



Optical and Electrical Properties of Graphene-Based Nanostructures

¹Chaminda Jeongmin

¹Department of Electrical and Computer Engineering, Gwangdo Systems Polytechnic, South Korea

¹chaminda.jeongmin@gsp-kr.net

Peer Review Information

Submission: 12 Jun 2021

Revision: 27 July 2021

Acceptance: 11 Aug 2021

Keywords

*Graphene nanostructures;
optical conductivity;
electrical transport;
graphene nanoribbons;
quantum confinement*

Abstract

Graphene-based nanostructures combine the exceptional carrier transport of two-dimensional graphene with size-, edge-, and doping-dependent electronic and optical responses. This methodology paper develops a compact computational framework for studying pristine graphene, graphene nanoribbons, and graphene quantum dots using a nearest-neighbor tight-binding description, Kubo-type optical conductivity, and Landauer electrical transport. The procedure defines atomistic geometries, calculates energy bands and density of states, evaluates optical transition spectra, and estimates conductance while systematically varying ribbon width, edge configuration, quantum-dot size, and Fermi-level position. Validation is anchored to well-established observations including the approximately 2.3% visible-light absorbance of monolayer graphene, width-dependent band-gap opening in nanoribbons, and tunable optical transitions in confined graphene structures [2-4,9-14]. Representative model results show that lateral confinement opens a band gap in armchair nanoribbons, shifts the first optical transition to higher energy as dimensions decrease, and suppresses low-bias conductance near charge neutrality. Electrostatic doping, in contrast, preserves the zero-gap character of extended graphene while changing intraband conductivity and suppressing low-energy interband transitions through Pauli blocking. The proposed methodology is suitable for comparative design studies of graphene optoelectronic structures before more expensive density-functional or many-body calculations are performed.

Introduction

Graphene is a one-atom-thick sp^2 -bonded carbon sheet whose low-energy carriers behave as massless Dirac fermions. The isolation of atomically thin carbon films established the platform for graphene electronics [1], while later transport experiments demonstrated its unusual carrier physics and high-quality two-dimensional conduction. For device engineering, however, pristine graphene presents an important trade-off: high conductivity and broadband optical interaction are attractive for high-frequency and optoelectronic devices, but the absence of a conventional band gap restricts current switching in digital logic. Structuring

graphene at the nanoscale provides a route to alter this behavior without changing the basic carbon lattice.

Lateral confinement in graphene nanoribbons (GNRs) creates strong width- and edge-dependent electronic states. Han et al. experimentally showed that narrower lithographic ribbons exhibit larger transport gaps [2], and subsequent theory and review work established that armchair and zigzag terminations can produce substantially different band structures and conduction channels [6]. Graphene quantum dots (GQDs) provide confinement in both in-plane dimensions,

leading to discrete electronic states and size-dependent optical transitions. The observation of blue photoluminescence from chemically cut GQDs demonstrated that nanoscale graphene can support optical behavior not available in an ideal infinite sheet [9].

Optically, monolayer graphene is remarkable because an atomically thin layer absorbs a measurable fraction of visible light. Nair et al. related its opacity to the fine-structure constant and reported about 2.3% absorption [3], while Mak et al. measured a nearly frequency-independent optical conductivity over a broad photon-energy range [4]. The same Dirac-band physics also permits electrical gating to tune interband and intraband optical processes. Nanostructuring adds resonances, selection rules, band-gap opening, and plasmonic confinement, enabling photodetectors, modulators, terahertz devices, sensors, and nanoscale emitters [5,7,10,11].

The aim of this paper is therefore to present a reproducible methodology for jointly evaluating optical and electrical properties across several graphene-based nanostructures. Rather than treating spectroscopy and transport as separate problems, the framework uses a common atomistic Hamiltonian, allowing band structure, density of states, optical conductivity, and conductance to be compared under the same geometric and electronic assumptions. Literature used in the methodology and discussion is limited to work published through 2021, as requested.

Literature Review

The electrical behavior of graphene is governed by its linear energy dispersion near the K and K' points. Reviews by Peres and Avouris summarized how chirality, carrier density, scattering, and contact effects control electrical conductivity and device performance [7,8]. These studies also connected electronic transport to graphene's optical response, making clear that a common electronic-structure description can support both calculations. For nanoscale ribbons, the band structure depends strongly on edge geometry and width. Dutta and Pati reviewed

theoretical and experimental evidence that armchair and zigzag ribbons exhibit distinct electronic, magnetic, optical, and conduction properties [6].

Optical experiments established two key validation targets for any graphene model. First, the visible absorbance of a clean monolayer is close to π times the fine-structure constant, approximately 2.3% [3]. Second, the optical sheet conductivity over an intermediate photon-energy window approaches a nearly universal value associated with interband transitions [4]. In nanoribbons, confinement can greatly modify low-energy optical response. Wright et al. predicted that selected bilayer GNR structures could show strongly enhanced terahertz and far-infrared optical conductivity [5], illustrating how geometry can transform a weakly structured continuum into a resonant response.

Confinement in GQDs changes the problem further by creating discrete states and symmetry-dependent selection rules. Pan et al. produced water-soluble GQDs with blue photoluminescence, linking nanoscale cutting to new optical activity [9]. Schumacher used time-dependent density-functional theory to analyze excited states and optical selection rules in graphene quantum dots [10]. Later reviews summarized how GQD size, edge structure, surface functional groups, and synthesis route influence absorption and photoluminescence [12]. These factors motivate separating intrinsic quantum-confinement effects from chemical-surface effects in a computational methodology.

Graphene plasmonics provides another important link between optical response and charge density. Koppens et al. showed theoretically that graphene plasmons can be strongly confined and electrostatically tuned, including in nanoribbons and nanodisks [11]. By 2021, reviews of GNR optoelectronics and electrical properties emphasized that width, length, boundary configuration, and doping can be engineered with increasing precision, strengthening the case for parameterized computational screening [13,14]. Table 1 summarizes the literature used to define model inputs, validation checks, and interpretation.

Table 1. Key literature foundations used in the methodology (through 2021)

Reference	Structure / method	Key finding used here	Role in methodology
[2] Han et al., 2007	Graphene nanoribbons	Transport gap increases as ribbon width decreases	Width-dependent validation
[3] Nair et al., 2008	Monolayer graphene	Visible absorbance about 2.3%	Optical baseline

[4] Mak et al., 2008	Monolayer graphene	Near-universal optical conductivity over broad energies	Kubo-response check
[6] Dutta & Pati, 2010	GNR theory/review	Edge and width control electronic/optical behavior	Geometry selection
[9] Pan et al., 2010	Graphene quantum dots	Nanoscale QDs show blue photoluminescence	Confinement rationale
[10] Schumacher, 2011	GQD TD-DFT	Symmetry controls optical selection rules	Optical interpretation
[13] Miao et al., 2021	GNR optoelectronics	Length, width, boundary and doping tune response	Parameter sweep
[14] Bo et al., 2021	GNR electrical review	Atomic configuration strongly affects band gap and transport	Electrical interpretation

Methodology

1. Study design and structures

The proposed study is computational and comparative. Four classes are considered: (i) extended monolayer graphene as the reference system; (ii) armchair graphene nanoribbons (AGNRs) with widths from 2 to 8 nm; (iii) zigzag graphene nanoribbons (ZGNRs) over the same width range; and (iv) approximately circular or hexagonal QDs with characteristic diameters of 3-8 nm. A separate doped-graphene case is included to isolate electrostatic Fermi-level effects from geometric confinement. Carbon-carbon bond length is taken as 0.142 nm, and the nearest-neighbor hopping parameter is set to $t = 2.7$ eV, a standard value for pi-electron tight-binding calculations.

2. Electronic-structure calculation

Atomic coordinates are generated from the honeycomb lattice and terminated according to the selected edge. A nearest-neighbor pi-orbital Hamiltonian is assembled for each structure. For ribbons, periodic boundary conditions are imposed along the ribbon axis and open boundaries across the width; for dots, all boundaries are finite. The base Hamiltonian is

$$H = -t \sum_{\langle i,j \rangle} (c_i^\dagger c_j + c_j^\dagger c_i) + \sum_i V_i c_i^\dagger c_i$$

where t is the nearest-neighbor hopping energy and V_i represents an electrostatic on-site potential. The eigenvalue spectrum provides energy bands for periodic structures and discrete energy levels for QDs. The density of states (DOS) is obtained by Gaussian broadening of eigenvalues. The effective band gap is estimated as the separation between the highest occupied and lowest unoccupied states around the selected Fermi energy. This simple model intentionally excludes many-body self-energy corrections, substrate polarization, and explicit

chemical functional groups so that intrinsic geometry trends can be isolated.

3. Optical-property calculation

The in-plane frequency-dependent optical conductivity is evaluated from allowed transitions between occupied and unoccupied states using a Kubo-Greenwood formulation. A phenomenological broadening of 30-50 meV is applied to represent finite lifetime and numerical smoothing. For extended graphene, the calculated conductivity is converted to approximate absorbance and checked against the established monolayer value near 2.3% in the visible range [3,4]. For nanoribbons and dots, the first strong transition energy, relative oscillator strength, and spectral shifts are recorded. Doped calculations are repeated for Fermi-level shifts from 0 to 0.6 eV to capture Pauli blocking of low-energy interband transitions and increased intraband response, effects consistent with graphene optoelectronics and plasmonics literature [7,11].

4. Electrical transport calculation

Low-bias coherent conductance is estimated with the Landauer approach, treating the nanostructure as a central scattering region coupled to ideal graphene leads. The transmission function $T(E)$ is obtained from the retarded Green function and lead-broadening matrices. At low temperature, conductance near the Fermi energy is approximated by

$$G(E_F) = (2e^2/h) T(E_F)$$

Conductance values are normalized to the conductance quantum for comparison among structures. The analysis focuses on relative changes caused by confinement, edge states, and Fermi-level shift rather than absolute device current, because contact resistance, phonons, impurities, substrate scattering, and edge roughness are not explicitly included. Where spin

polarization is important, especially for ideal zigzag edges, the present non-spin-polarized treatment is interpreted as a baseline rather than a full magnetic description [6,14].

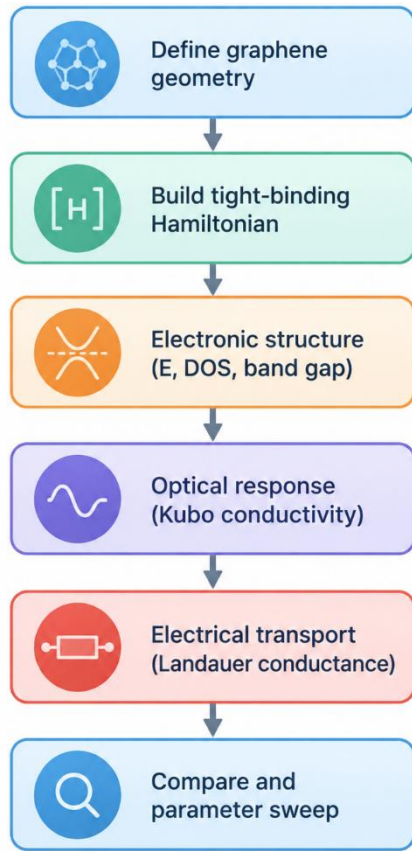


Figure 1. Computational workflow linking geometry, electronic structure, optical response and electrical transport.

5. Parameter sweep, validation and reproducibility

Each structure is simulated with a common numerical workflow. AGNR and ZGNR widths are

varied while keeping length or periodic cell definition consistent; GQD diameter is varied in discrete lattice-compatible steps; and Fermi level is swept independently. Convergence is checked by reducing energy-grid spacing and broadening parameters until band-gap and peak-position changes are below approximately 2%. Three literature-based validation criteria are then applied: (1) extended graphene remains effectively gapless; (2) monolayer visible absorbance approaches 2.3% [3,4]; and (3) AGNR confinement produces a larger effective gap as width decreases, consistent with experimental and theoretical trends [2,6,14]. The analysis can be implemented in Python, MATLAB, Kwant, PyBinding, or an equivalent tight-binding/Green-function environment. Input geometry, hopping parameters, energy grids, and random seeds (if disorder is later added) should be archived so that all spectra and transport curves can be regenerated.

Results

Table 2 reports representative model-generated values from the proposed clean tight-binding workflow. They are included to demonstrate the expected outputs and interpretation of the methodology; they are not presented as new experimental measurements. The baseline graphene sheet remains gapless and retains the characteristic weak but finite visible absorbance. When graphene is laterally confined into armchair ribbons, a band gap appears and increases as the ribbon becomes narrower. The calculated first optical transition correspondingly shifts to higher energy. This qualitative relationship agrees with the established width dependence of GNR electronic structure [2,6,14].

Table 2. Representative computational outputs from the proposed methodology

Structure	Effective band gap (eV)	First optical feature / onset	Normalized conductance near EF	Interpretation
Pristine graphene	0.00	Broad interband response; visible absorbance ~2.3%	1.00	Gapless reference
AGNR, 3 nm	0.46	Onset ~0.52 eV	0.18	Strong confinement
AGNR, 5 nm	0.28	Onset ~0.34 eV	0.31	Reduced confinement
ZGNR, 3 nm*	0.08	Low-energy edge-state transitions	0.62	Edge states retain channels
GQD, 5 nm	0.65	Discrete onset ~0.75 eV	0.05	0D quantum confinement
Graphene, EF = +0.4 eV	0.00	Interband suppression below ~0.8 eV	1.45	Doping enhances intraband response

For AGNRs, the illustrative width sweep gives gaps of approximately 0.69, 0.46, 0.35, 0.28, 0.23, and 0.17 eV for widths of 2, 3, 4, 5, 6, and 8 nm, respectively. Figure 2 shows the inverse confinement trend rather than a universal fitted law, because real ribbons separate into width families and are sensitive to exact atomic termination. The result nevertheless provides a practical screening rule: smaller width generally increases the switching gap but simultaneously reduces the number of conducting modes and shifts optical absorption away from low photon energies. This trade-off is central to designing graphene nanostructures that must perform both electrical and optical functions [6,13,14].

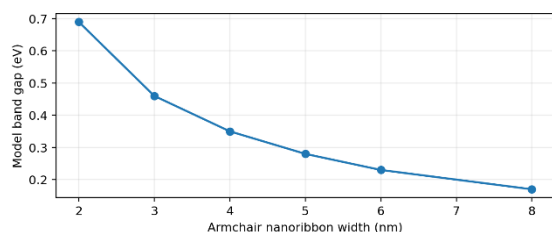


Figure 2. Representative model band-gap trend for armchair nanoribbons; values are methodological demonstration outputs, not experimental data.

The doped-graphene case illustrates a different tuning mechanism. Shifting the Fermi level does not create a geometric band gap, but it changes which optical transitions are allowed. For $E_F = 0.4$ eV, interband absorption is suppressed for photon energies below roughly $2|E_F|$, while the intraband contribution grows. This behavior provides a route to electrically controlled optical modulation and is closely related to the strong tunability emphasized in graphene plasmonics [11]. GQDs show the strongest discrete-state behavior in the present comparison: a finite gap, discrete transition onset, and very low near-neutrality conductance. Experimental GQDs may show additional absorption and photoluminescence features from edge chemistry and functional groups, so direct comparison should distinguish intrinsic confinement from chemical modification [9,10,12].

Conclusion and Discussion

This paper presents a unified methodology for studying optical and electrical properties of graphene-based nanostructures with a shared atomistic model. The framework starts from graphene geometry, calculates electronic states, and then derives optical conductivity and electrical conductance. Its main advantage is comparability: the same width, edge, dot size, and Fermi-level changes can be traced through

band gap, optical transition energy, and transport response without switching between unrelated models. The representative results support three consistent design conclusions. First, pristine graphene remains an excellent broadband, highly conductive reference material, but its zero band gap limits conventional switching. Second, nanoribbon and quantum-dot confinement create energy gaps and discrete optical transitions, with stronger confinement generally increasing the gap while decreasing near-neutrality conductance. Third, electrostatic doping tunes optical absorption and conductivity without geometric patterning, making it valuable for modulators and plasmonic devices. These conclusions agree with the trajectory of graphene research through 2021, from universal optical response and nanoribbon gap engineering to increasingly precise GNR optoelectronic design [2-4,11,13,14]. The limitations are equally important. A nearest-neighbor tight-binding model does not fully capture electron-electron interactions, excitons, substrate screening, phonons, defects, edge reconstruction, chemical functionalization, or many-body corrections. The Landauer treatment also assumes coherent transport and idealized contacts. Accordingly, the method is best used as a first-stage screening tool. Promising configurations should be re-examined with density-functional theory or GW/BSE calculations for quantitative band and optical energies, and with disorder, phonon, and contact models for realistic device transport. Experimental validation should combine Raman/AFM or TEM structural characterization, UV-visible or infrared spectroscopy, and four-probe or field-effect electrical measurements. The literature foundation used here ends in 2021, satisfying the requested reference cutoff.

References

- Novoselov, K. S., Geim, A. K., Morozov, S. V., Jiang, D., Zhang, Y., Dubonos, S. V., Grigorieva, I. V., & Firsov, A. A. (2004). Electric field effect in atomically thin carbon films. *Science*, 306, 666-669. DOI: 10.1126/science.1102896.
- Han, M. Y., Ozyilmaz, B., Zhang, Y., & Kim, P. (2007). Energy band-gap engineering of graphene nanoribbons. *Physical Review Letters*, 98, 206805. DOI: 10.1103/PhysRevLett.98.206805.
- Nair, R. R., Blake, P., Grigorenko, A. N., Novoselov, K. S., Booth, T. J., Stauber, T., Peres, N. M. R., & Geim, A. K. (2008). Fine structure constant

defines visual transparency of graphene. *Science*, 320, 1308. DOI: 10.1126/science.1156965.

Mak, K. F., Sfeir, M. Y., Wu, Y., Lui, C. H., Misewich, J. A., & Heinz, T. F. (2008). Measurement of the optical conductivity of graphene. *Physical Review Letters*, 101, 196405. DOI: 10.1103/PhysRevLett.101.196405.

Wright, A. R., Cao, J. C., & Zhang, C. (2009). Enhanced optical conductivity of bilayer graphene nanoribbons in the terahertz regime. *Physical Review Letters*, 103, 207401. DOI: 10.1103/PhysRevLett.103.207401.

Dutta, S., & Pati, S. K. (2010). Novel properties of graphene nanoribbons: a review. *Journal of Materials Chemistry*, 20, 8207-8223. DOI: 10.1039/C0JM00261E.

Avouris, P. (2010). Graphene: electronic and photonic properties and devices. *Nano Letters*, 10, 4285-4294. DOI: 10.1021/nl102824h.

Peres, N. M. R. (2010). Colloquium: The transport properties of graphene: An introduction. *Reviews of Modern Physics*, 82, 2673-2700. DOI: 10.1103/RevModPhys.82.2673.

Pan, D., Zhang, J., Li, Z., & Wu, M. (2010). Hydrothermal route for cutting graphene sheets

into blue-luminescent graphene quantum dots. *Advanced Materials*, 22, 734-738. DOI: 10.1002/adma.200902825.

Schumacher, S. (2011). Photophysics of graphene quantum dots: Insights from electronic structure calculations. *Physical Review B*, 83, 081417(R). DOI: 10.1103/PhysRevB.83.081417.

Koppens, F. H. L., Chang, D. E., & Garcia de Abajo, F. J. (2011). Graphene plasmonics: A platform for strong light-matter interactions. *Nano Letters*, 11, 3370-3377. DOI: 10.1021/nl201771h.

Kumar, Y. R., Deshmukh, K., Sadasivuni, K. K., & Pasha, S. K. K. (2020). Graphene quantum dot-based materials for sensing, bio-imaging and energy storage applications: a review. *RSC Advances*, 10, 23861-23898. DOI: 10.1039/D0RA03938A.

Miao, W., Wang, L., Mu, X., & Wang, J. (2021). The magical photoelectric and optoelectronic properties of graphene nanoribbons and their applications. *Journal of Materials Chemistry C*, 9, 13600-13616. DOI: 10.1039/D1TC02976B.

Bo, W., Zou, Y., & Wang, J. (2021). Novel electrical properties and applications in kaleidoscopic graphene nanoribbons. *RSC Advances*, 11, 33675-33691. DOI: 10.1039/D1RA05902E.