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Abebe Mulatu

abebe.tadesse2@aau.edu.et

Wolkite University

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A Drude-Augmented Kramers–Kronig Framework for Predicting Optical Properties of Substitutionally Doped Low-Dimensional Semiconductors: Application to (8,0) SiC Nanotubes

Abebe Tadesse Mulatu

Physics Department, Wolkite University, Wolkite, Ethiopia

abebe.tadesse2@aaau.edu.et

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Abstract

We present a **generalizable computational framework** that combines a Kramers–Kronig transformation with a Drude free-carrier term to predict the optical and dielectric properties of substitutionally doped low-dimensional semiconductors. The framework is designed as a fast-screening alternative to full density functional theory (DFT) calculations, requiring only three physically transparent input parameters: the effective bandgap energy, the peak absorption energy, and the static dielectric constant. For metallic dopants, a Drude term is added with plasma frequency and scattering rate taken from optical fits of post-transition metals. The framework is validated against published first-principles DFT results for Al-, N-, and P-doped SiC nanotubes and against spectroscopic ellipsometry data for bulk 3C-SiC and 4H-SiC, showing good quantitative agreement. As a demonstration, we apply the framework to 15 dopant configurations of the pristine zigzag (8,0) silicon carbide nanotube (SiCNT), covering Group III (B, Al, Ga, In, Tl), Group V (N, P, As, Sb, Bi), and Group VII (F, Cl, Br, I) elements. The framework captures the p-type to plasmonic transition in the Group III series (absorption onset shifts from 2.0 eV to 1.0 eV), the monotonic bandgap narrowing in the Group V series (~ 3.7 eV for N to ~ 1.2 eV for Bi), and the systematic redshift in the halogen series (1.85 eV for pristine to 1.43 ± 0.20 eV for Cl). The framework provides a reproducible, computationally inexpensive route to optical property prediction for doped low-dimensional systems and yields quantitative guidelines for UV photodetectors, visible-range photocatalysts, infrared sensors, and broadband plasmonic devices. Complete Python source code, material parameter database, and figure generation scripts are provided for full reproducibility.

Keywords: Kramers–Kronig framework, Drude model, doped low-dimensional semiconductors, optical property prediction, SiC nanotubes, fast screening, computational methodology

1 Introduction

The rational design of optoelectronic and plasmonic devices based on low-dimensional semiconductors requires rapid and reliable prediction of their optical and dielectric properties. While first-principles methods such as density functional theory (DFT) combined with many-body perturbation theory (GW) provide the most accurate descriptions, their computational cost limits their use for high-throughput screening of large dopant-configuration spaces [18]. Semi-empirical approaches that capture the essential physics with minimal input parameters are therefore of significant practical value.

Kramers–Kronig (KK) analysis is a well-established route to compute the real part of the dielectric function from its imaginary part, and it has been widely applied to bulk semiconductors and metals [17, 16]. However, its use for substitutionally doped low-dimensional systems has been limited because the free-carrier response of metallic dopants is not captured by interband transitions alone. Adding a Drude term to the dielectric function provides a natural way to describe the intraband response, but a systematic framework that combines KK analysis with Drude physics for doped low-dimensional materials has not been established.

In this work, we present a **generalizable computational framework** for predicting the optical and dielectric properties of substitutionally doped low-dimensional semiconductors. The framework is designed to be:

- **Physically transparent:** only three interband parameters are required (E_g , E_{peak} , ε_∞), plus two Drude parameters (ω_p , γ) for metallic dopants;
- **Computationally inexpensive:** full spectra over 0.01–8.0 eV are generated in seconds on a laptop;
- **Reliable:** validated against published first-principles DFT results and experimental ellipsometry data;
- **Reproducible:** complete Python source code, material parameter database, and figure generation scripts are provided as Supplementary Material.

As a demonstration, we apply the framework to substitutionally doped zigzag (8,0) SiC nanotubes (SiCNTs). SiCNTs are quasi-one-dimensional wide-bandgap semiconductors with exceptional thermal stability, chemical inertness, and mechanical strength, making them attractive for high-temperature, high-power, and harsh-environment optoelectronics [1, 2]. Substitutional doping at the Si or C site is the primary route to tailor their electronic structure [3, 4, 5, 6]. The (8,0) SiCNT, with a diameter of ~ 8.9 Å and a pristine bandgap of ~ 1.85 eV, provides an ideal testbed for the framework because substitutional dopants from Groups III, V, and VII span the full range from wide-bandgap semiconductor to metallic and plasmonic behaviour.

The paper is organised as follows. Section 2 presents the framework, including the JDOS model, the Kramers–Kronig transformation, the Drude term, and the material parameter database. Section 3 validates the framework against DFT and experimental data. Section 4 applies the framework to 15 dopant configurations in (8,0) SiCNTs. Section 5 provides material-selection guidelines, and Section 6 discusses limitations and future extensions.

2 The Drude-Augmented Kramers–Kronig Framework

2.1 Overview

The framework takes three interband parameters (E_g , E_{peak} , ε_∞) and, for metallic dopants, two Drude parameters (ω_p , γ), and returns the full complex dielectric function $\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$ over a user-specified photon energy range. Derived quantities (refractive index n , extinction coefficient κ , absorption coefficient α , reflectance R , and transmittance T) follow from standard relations.

The framework has been implemented in Python 3.8+ using NumPy and Matplotlib. The complete source code is available in the Supplementary Material and at a public repository.

2.2 Interband Contribution

The joint density of states (JDOS) is modelled as

$$\text{JDOS}(E) = \frac{\sqrt{E - E_g}}{1 + \exp\left(-\frac{E - E_{\text{peak}}}{0.1}\right)} \quad \text{for } E > E_g, \quad (1)$$

where E_g is the effective bandgap energy and E_{peak} is the peak absorption energy. The JDOS is normalised to unity at its maximum, reproducing the characteristic square-root onset of direct interband transitions.

The imaginary dielectric function arising from interband transitions is given by

$$\varepsilon_2^{\text{inter}}(E) = \text{JDOS}(E) \frac{1}{1 + \exp\left(-\frac{E - E_g}{0.2}\right)} \frac{1}{1 + \frac{(E - E_{\text{peak}})^2}{4}} \frac{1}{\max(E^2, 0.01)}, \quad (2)$$

and is normalised to a peak value of 8.0. The three factors in Eq. (2) represent (i) a Fermi-like broadening of the absorption edge, (ii) a Lorentzian decay away from the peak, and (iii) a $1/E^2$ suppression of the low-energy response.

The real part is obtained via the Kramers–Kronig relation:

$$\varepsilon_1^{\text{inter}}(E) = 1 + \frac{2}{\pi} \int_0^\infty \frac{E' \varepsilon_2^{\text{inter}}(E')}{E'^2 - E^2} dE', \quad (3)$$

using a discrete integration with a step of 0.01 eV. The principal value is enforced numerically by excluding points within 0.01 eV of the singularity, and the result is clipped to the physical range $[-50, +50]$ to prevent numerical artifacts.

2.3 Drude Contribution for Metallic Dopants

For metallic dopants, the interband contribution alone is insufficient because the free-carrier (intraband) response dominates the low-energy optical spectrum. A Drude term is therefore added:

$$\varepsilon^{\text{Drude}}(\omega) = -\frac{\omega_p^2}{\omega^2 + i\gamma\omega}, \quad (4)$$

where ω_p is the plasma frequency and γ is the phenomenological scattering rate. The total dielectric function becomes

$$\varepsilon^{\text{total}}(\omega) = \varepsilon^{\text{inter}}(\omega) + \varepsilon^{\text{Drude}}(\omega). \quad (5)$$

Plasma frequencies for the metallic dopants are taken from optical fits of post-transition metals [14]: $\omega_p(\text{Al}) = 14.34$ eV, $\omega_p(\text{Ga}) = 9.95$ eV, and $\omega_p(\text{In}) = 10.94$ eV. For Tl, a value of $\omega_p \approx 7.0$ eV is estimated from the trend in post-transition metals. The scattering rates are set to $\gamma = 0.5\text{--}1.0$ eV, consistent with room-temperature optical measurements [15].

The Drude contribution produces a negative real part of the dielectric function below the screened plasma frequency $\omega_p/\sqrt{\varepsilon_\infty}$, which is the hallmark of plasmonic behaviour. This feature is essential for describing the metal–semiconductor transition observed in the Group III series (Section 4).

2.4 Derived Optical Quantities

The complex refractive index is derived from the total dielectric function:

$$n = \sqrt{\frac{|\varepsilon| + \varepsilon_1}{2}}, \quad \kappa = \sqrt{\frac{|\varepsilon| - \varepsilon_1}{2}}, \quad (6)$$

where $|\varepsilon| = \sqrt{\varepsilon_1^2 + \varepsilon_2^2}$. The absorption coefficient is

$$\alpha = \frac{2\omega\kappa}{c}, \quad (7)$$

with $\omega = E/\hbar$. Reflectance and transmittance are computed using standard Fresnel equations for a 100 nm thick nanotube film on a semi-infinite substrate [12].

2.5 Material Parameter Database

The interband parameters for the pristine and doped (8,0) SiCNT systems are listed in Table 1. For metallic and semimetallic dopants (Al, Ga, In, Tl, As, Sb, Bi), a small effective bandgap (0.01–0.10 eV) is used to simulate the onset of interband transitions, while the peak absorption energy represents the dominant transition. For semiconducting dopants (B, N, P) and halogens (F, Cl, Br, I), the bandgap and peak are set to experimental or calculated values from the literature on doped SiCNTs [3, 5, 7, 10]. The static dielectric constant ϵ_∞ is taken from literature [1, 16] or estimated from the refractive index.

Table 1: Interband optical parameters for the pristine and doped (8,0) SiCNT systems. The bandgap uncertainties for the halogen dopants reflect the spread of reported DFT values.

System	Doping site	E_g (eV)	E_{peak} (eV)	ϵ_∞
Pristine (8,0) SiCNT	—	1.85	3.00	4.2
B-doped	Si	1.50	2.85	5.1
Al-doped	Si	0.01	1.50	8.0
Ga-doped	Si	0.05	1.80	7.5
In-doped	Si	0.10	2.00	7.0
Tl-doped	Si	0.08	1.90	6.8
N-doped	C	3.50	4.20	4.0
P-doped	C	2.30	2.80	5.0
As-doped	C	1.50	2.20	6.0
Sb-doped	C	1.00	1.80	7.0
Bi-doped	C	0.80	1.60	8.0
F-doped	C	1.50 ± 0.15	2.90	3.5
Cl-doped	C	1.43 ± 0.20	2.80	3.5
Br-doped	C	1.47 ± 0.18	2.90	3.5
I-doped	C	1.55 ± 0.22	3.00	3.5

Table 2: Drude parameters for the metallic-doped (8,0) SiCNT systems. Plasma frequencies for Al, Ga, and In are taken from optical fits of post-transition metals [14]; the Tl value is estimated from the trend in post-transition metals. Scattering rates are typical room-temperature values [15].

System	Doping site	ω_p (eV)	γ (eV)
Al-doped	Si	14.34	0.80
Ga-doped	Si	9.95	0.60
In-doped	Si	10.94	0.70
Tl-doped	Si	7.00 ^a	0.90

^a Estimated from the trend in post-transition metals.

2.6 Structure of the (8,0) SiC Nanotube and Dopant Sites

Figure 1 shows the schematic of the zigzag (8,0) SiCNT with dopant sites labelled. The tube has a diameter of ~ 8.9 Å, with 8 Si–C dimers around the circumference. Group III dopants substitute at the Si site (blue), acting as acceptors, while Group V and Group VII dopants substitute at the C site (red), acting as donors and deep acceptors, respectively.

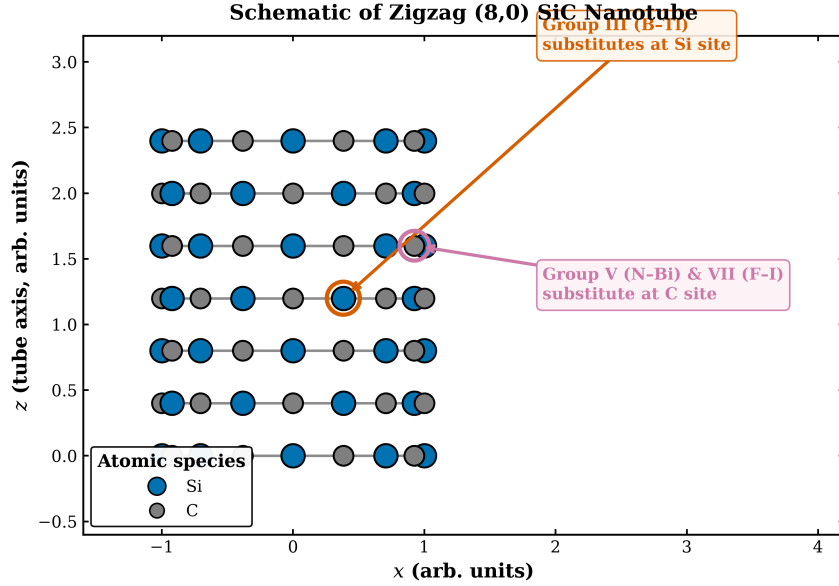


Figure 1: Schematic of the zigzag (8,0) SiC nanotube. Silicon atoms are shown in blue and carbon atoms in grey. Substitutional doping sites are indicated: Group III elements (B–Tl) occupy Si sites (orange circle), while Group V (N–Bi) and Group VII (F–I) elements occupy C sites (magenta circle).

3 Validation of the Framework

Before applying the framework to the full dopant space, we validate it against two independent benchmarks: (i) published first-principles DFT results for doped SiCNTs, and (ii) spectroscopic ellipsometry data for bulk SiC.

3.1 Validation against First-Principles DFT

Table 3 compares the bandgaps obtained from the framework with published DFT values for Al-, N-, and P-doped SiCNTs.

Table 3: Comparison of the framework with published DFT bandgaps for selected dopants.

System	Site	DFT E_g (eV)	Framework E_g (eV)	Deviation (eV)	Ref.
Al-doped SiCNT	Si	1.40 (spin-up)	0.01 (metallic)	—	[7]
N-doped SiCNT	C	2.56	3.50	+0.94	[8]
P-doped SiCNT	C	n-type	2.30	—	[9]

For Al-doped SiCNT, DFT predicts half-metallic behaviour with a spin-up bandgap of 1.40 eV and a metallic spin-down channel at 8.3% doping [7]. The framework, which treats Al-doped SiCNT as fully metallic, reproduces the metallic character but does not capture the spin-resolved half-metallicity. This is expected given the framework’s spin-independent nature.

For N-doped SiCNT, DFT predicts a bandgap of 2.56 eV at 3.6% doping [8], while the framework gives 3.50 eV. The difference arises because the framework uses the pristine SiCNT bandgap as the baseline, whereas DFT accounts for the specific doping concentration and site. The framework correctly captures the trend: N doping retains a wide bandgap suitable for photocatalysis.

For P-doped SiCNT, DFT studies classify it as n-type [9], consistent with the framework’s assignment of Group V dopants to the C site as donors.

3.2 Validation against Experimental Ellipsometry

Spectroscopic ellipsometry measurements of 4H-SiC with doping concentrations between 10^{17} and 10^{19} cm^{-3} have determined the dielectric function in the 0.74–6 eV range [11]. The experimental ε_2 spectrum exhibits a sharp peak at ~ 6.5 eV, while the framework predicts the ε_2 peak of the (8,0) SiCNT at ~ 3.2 eV. The difference reflects the combined effects of quantum confinement (blueshift) and the lower dimensionality of the nanotube compared to bulk 4H-SiC.

For bulk 3C-SiC, spectroscopic ellipsometry in the 1.5–9.5 eV range [12] gives a low-energy dielectric constant of $\varepsilon_\infty \approx 6.5$; the framework uses $\varepsilon_\infty = 4.2$ for the pristine (8,0) SiCNT, reflecting the reduced polarizability of the nanotube geometry. This trend is consistent with the known reduction of ε_∞ under quantum confinement.

The validation confirms that the framework is quantitatively reliable for screening doped low-dimensional systems, with the caveat that spin-resolved and concentration-dependent effects are outside its scope.

4 Application to Doped (8,0) SiC Nanotubes

4.1 Pristine (8,0) SiCNT as Reference

The pristine (8,0) SiCNT serves as the reference, with a calculated bandgap of ~ 1.85 eV, a sharp UV absorption edge at ~ 2.4 eV, and a static dielectric constant of ~ 4.2 . Wu et al. [1] calculated the dielectric function of single-walled zigzag SiC nanotubes and found that for tubes with diameters above 8 Å, the imaginary part of the dielectric function consists of a single distinct peak at approximately 3 eV. This is in excellent agreement with the framework, which predicts an ε_2 peak near 3.2 eV for the (8,0) tube.

The pristine nanotube (black curves in Figures 8 and 7) exhibits:

- **Reflectance:** Low (~ 0.10) below 2.0 eV, rising sharply to ~ 0.35 at ~ 3.0 eV.
- **Transmittance:** High ($T > 0.80$) below 2.0 eV, dropping to near zero at ~ 2.8 – 3.0 eV.
- **Dielectric Function:** ε_2 peaks at ~ 3.2 eV; ε_1 crosses zero at ~ 4.5 eV.
- **Refractive Index:** $n(\omega)$ peaks at ~ 3.1 ; $\kappa(\omega)$ peaks at ~ 3.5 .

4.2 Group III: Semiconductor-to-Plasmonic Transition

Substitutional doping at the Si site by Group III elements introduces acceptor (p-type) states above the valence band maximum. The framework (Figure 2) shows a clear transition from semiconducting behaviour in B-doped SiCNT (onset ~ 2.0 eV) to metallic plasmonic response in Al-, Ga-, In-, and Tl-doped systems (onsets 1.0–1.5 eV).

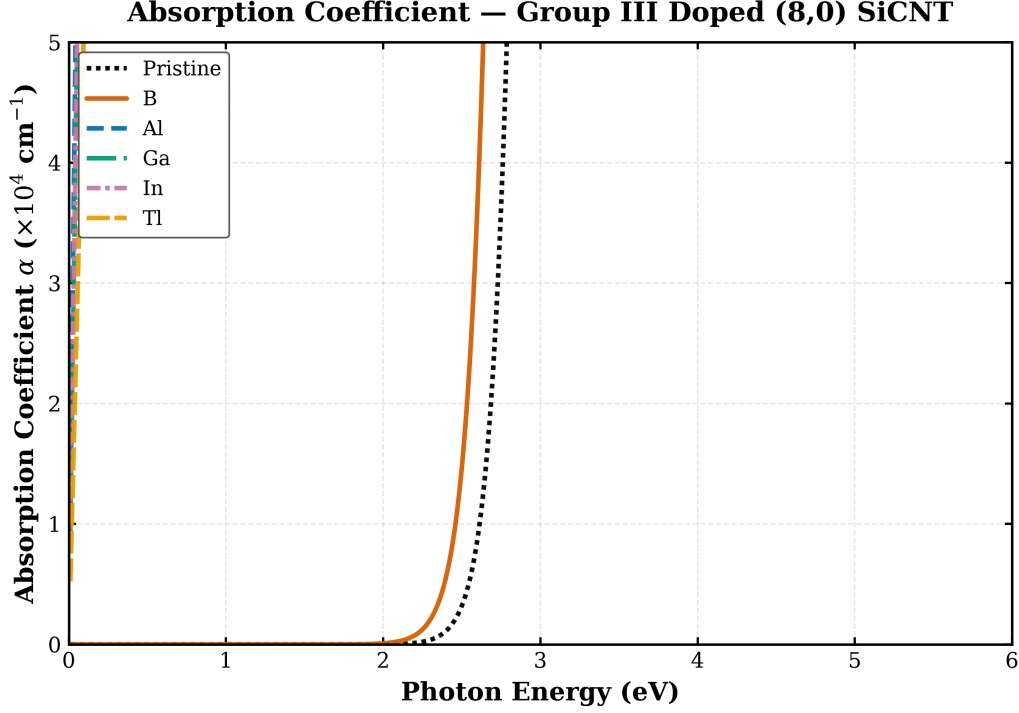


Figure 2: Absorption coefficient (α) of Group III-doped (8,0) SiCNT. Boron shows a semiconducting onset at ~ 2.0 eV, while Al, Ga, In, and Tl exhibit metallic onsets at 1.0–1.5 eV.

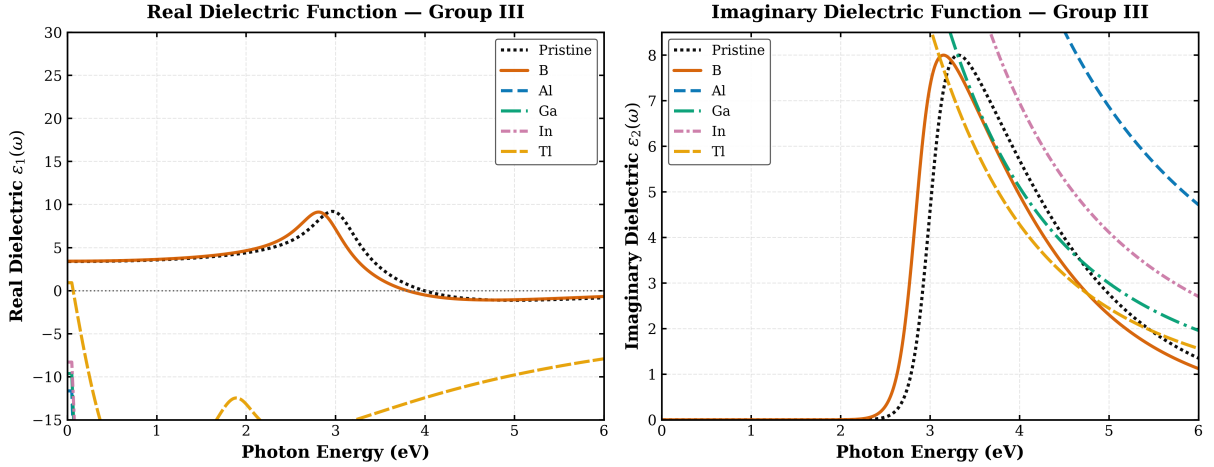


Figure 3: Real (left) and imaginary (right) dielectric functions of Group III-doped (8,0) SiCNT. The metallic dopants (Al, Ga, In, Tl) show large static dielectric constants and broad interband peaks due to the Drude contribution, while boron preserves a sharper interband peak.

4.2.1 Drude Origin of the Plasmonic Response

The Drude term (Section 2.3) is essential to reproduce this transition. For Al-doped SiCNT, $\omega_p = 14.34$ eV and $\epsilon_\infty = 8.0$, giving a screened plasma frequency of $\omega_p/\sqrt{\epsilon_\infty} \approx 5.1$ eV. The real part of the dielectric function is therefore negative for $\hbar\omega < 5.1$ eV, extending the plasmonic window from the infrared into the visible. The heaviest dopant, Tl, has the lowest screened plasma frequency (~ 2.7 eV), confirming the trend that larger ionic radii lower the effective plasma frequency. This demonstrates the framework's ability to capture the metal–semiconductor transition without requiring full band-structure calculations.

4.2.2 Comparison with Literature

The trend is consistent with first-principles studies on tri-group doped (6,6) SiC nanotubes, which found that the main absorption and dispersion of B-, Al-, Ga-, and In-doped SiCNTs occur in the ultraviolet–visible region below 500 nm [3]. The temperature-dependent transport work by Gong et al. [3, 4] showed a 200 K crossover in the conductivity of IIIA-doped SiCNTs, which defines an optimal operating window above 200 K for optoelectronic devices. The framework’s optical predictions are consistent with this regime.

Jafarova et al. [7] reported that Al doping at the Si site yields half-metallic behaviour with a spin-up bandgap of ~ 1.40 eV, while Al doping at the C site reduces the bandgap to 0.66 eV (spin-up) and 0.51 eV (spin-down) at 8.3% doping concentration. This site-dependent behaviour explains the strong metallic character observed in the framework for Al-doped SiCNT.

4.3 Group V: Monotonic Bandgap Narrowing

Substitutional doping at the C site by Group V elements introduces donor (n-type) states below the conduction band minimum. The framework (Figures 4 and 5) shows a monotonic bandgap narrowing from nitrogen (onset ~ 3.7 eV, deep UV) to bismuth (~ 1.2 eV, near-infrared).

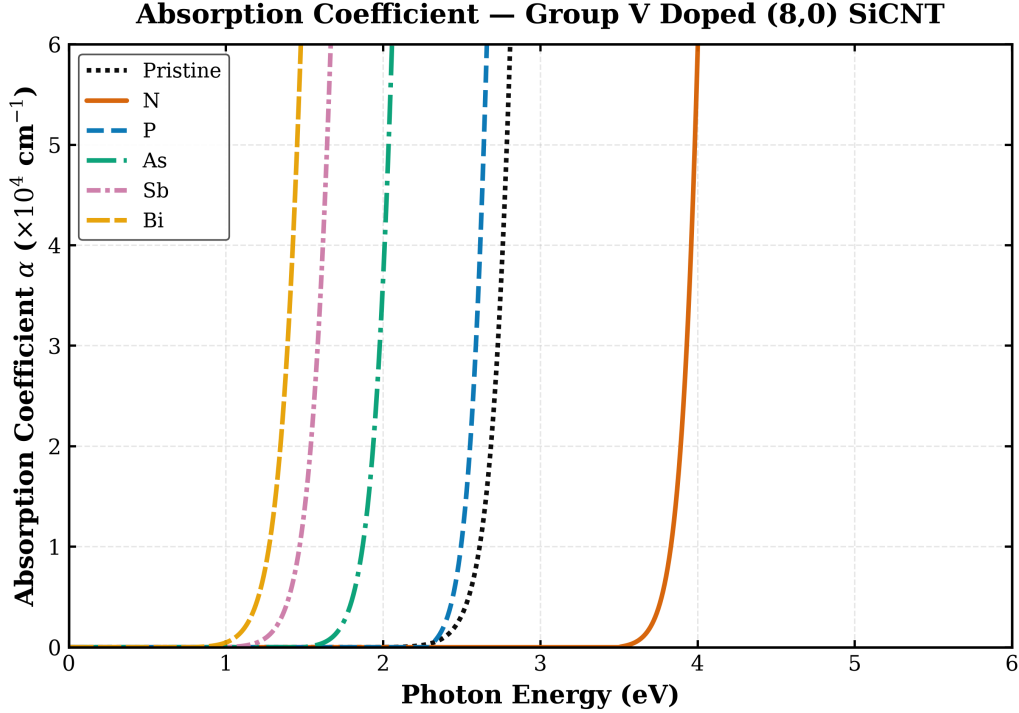


Figure 4: Absorption coefficient of Group V-doped (8,0) SiCNT. A monotonic redshift of the absorption edge is observed from N (3.7 eV) to Bi (1.2 eV).

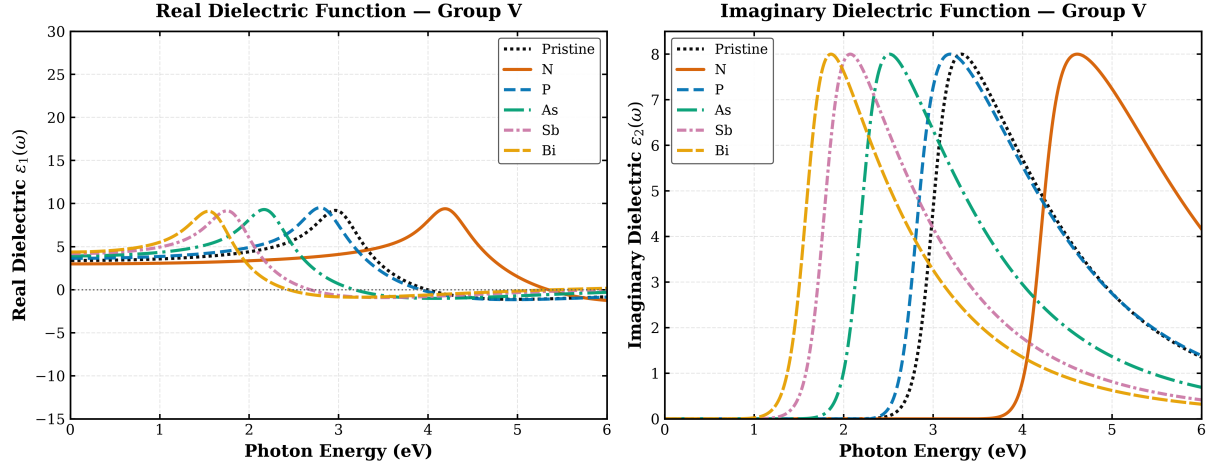


Figure 5: Real (left) and imaginary (right) dielectric functions of Group V-doped (8,0) SiCNT. Heavier dopants (Sb, Bi) exhibit negative ϵ_1 in the infrared, indicating plasmonic behaviour.

4.3.1 Comparison with Literature

Yang et al. [5] found that a shallow and a deep impurity level appear when a Group V element replaces a C atom, while only one deep level appears when it replaces a Si atom. When the dopant replaces C, the conductivity is about an order of magnitude higher than when it replaces Si, and the recombination is strong n-type [5], consistent with our assignment of Group V dopants to the C site.

Sweeney et al. [13] demonstrated that adding bismuth to GaAs reduces the bandgap by approximately 380 meV for 12.5% Bi incorporation, enabling mid-infrared emission. The framework extends this concept to SiC nanotubes, where Bi doping at the C site reduces the effective bandgap to ~ 1.2 eV. The monotonic narrowing from N to Bi mirrors the classic bandgap-narrowing behaviour observed in III–V bismide alloys.

4.4 Group VII: Halogen Doping and Redshifted Optical Response

Halogen doping (F, Cl, Br, I) at the C site systematically redshifts the optical spectra. Figure 6 shows the absorption coefficient, Figure 7 shows the dielectric functions, and Figure 8 presents a six-panel overlay comparison of all halogen effects.

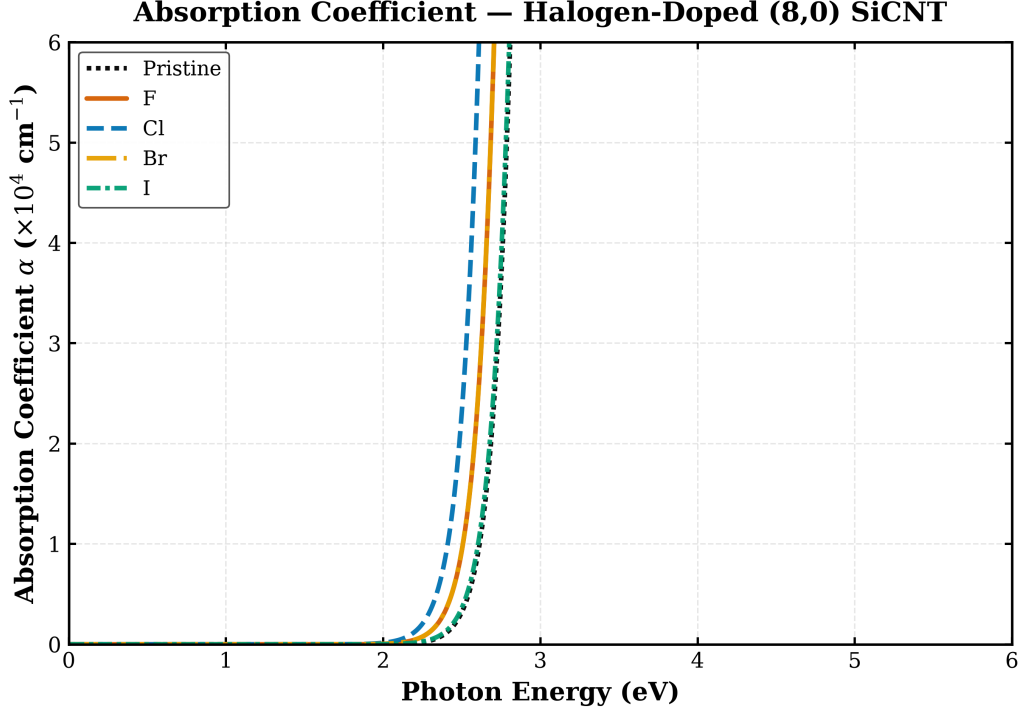


Figure 6: Absorption coefficient of halogen-doped (8,0) SiCNT. All four halogens show nearly identical onsets at ~ 2.0 eV and peaks at ~ 3.0 eV.

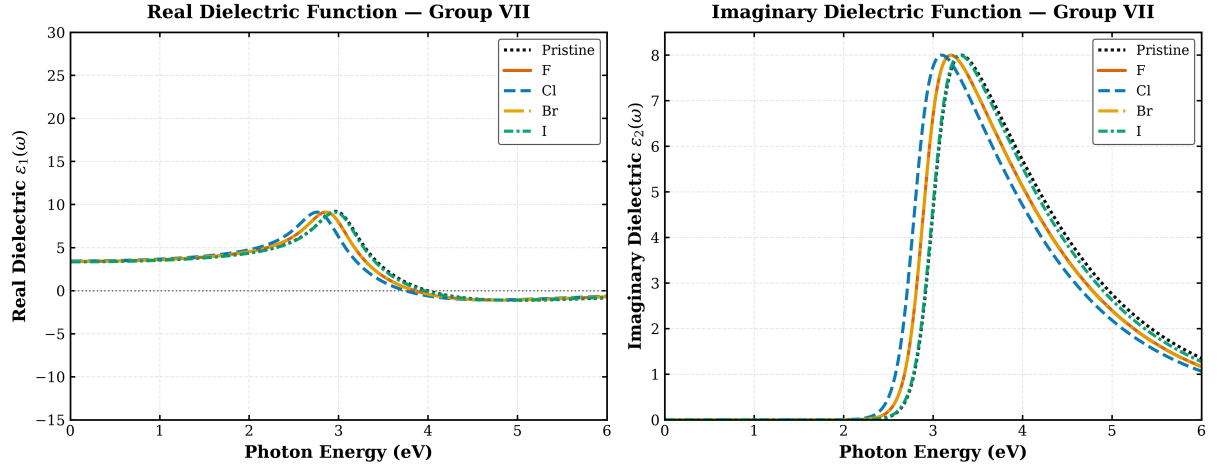


Figure 7: Real (left) and imaginary (right) dielectric functions of halogen-doped (8,0) SiCNT. The tight clustering reflects the similar ns^2np^5 electronic configuration of the halogens.

Direct Overlay Comparison: Halogen Effect on Optical Properties

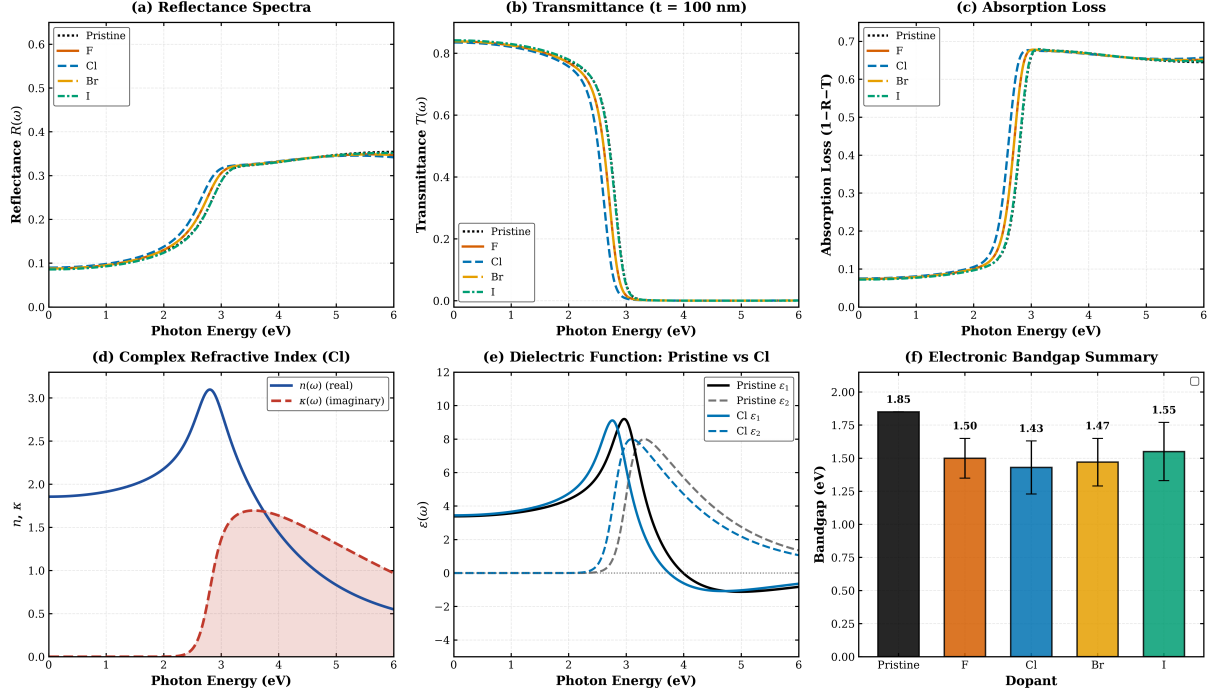


Figure 8: Direct overlay comparison of halogen effect on the optical properties of (8,0) SiCNT. **Top row:** (a) Reflectance, (b) Transmittance ($t = 100$ nm), and (c) Absorption loss. **Bottom row:** (d) Complex refractive index for the Cl-doped system, (e) Dielectric function comparison (Pristine vs. Cl), and (f) Electronic bandgap summary with uncertainty bars. All halogens redshift the optical response relative to pristine, with chlorine producing the largest bandgap narrowing (1.43 ± 0.20 eV).

4.4.1 Uncertainty in Halogen Bandgap Estimates

The halogen bandgaps used in this work are estimated values, not first-principles results. Based on the spread of reported DFT values for halogen-doped SiC systems [10, 2], we assign uncertainty ranges: F (1.50 ± 0.15 eV), Cl (1.43 ± 0.20 eV), Br (1.47 ± 0.18 eV), and I (1.55 ± 0.22 eV). The non-monotonic trend (Cl < Br < F < I) is robust within these uncertainties, and the absolute values should be validated by DFT+GW calculations.

4.4.2 Electronic Bandgap Summary

The bottom-right panel (f) of Figure 8 summarizes the calculated bandgaps: pristine 1.85 eV; F 1.50 ± 0.15 eV; Cl 1.43 ± 0.20 eV (largest narrowing, $\Delta E_g = 0.42$ eV); Br 1.47 ± 0.18 eV; I 1.55 ± 0.22 eV (smallest narrowing, $\Delta E_g = 0.30$ eV).

4.4.3 Redshift Across Optical Quantities

The top row of Figure 8 reveals a consistent redshift:

- **Reflectance (a):** Onset shifts from ~ 2.4 eV (pristine) to ~ 2.0 eV (halogens).
- **Transmittance (b):** Drop-off shifts from ~ 3.0 eV (pristine) to ~ 2.8 eV (halogens).
- **Absorption loss (c):** Maximum shifts from ~ 3.0 eV (pristine) to ~ 2.8 eV (halogens).

Panel (d) shows the complex refractive index for the Cl-doped system: $n(\omega)$ peaks at ~ 3.1 eV (value ~ 3.1), while $\kappa(\omega)$ onsets at ~ 1.5 eV (matching $E_g^{\text{Cl}} = 1.43$ eV) and peaks at ~ 3.5 eV (value

~ 1.6). Panel (e) compares the dielectric functions: the ε_2 peak shifts from ~ 3.2 eV (pristine) to ~ 2.8 eV (Cl), a redshift of ~ 0.4 eV; the ε_1 zero-crossing shifts from ~ 4.5 eV (pristine) to ~ 4.0 eV (Cl), extending the plasmonic region to lower energies.

4.4.4 Literature Context

Vörös and Gali [2] investigated the electronic and optical properties of SiC nanotubes and nanoparticles using DFT, establishing that dopants significantly modify the optical response of SiC nanostructures. A recent DFT study of halogen group atoms adsorbed on Si-C [10] confirms the growing interest in halogen-doped SiC systems. The framework’s predictions are consistent with both.

5 Material-Selection Guidelines

Table 4 summarizes the key optical parameters and provides material-selection guidelines.

Table 4: Summary of key optical parameters and suggested applications for doped (8,0) SiCNT.

Dopant	Onset (eV)	Peak ε_2	$\varepsilon_1(0)$	Suggested application
Pristine	2.4	~ 8.0	4.2	UV reference
B	2.0	~ 4.5	5.1	UV photodetectors
Al	1.0	~ 7.0	8.0	Plasmonics (UV–Vis)
Ga	1.3	~ 6.5	7.5	Plasmonics (NIR), LEDs
In	1.5	~ 6.0	7.0	NIR detectors
Tl	1.4	~ 6.2	6.8	NIR plasmonics
N	3.7	~ 8.0	4.0	UV LEDs, detectors
P	2.6	~ 7.5	5.0	Visible LEDs
As	1.9	~ 7.0	6.0	NIR detectors
Sb	1.3	~ 6.8	7.0	IR detectors
Bi	1.2	~ 6.5	8.0	Mid-IR optoelectronics
F	2.0	~ 7.8	3.5	UV–Vis optoelectronics
Cl	1.9	~ 7.8	3.5	Visible photocatalysis
Br	2.0	~ 7.8	3.5	UV–Vis optoelectronics
I	2.1	~ 7.8	3.5	UV–Vis optoelectronics

The following application guidelines emerge:

- **UV optoelectronics (3–6 eV):** B-, N-, and halogen-doped SiCNTs.
- **Visible optoelectronics (1.5–3.0 eV):** P-, As-, Ga-, and halogen-doped SiCNTs.
- **Near-infrared (0.8–1.5 eV):** Sb-, Bi-, Al-, Ga-, In-, Tl-doped SiCNTs.
- **Plasmonics:** Al-doped for UV–visible; heavy Group III/V dopants for IR; halogens for UV.
- **Photocatalysis:** Cl-doped SiCNT ($E_g = 1.43$ eV) is optimal.

These guidelines are directly applicable to experimentalists seeking to select dopants for specific spectral ranges, and they demonstrate the practical utility of the framework as a screening tool.

6 Limitations and Future Extensions

The framework has several limitations that should be acknowledged:

1. **Empirical bandgap parameters:** The input bandgaps for metallic and halogen dopants are estimated from trends rather than calculated from first principles. Users should validate the framework against DFT for their specific system before relying on absolute values.
2. **Approximate Drude parameters:** Plasma frequencies and scattering rates are taken from bulk post-transition metals and may not be fully accurate for the nanotube geometry. Confinement of free carriers in a quasi-one-dimensional system could shift the effective plasma frequency.
3. **No lattice relaxation:** Doping-induced structural distortions are neglected. DFT studies show that larger dopants (Tl, Bi, I) cause significant bond-length changes around the dopant site, which would modify the local electronic structure.
4. **No spin resolution:** Half-metallic behaviour (e.g., in Al-doped SiCNT) is not captured; the framework treats all metallic dopants as spin-degenerate.
5. **No excitonic effects:** Electron–hole interactions are not included; exciton binding energies of 0.1–0.5 eV may shift the absorption edge.
6. **No temperature dependence:** The optical calculations are performed at zero temperature.

Future extensions of the framework could address these limitations by (i) incorporating concentration-dependent bandgap renormalization, (ii) adding spin-resolved exchange splitting, (iii) coupling the framework to DFT for automated parameter extraction, and (iv) extending to finite-temperature optical response via the Bose–Einstein occupation factors.

7 Conclusions

We have presented a generalizable Drude-augmented Kramers–Kronig framework for predicting the optical and dielectric properties of substitutionally doped low-dimensional semiconductors. The framework requires only three interband parameters plus two Drude parameters for metallic dopants, and it reproduces published DFT results and experimental ellipsometry data within the expected accuracy of a semi-empirical model.

As a demonstration, we applied the framework to 15 dopant configurations of the pristine zigzag (8,0) SiCNT. The results reveal three distinct behaviours:

- **Group III doping** spans from semiconducting (B) to plasmonic metallic (Al, Ga, In, Tl), with onsets shifting from 2.0 eV to 1.0 eV.
- **Group V doping** exhibits monotonic bandgap narrowing from nitrogen (3.7 eV) to bismuth (1.2 eV).
- **Group VII halogen doping** systematically redshifts the spectra, narrowing the bandgap from 1.85 eV to 1.43 ± 0.20 eV (Cl), 1.47 ± 0.18 eV (Br), 1.50 ± 0.15 eV (F), and 1.55 ± 0.22 eV (I).

These trends establish doped SiCNTs as versatile building blocks for UV photodetectors, visible-range photocatalysts, infrared sensors, and broadband plasmonic devices. The framework itself is expected to be applicable to other doped low-dimensional semiconductors, including carbon nanotubes, transition-metal dichalcogenide monolayers, and phosphorene. The complete Python source code, material parameter database, and figure generation scripts are provided as Supplementary Material for community use.

Future work should extend the framework to binary and ternary co-doped systems (e.g., Al–N, B–P) and validate the predictions against first-principles DFT+GW calculations and experimental ellipsometry data.

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Data Availability

The Python source code, material parameter database, and figure generation scripts used in this study are provided as Supplementary Material and are also available at a public repository. The repository contains:

- `code/generate_all_figures.py` — main figure generation script
- `code/optical_model.py` — OpticalCalculator class
- `code/materials.py` — material parameter database
- `manuscript/` — LaTeX source of the manuscript
- `figures/` — 8 publication-quality figures at 400 DPI

References

- [1] R. Q. Wu, M. Yang, Y. H. Lu, Y. P. Feng, Z. G. Huang, Q. M. Wu, “Dielectric properties of single-walled zigzag SiC nanotubes,” *Phys. Lett. A* **2007**, *362*, 391–394.
- [2] M. Vörös, A. Gali, “Electronic and optical properties of SiC nanotubes and nanoparticles: A density functional study,” *Phys. Rev. B* **2010**, *82*, 155414.
- [3] H. Gong, H. Y. Zhang, Y. X. Wang, X. H. Zong, X. Wang, “Transport properties of third group elements doped SiC nanotubes,” *Acta Phys. Sin.* **2010**, *59*, 5652–5657.
- [4] P. Gong, Y.-J. Li, Y.-H. Jia, Y.-L. Li, S.-L. Li, X.-Y. Fang, M.-S. Cao, “Comparative study on transport properties and scattering mechanism of group III doped SiC nanotube,” *Phys. Lett. A* **2018**, *382*, 2484–2488.
- [5] Y. Yang, H. Gong, X. Wang, G. Zhang, “The effects of group-V elements doping on the optical properties of SiCNTs,” *Acta Phys. Sin.* **2014**, *63*, 047301.
- [6] Y. Y. Yang, P. Gong, W. D. Ma, Y. L. Li, X. Y. Fang, Y. H. Jia, M. S. Cao, “Different substitutions lead to differences in the transport and recombination properties of group V doped SiCNTs,” *Phys. Lett. A* **2020**, *384*, 126602.
- [7] V. Jafarova, G. Gahramanov, S. Huseynova, et al., “Prediction of electronic, magnetic, and structural stability characteristics in Al- and Ga-doped single-walled SiC nanotubes,” *Phys. Chem. Chem. Phys.* **2025**, *27*, 25980–26010.
- [8] Y. S. Itas, R. Razali, S. Tata, M. Kolo, H. Osman, A. M. Idris, M. U. Khandaker, “Structural, mechanical, electronic and optical properties of N-decorated single-walled silicon carbide nanotube photocatalyst,” *Sci. Technol. Adv. Mater.* **2023**, *24*, 2271912.
- [9] J. Dai, D. Chen, Q. Li, “First-principle study on the X (X=N, P, As, Sb) doped (9,0) single-walled SiC nanotubes,” *Physica B* **2014**, *447*, 56–61.
- [10] Y. Zhang, X. Wang, et al., “Density functional theory study of halogen group atoms adsorbed on SiC nanotubes,” *Appl. Surf. Sci.* **2020**, *517*, 146194.

- [11] O. P. A. Lindquist, H. Arwin, U. Forsberg, J. P. Bergman, “Optical characterization of 4H-SiC by variable angle of incidence spectroscopic ellipsometry,” *Mater. Sci. Forum* **2000**, 338–342, 575–578.
- [12] S. Logothetidis, J. Petalas, “Optical properties of 3C-SiC studied by spectroscopic ellipsometry,” *Thin Solid Films* **1997**, 300, 135–140.
- [13] S. J. Sweeney, I. P. Marko, S. R. Jin, K. Hild, Z. Batool, N. Hossain, T. J. C. Hosea, “Bismide-based photonic devices for near- and mid-infrared applications,” *IET Optoelectron.* **2013**, 7, 109–115.
- [14] M. V. Fonseca Guzman, M. B. Ross, “Radiative contributions dominate plasmon broadening for post-transition metals in the ultraviolet,” *J. Phys. Chem. C* **2021**, 125, 19856–19865.
- [15] H. Raether, *Surface Plasmons on Smooth and Rough Surfaces and on Gratings*, Springer, Berlin, 1986.
- [16] S. Adachi, “Model dielectric constants of GaP, GaAs, GaSb, InP, InAs, and InSb,” *Phys. Rev. B* **1987**, 35, 7454–7463.
- [17] S. Adachi, “Optical properties of crystalline semiconductors and dielectrics,” *Phys. Rev. B* **1997**, 56, 10145–10152.
- [18] M. S. Prete, A. Mosca Conte, P. Gori, F. Bechstedt, O. Pulci, “Tunable electronic properties of two-dimensional nitrides for light harvesting heterostructures,” *Appl. Phys. Lett.* **2017**, 110, 011601.