Symmetry Adapted Analysis of Screw Dislocation: Electronic Structure and Carrier Recombination Mechanisms in GaN

Yuncheng Xie, Haozhe Shi, Menglin Huang, Weibin Chu, Shiyou Chen, Xin-Gao Gong

Department of Physics; State Key Laboratory of Surface Physics; Key Laboratory of Computational Physical Sciences (MOE); College of Integrated Circuits and Micro-Nano Electronics, Fudan University, Shanghai 200433, China

arXiv:2601.19240 Accepted for publication in *Physical Review B*.

Motivation and Model

- Screw dislocations reshape carrier dynamics in wide-bandgap semiconductors.
- Standard supercells capture the geometry but hide the helical symmetry.
- We restore the screw group algebra inside the atomistic GaN nanowire model.

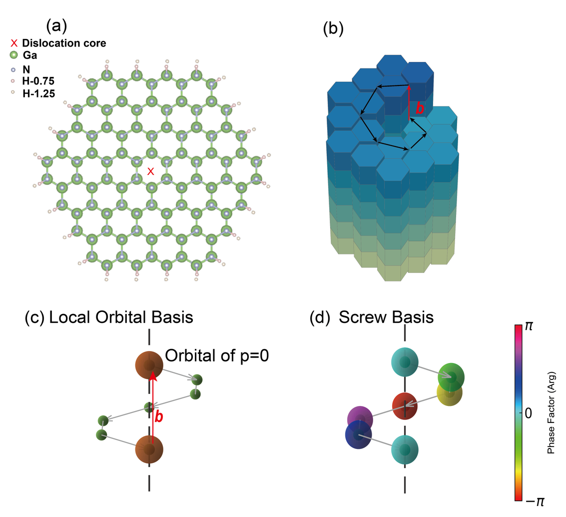

Figure. Passivated GaN nanowire with Burgers vector $\mathbf{b} = [0001]c$ and 6_2 screw symmetry. Localized atomic orbitals are symmetrized into screw-adapted basis functions.

DFT input. HSE06/ABACUS defines H; screw projectors recover μ channels.

Screw Projectors

For an n-fold screw rotation followed by translation mc/n,

$$\lambda_\mu(k_z) = \exp\left[i\left(k_z\frac{mc}{n} + \mu\frac{2\pi}{n}\right)\right].$$

Localized-orbital screw states are constructed by a discrete Fourier projection:

$$|\chi_{p\alpha k\mu}\rangle = \frac{1}{\sqrt{n}}\sum_{j=0}^{n-1} e^{-ij\mu 2\pi/n} \times U_j^{(\alpha)}\,|p,j;\alpha;k\rangle.$$

$$P_\mu(k) = \frac{1}{n}\sum_{j=0}^{n-1}\lambda_\mu(k)^{-j}S^j$$

$$\hat{H} = \bigoplus_{\mu=0}^{5} H_\mu(k)$$

- If $[H,S] = 0$, matrix elements between different μ sectors vanish.
- Each block is diagonalized independently and assigned a screw quantum number.
- The six blocks make μ a working quantum number.
- These labels constrain optical and recombination channels.

Band Flow

For $S = \{C_6 \mid c/3\}$, translating k by $G = 2\pi/c$ shifts the screw label:

$$\lambda_\mu(k+G) = \lambda_{\mu+2}(k).$$

$$\Delta\mu = +2 \pmod 6 \quad \text{for} \quad k \mapsto k+G$$

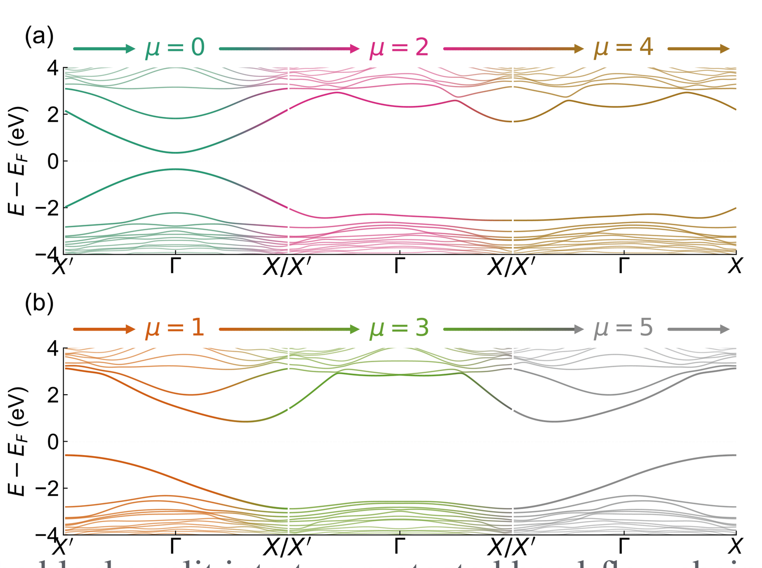

Figure. The blocks split into two protected band-flow chains: $0 \to 2 \to 4 \to 0$ and $1 \to 3 \to 5 \to 1$.

Block-Diagonal Hamiltonian

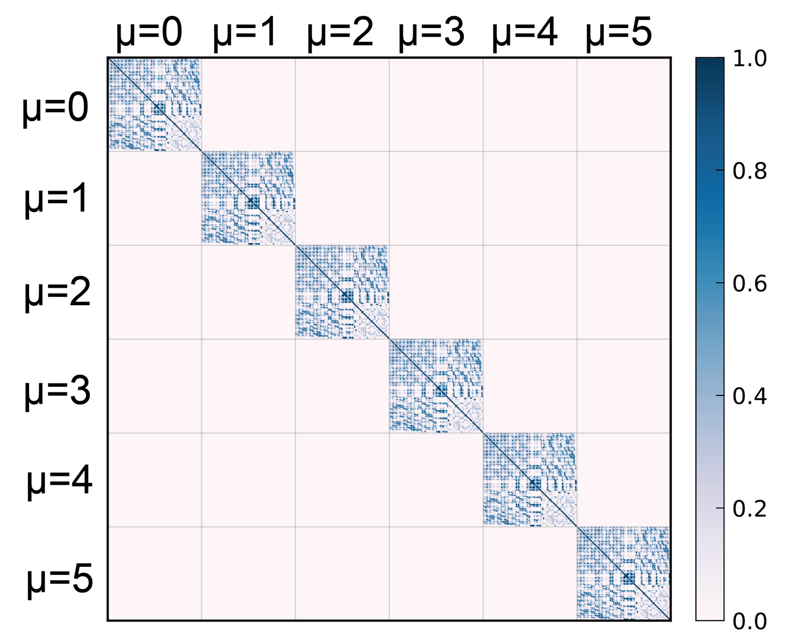

Figure. In the screw basis, the localized-orbital Hamiltonian separates into six independent symmetry blocks.

- **Projector verification:** the heatmap directly checks the screw-adapted construction.
- **No spurious mixing:** different screw representations remain separated.
- **Good quantum number:** eigenstates are labeled by $\mu = 0, \ldots, 5$.

Electronic Structure

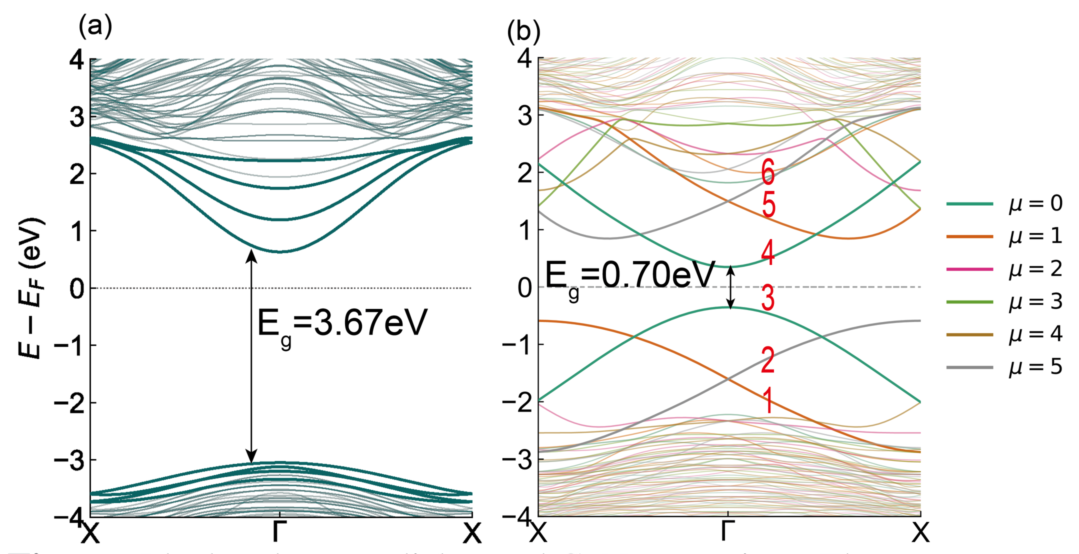

Figure. Ideal and screw-dislocated GaN nanowires. The screw core creates six localized gap states and reduces the gap from 3.68 eV to 0.70 eV. Colors label the dominant μ character.

- **Core-localized states** originate mainly from $\mu = 0, 1, 5$.
- **States 3 and 4** closest to the Fermi level both belong to $\mu = 0$.
- **Gap collapse:** the screw core creates a 0.70 eV infrared channel.

$\mu_3 = \mu_4 = 0$: symmetry allowed, but spatially weak.

Optical Selection Rules

The dipole component $d^{(m)}$, with $m = 0, \pm1$, carries angular momentum under the screw rotation:

$$\langle \psi_f^{(\mu_f)}|d^{(m)}|\psi_i^{(\mu_i)}\rangle \neq 0 \;\Rightarrow\; \mu_f - \mu_i \equiv m \pmod 6.$$

Polarization	m	Rule	Meaning
$\boldsymbol{E} \parallel \hat{z}$	0	$\Delta\mu = 0$	intra-block
σ^+	+1	$\Delta\mu = +1$	screw momentum +1
σ^-	−1	$\Delta\mu = -1$	screw momentum −1
$\boldsymbol{E} \perp \hat{z}$	±1	$\Delta\mu = \pm1$	transverse

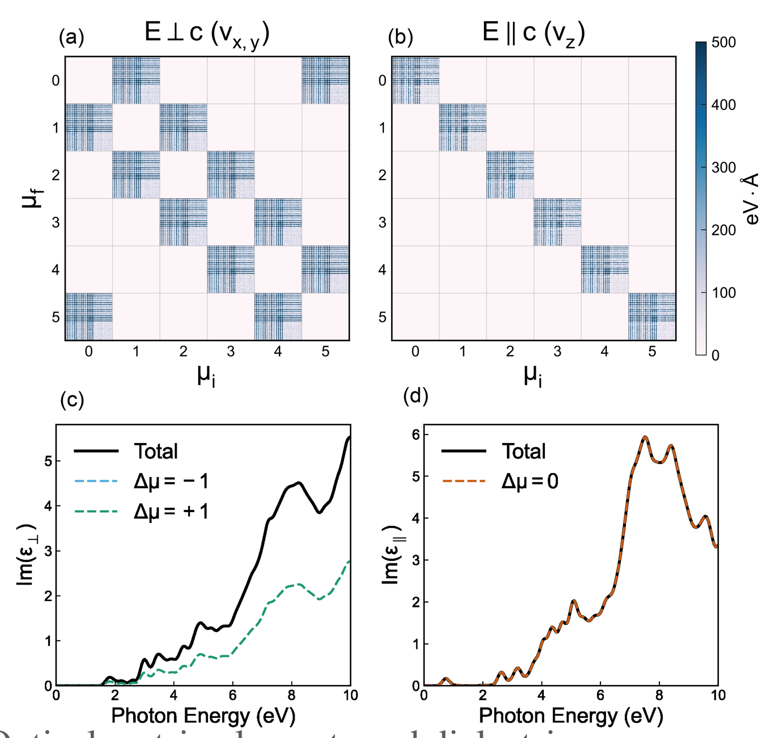

Figure. Optical matrix elements and dielectric response confirm the rule: transverse components occupy $\Delta\mu = \pm1$, while axial polarization remains in $\Delta\mu = 0$.

Carrier Separation

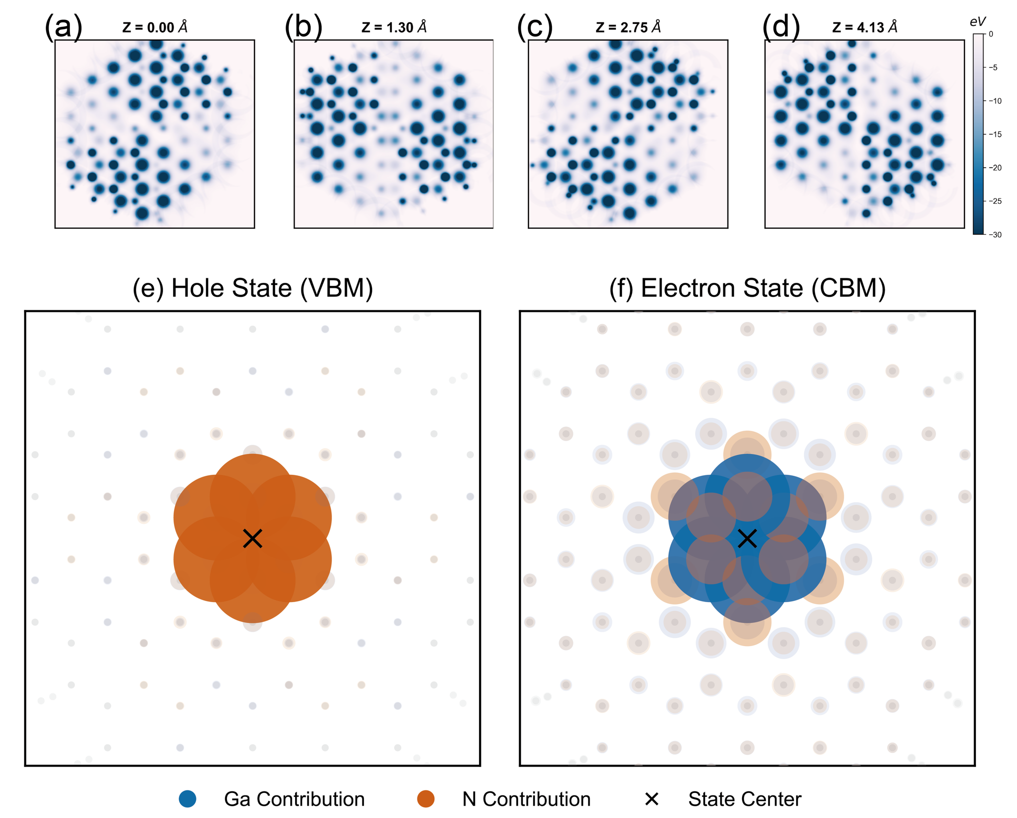

Figure. The screw core produces a rotating electrostatic potential. State 3 is N dominated, while state 4 is Ga dominated, giving spatially separated hole and electron densities.

- **Screw piezoelectric fields** separate carriers near the core.
- **Quasi-quantum-well behavior** weakens electron-hole wave-function overlap.
- **Dipole quenching:** spontaneous emission scales with $|\mathbf{d}_{fi}|^2$.

Radiative Suppression

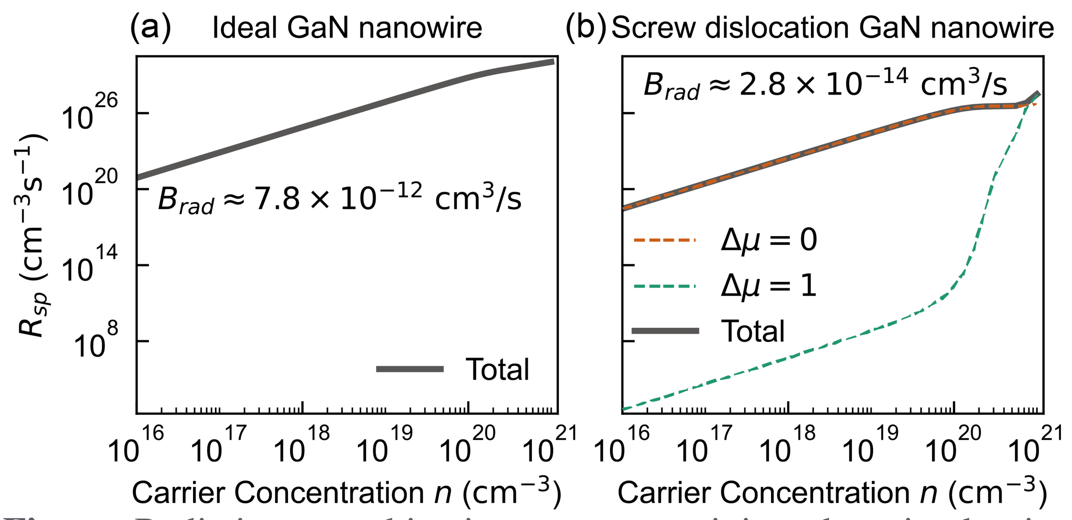

Figure. Radiative recombination rates versus injected carrier density. The screw core suppresses radiative recombination by two to three orders of magnitude relative to the ideal nanowire.

The dominant low-density radiative transition is the $\Delta\mu = 0$ channel between states 3 and 4 near Γ. It emits near 0.7 eV with polarization parallel to the screw line.

$$B_{\text{rad}} = 2.8 \times 10^{-14}\ \text{cm}^3\ \text{s}^{-1}$$

- **Two to three orders lower** than the ideal nanowire.
- **Symmetry allowed** yet spatially quenched by carrier separation.

Nonradiative Capture

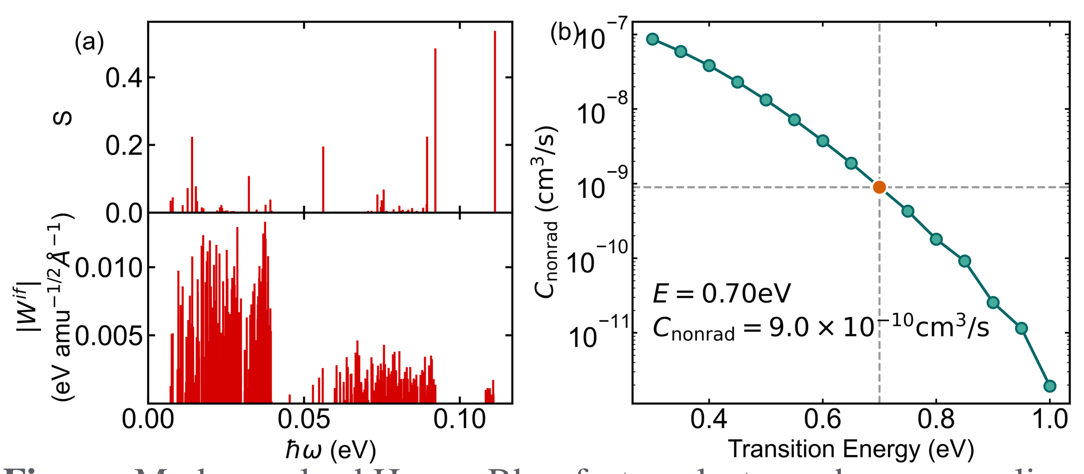

Figure. Mode-resolved Huang-Rhys factor, electron-phonon coupling, and nonradiative capture coefficient. Low-frequency modes dominate the electron-phonon coupling.

Although the total Huang-Rhys factor is moderate, $S = 2.6$, the small 0.70 eV gap enables efficient multiphonon capture:

$$C_{\text{nonrad}} = 9.0 \times 10^{-10}\ \text{cm}^3\ \text{s}^{-1} \quad (300\,\text{K}).$$

- **Dominant loss channel:** nonradiative capture takes over after the gap collapses.
- **Low-frequency modes** supply the strongest electron-phonon coupling.

At room temperature, the screw core favors fast nonradiative decay.