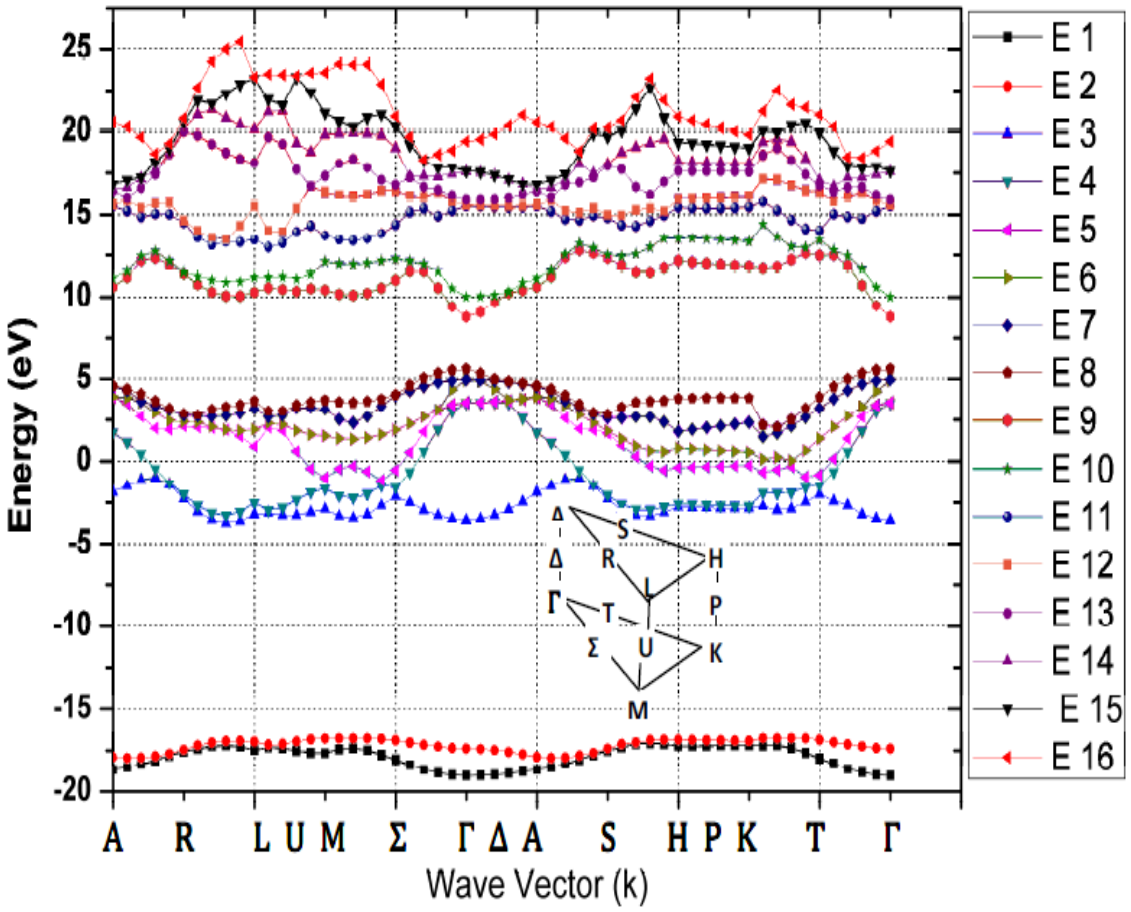
with $k^2 = k_x^2 + k_y^2 + k_z^2 = \frac{2mE}{\hbar^2}$

- ❑ The velocity, **v, of a particle represented by a wave packet** centered around the crystal momentum, **k, is obtained from** the *dispersion relation between* ***k and the energy E as***

$$E_k = \frac{\hbar^2 k^2}{2m} \dots\dots\dots\dots v = < \left|\frac{\hbar}{i}\nabla\right| >= \frac{1}{\hbar}\nabla_k E_k = \frac{\hbar k}{m} \qquad D(E)dE = \frac{2m^{3/2}E^{1/2}}{\sqrt{2}\pi^2\hbar^3}dE$$

Full Band Simulator

- Electronic structure of IV, III-V and II-VI alloys is simulated using standard lattice constant “a” of the compounds.
- Virtual Crystal Approximation used to obtain “a” for ternary alloys.
- Inclusion of a semi-empirical disorder contribution.
- Non-Parabolicity & Parabolicity effects include
- The different parameter of carriers in different bands and valleys.
- The absolute minima of the conduction band of most III-V and II-VI semiconductors lie at the ɾ point.
- Main valleys energies, effective masses with non-parabolicity factors, carrier group velocity, DOS etc.



Full Band Simulator

An optimized Empirical Pseudopotential Method (EPM) in conjunction with Virtual Crystal Approximation (VCA) and the compositional disorder effect are inbuilt in ***FBS Simulator*** for simulation to extract the *ACCURATE* full electronic band structure of various elemental & compound semiconductors to ensure excellent agreement with the experiments.

- Electronic band structure can accurately predict electronic as well as optical properties and work as a source of factual information about semiconductors.
- Electronic band structure is calculated by solution of one electron Schrodinger wave equation
- Relatively easy for calculation of the electronic band structure in contrast to ab-initio methods
- Only valence electrons contribute in calculation of electronic band structure
- Bandgap engineering by introducing impurity can provide useful design guidelines

Group-III Nitrides: Full Band Analysis

Energy difference obtained using FullBand simulator based on the proposed model compared with those reported earlier, with those computed from reported various density functional theory (DFT) techniques and with experimental results

Material	Previously reported values of E_g	E^{LDA}	$E^{LDA-1/2}$	DFT^{PBE}	DFT^{HSE}	Experiments	$E^{This\ work}$
AlN	6.54[7], 6.23[10]	4.50[5,7]	6.06[5]	4.13[7], 4.02[20]	6.42[7], 6.29[20]	6.23[5], 6.026[17], 6.1-6.2[7,20]	**6.20**
GaN	3.5[7], 3.507[10]	2.02[5], 2.11[7]	3.52[5]	1.69[7,20]	3.55[7,] 3.55[20]	3.507[5], 3.35[22], 3.51[20]	**3.47**
InN	0.7–1.0[7,8], 0.7-1.9[10]	-0.03[5], -0.24[7]	0.95[5]	– 0.42[7,20]	0.86[7], 0.86[20]	0.7-1.9[5], 0.6-0.7[20]	**0.7**
$Al_{0.2}Ga_{0.8}N$	3.99*	2.353[5]	3.951[5]	4.570[12]	4.569[12]	3.962[24]	**3.94**
$In_{0.2}Ga_{0.8}N$	2.72-2.78*	1.52[5]	2.76[5]	2.272[5]	1.925[12]	2.625[23]	**2.66**
$In_{0.2}Al_{0.8}N$	4.7 - 4.76*	3.431[5]	4.409[5]	3.445[12]	2.976[12]	4.515[25]	**4.71**

* Scientific Reports, Nature **Journal** **2020**

ZnO: Full Band Analysis

Different DFT based calculated energy band gap of ZnO materials within the conventional DFT (LDA and PBE functional), LDA + U functional, and hybrid functional (HSE06) along with the lattice parameters, structural internal parameters (u) and disorder constants (P). The calibrated energy gap of ZnO materials using FullBand simulator and Experimental band gap are also included for comparison.

DFT Methods	LDA	PBE	HSE06	LDA+U	Experimental	This Work
a (Å)	3.210[3]	3.284[4.5]	3.262[4.5]	3.197[6]	3.253[19-21]	**3.254**
c (Å)	5.136[3]	5.296[4.5]	5.212[4.5]	5.154[6]	5.205[19-21]	**5.21**
u	0.380	0.378	0.381	0.378	0.380	**0.380**
P*	0.000	0.002	-0.001	0.002	0.000	**0.000**
Eg (eV)	**0.7941**[3]	**3.413**[4.5]	**2.464**[4.5]	**1.1541**[6]	**3.44**[3-5]	**3.428**

* Journal of Electronic Materials (under Review).

ZnO: Full Band Analysis

ZnO Samples	t_{DS} (nm)			t_{WH} (nm)	Strain	Lattice Constant		Internal Parameter	Bond Length (Å)	Optical Band gap (eV)	Simulated Band gap (eV)
	(100)	(002)	(101)			a (Å)	c (Å)	u(P)			
Undoped	11	18	10	26	6.5×10^{-3}	3.246	5.238	0.398	2.013	3.22	**3.22**
1at.% **Cd**	16	20	17	13	-8.0×10^{-3}	3.328	5.190	0.4023	2.009	3.20	**3.19**
2at.% **Cd**	19	21	19	26	1.5×10^{-3}	3.332	5.161	0.4025	2.007	3.19	**3.22**
3at.% **Cd**	11	18	10	31	10.0×10^{-3}	3.313	5.225	0.4040	2.006	3.15	**3.15**
1at.% **Sr**	14	10	17	7.48	-1.64×10^{-2}	3.256	5.194	0.389	1.978	3.25	**3.27**
2at.% **Sr**	21	9	16	10.27	4.27×10^{-2}	3.251	5.194	0.389	1.976	3.26	**3.26**
3at.% **Sr**	9	6	6	4.14	9.95×10^{-2}	3.271	5.223	0.389	1.988	3.28	**3.33**
1at.% **Fe**	5	8	9	1.43	-14.8×10^{-2}	3.236	5.194	0.380	1.967	3.24	**3.26**
2at.% **Fe**	3	5	7	0.65	-34.5×10^{-2}	3.231	5.194	0.380	1.968	3.26	**3.25**
3at.% **Fe**	8	5	7	9.06	6.6×10^{-2}	3.231	5.186	0.380	1.970	3.29	**3.25**

Undoped, Cd, Sr and Fe doped ZnO thin films prepared by Sol gel technique along with optical and simulated energy band gaps.

* Journal of Electronic Materials 2021

ZnO: Full Band Analysis

Extracted Alloy disorder parameters for Cd, Sr and Fe doped ZnO thin films deposited by sol-gel spin coating method.

ZnO Samples	Alloy Disorder Parameters (P)
1at.% Cd doped	0.01544
2at.% Cd doped	0.014562
3at.% Cd doped	0.019986
1at.% Sr doped	0.008008
2at.% Sr doped	0.00841
3at.% Sr doped	0.008263
1at.% Fe doped	0.000613
2at.% Fe doped	0.001012
3at.% Fe doped	0.000614

Full Band Simulator

Energy difference at various valleys locations (difference of energies band 9 and band 8) of undoped, Cd, Sr and Fe doped ZnO thin films.

Valley Locations	1%Cd	2%Cd	3%Cd	1%Sr	2%Sr	3%Sr	1%Fe	2%Fe	3%Fe
A	6.022	6.087	6.043	5.659	5.643	5.740	5.488	5.469	5.467
R	8.520	8.563	8.533	8.274	8.265	8.329	8.156	8.143	8.141
L	6.644	6.669	6.620	6.687	6.679	6.736	6.714	6.697	6.692
M	6.712	6.787	6.731	6.377	6.355	6.474	6.229	6.215	6.207
Σ	6.971	6.990	6.936	6.695	6.677	6.787	6.564	6.542	6.535
Γ	3.193	3.222	3.156	3.271	3.255	3.331	3.268	3.253	3.245
A	6.021	6.086	6.043	5.659	5.643	5.740	5.488	5.469	5.467
S	9.499	9.496	9.490	9.541	9.540	9.544	9.551	9.549	9.548
H	8.367	8.368	8.335	8.559	8.551	8.572	8.701	8.700	8.690
K	8.011	8.020	7.980	8.193	8.185	8.214	8.341	8.339	8.328
T	8.580	8.576	8.546	8.805	8.798	8.814	8.944	8.941	8.934

TNL

Thank You

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