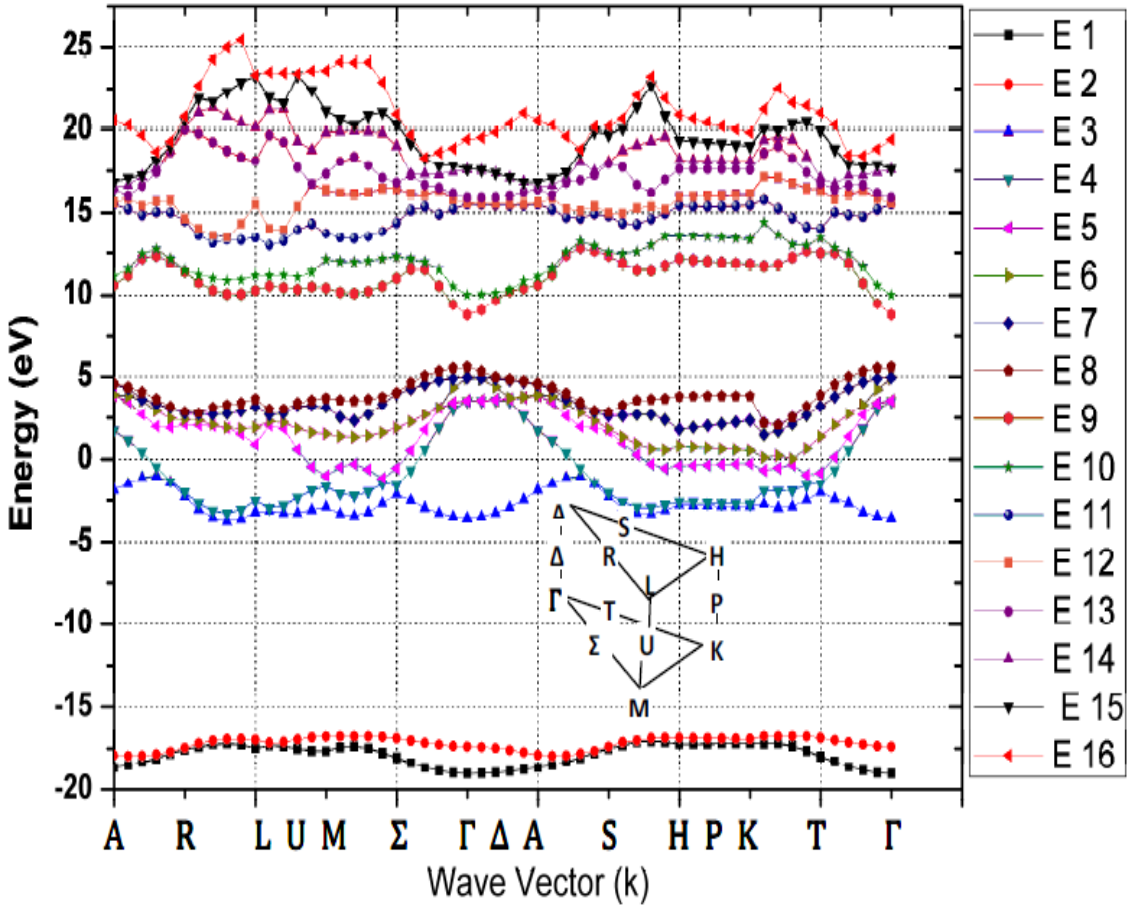
# FullBand Simulator – TNL FBS Simulator

## Case Studies

1. **A detailed full band analysis for Group-III Nitrides (GaN, AlN, InN, InGaN, AlGaN, AlInN etc), Lattice parameters 'a' and 'c' used as input parameters using *TNL-FBS Simulator* have been carried out.**

   **The bandgap at Γ valley have been calibrated against experiments and compared with DFT based calculated energy band gap.**

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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. For more details download full Article: https://www.technextlab.com/Scientific_Report_Nature.pdf

| **Material** | **Previously reported values of $E_g$ (eV)** | **$E^{LDA}$ (eV)** | **$E^{LDA-1/2}$ (eV)** | **$DFT^{PBE}$ (eV)** | **$DFT^{HSE}$ (eV)** | **Experiments (eV)** | **FullBand Simulator (eV)** |
|---|---|---|---|---|---|---|---|
| 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** |

**Here,** Energy difference $(E_g = \Gamma_1^c - \Gamma_8^v)$ obtained using FullBand simulator based on the proposed model compared with those reported earlier, with those computed from previously reported various density functional theory (DFT) techniques and with experimental results. Here suffix represents the reference numbers of above mentioned article.

LDA local density approximation, LDA-1/2 approximately includes the self-energy of excitations in semiconductors, PBE represents Perdew–Burke–Ernzerhof (PBE) exchange energy theory, HSE represents Heyd–Scuseria–Ernzerhof exchange–correlation functional uses an error function screened Coulomb potential to calculate the exchange portion of the energy.

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## 2. A detailed full band analysis for Undoped and Doped ZnO,

**Lattice parameters 'a' and 'c' used as input parameters. The bandgap at Γ valley have been calibrated against experiments and compared with DFT based calculated energy band gap.**

For more details download full Article: https://www.technextlab.com/publication.html

| Parameters | LDA | PBE | HSE06 | LDA+U | Experimental | FullBand Simulator |
|---|---|---|---|---|---|---|
| **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** |
| **$E_g$ (eV)** | **0.7941**[3] | **3.413**[4.5] | **2.464**[4.5] | **1.1541**[6] | **3.44**[3-5] | **3.428** |

Crystallite size determined by DS formula and WH plot, strain, lattice constants and anion-cation bond length for undoped and Cd doped ZnO thin films along with optical and simulated energy band gaps using EPM method with optimized internal parameter (u) at gamma valley.

| 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 | | | |
| Undoped | 11 | 18 | 10 | 26 | $6.5\times10^{-3}$ | 3.324 | 5.243 | 0.4035 | 2.013 | 3.22 | 3.21785 |
| 0.45at.% Cd doped | 16 | 20 | 17 | 13 | $-8.0\times10^{-3}$ | 3.328 | 5.190 | 0.4023 | 2.009 | 3.20 | 3.19845 |
| 0.51at.% Cd doped | 19 | 21 | 19 | 26 | $1.5\times10^{-3}$ | 3.332 | 5.161 | 0.4025 | 2.007 | 3.19 | 3.19286 |
| 0.56at.% Cd doped | 11 | 18 | 10 | 31 | $10.0\times10^{-3}$ | 3.313 | 5.225 | 0.4040 | 2.006 | 3.15 | 3.15996 |