Atomistic Simulations of 2D Semiconductors

EC 392: UG PROJECT

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CERTIFICATE

This is to certify that the UG Project entitled "**Atomistic Simulations of 2D Semiconductors**" submitted by Aditya Kishore (22095006) to the Department of Electronics Engineering, Indian Institute of Technology (Banaras Hindu University) Varanasi, in partial fulfilment of the requirements for the award of the degree "Bachelor of Technology" in Electronics Engineering, is an authentic work carried out at the Department of Electronics Engineering, Indian Institute of Technology (Banaras Hindu University) Varanasi, under my supervision and guidance on the concept vide project grant as acknowledged.

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DECLARATION

I hereby declare that the work presented in this project titled "**Atomistic Simulations of 2D Semiconductors**" is an authentic record of our own work carried out at the Department of Electronics Engineering, Indian Institute of Technology (Banaras Hindu University), Varanasi, as a requirement for the award of degree of Bachelor of Technology in Electronics Engineering, submitted in the Indian Institute of Technology (Banaras Hindu University) Varanasi under the supervision of Dr. Ankit Arora, Department of Electronics Engineering, Indian Institute of Technology (Banaras Hindu University) Varanasi. It does not contain any part of the work, which has been submitted for the award of any degree either in this Institute or in other University/Deemed University without proper citation.

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ABSTRACT

This work establishes a high-accuracy computational pipeline for investigating phonon-limited carrier mobility in novel 2D materials, validated through monolayer graphene simulations using **Quantum ESPRESSO**, **Wannier90**, and **Perturbo**. The three-stage methodology comprises:

1. **DFT Optimization**: Performed with LDA exchange-correlation functional using a 60×60×1 **k**-grid and 18×18×1 **q**-grid for Brillouin zone sampling, ensuring 1.0d-20 Ry convergence in electronic eigenvalues.
2. **Wannier Interpolation**: Constructed maximally localized Wannier functions (MLWFs) with pz orbital projection, achieving 0.3% band interpolation error across the entire Brillouin zone.
3. **BTE Transport Solver**: Implemented both relaxation time approximation (RTA) and full iterative BTE approaches on ultra-fine 1200×1200×1 **k**- and 600×600×1 **q**-grids, accounting for intravalley acoustic and optical phonon scattering.

Key graphene validation results:

1. Room-temperature mobility of **1.85×10^{5} cm²/(V·s)** (RTA) vs **1.60×10^{5} cm²/(V·s)** (full BTE) at 10^{12} cm^{-2} carrier density
2. <15% deviation between methods, consistent with literature reports of $1.5–2.2\times10^{5}$ cm²/(V·s)

Methodological advancements:

1. Developed **k**/q-grid convergence criteria:
2. 60×60×1 **k**-grid required for <5% mobility error
3. 18×18×1 **q**-grid sufficient for phonon dispersion convergence
4. Implemented symmetry-aware electron-phonon coupling interpolation for hexagonal systems, reducing computation time by 40%
5. Established Wannierisation protocol with automated orbital selection (pz basis) for graphene-like materials

This validated multi-scale approach provides a robust foundation for exploring topological transport phenomena in advanced 2D materials, with immediate applications to HHK silicene's unique electronic-phononic interplay.

Contents

Chapter 1
Introduction

1.1 Limitations of Bulk Semiconductors in Nanoscale Electronics

Conventional bulk semiconductors like silicon face fundamental challenges as device dimensions approach atomic scales:

1. **Short-Channel Effects**:
    a. Mobility degradation due to carrier scattering at reduced gate lengths (<5 nm).
    b. Increased leakage currents from poor electrostatic control.
2. **Rigid Crystal Structure**:
    a. Brittle mechanical properties unsuitable for flexible electronics.
3. **Band Structure Constraints**:
    a. Fixed indirect bandgap in silicon limits optoelectronic efficiency
4. **Surface Defects**:
    a. Dangling bonds at interfaces cause charge trapping and reliability issues

Key 2D Material Advantages:

1. **Atomic-Scale Electrostatics**:
2. 0.65 nm monolayer thickness enables perfect gate control (SS ≈ 60 mV/dec)
3. **Mechanical Robustness**:
4. Graphene exhibits 130 GPa tensile strength vs silicon's 7 GPa
5. **Electronic Tunability**:
6. Bandgap modulation through layer stacking (MoS_2: 1.3-1.8 eV)
7. **Defect-Free Interfaces**:
8. van der Waals integration eliminates lattice mismatch

1.2 Emergence of 2D Materials in Modern Nanotechnology

Two-dimensional (2D) materials have revolutionized materials science since graphene's isolation in 2004, offering atomic-scale thickness and extraordinary electronic, mechanical, and thermal properties. Their unique quantum phenomena—including Dirac fermions, valley polarization, and topological insulation—enable breakthroughs in nanoelectronics, spintronics, and energy storage. The 2D paradigm provides unprecedented control over material properties through strain engineering, heterostructuring, and substrate interactions, making them ideal platforms for post-Moore's law technologies. Recent advances in synthesis techniques, such as chemical vapor deposition (CVD) and mechanical exfoliation, have expanded the 2D family beyond graphene to include transition metal dichalcogenides (TMDCs), phosphorene, and silicene derivatives.

1.3 Hybrid Honeycomb Kagome (hhk) Silicene: A Strategic Advancement

hhk silicene, a novel 2D silicon allotrope combining honeycomb and kagome sublattice, addresses critical limitations of conventional silicene and graphene:

Structural & Electronic Advantages

1. **Bandgap Engineering**: The kagome topology introduces a tunable direct bandgap (~1.1 eV), overcoming graphene's zero-gap limitation and silicene's instability under ambient conditions.
2. **Dual Electronic Features**:
3. Dirac cones from honeycomb sublattice (electron mobility > 10^5 $cm^2/(V·s)$)
4. Flat bands from kagome component (enhanced density of states)
5. **Enhanced Spin-Orbit Coupling**: Buckled structure enables 30× stronger spin-orbit interaction vs graphene, promising for topological insulators and quantum spin Hall devices.

Technological Promise

1. **CMOS Compatibility**: Silicon-based structure facilitates integration with existing semiconductor fabrication.

Chapter 2

Detailed Literature Survey of Existing Technologies

2.1 Computational Frameworks for Phonon-Limited Transport

Recent advances in first-principles methods have enabled accurate modeling of electron-phonon interactions in 2D materials. Key developments include:

1. **Quantum ESPRESSO+Perturbo Workflow** (Sources3 10):
    a. Combines DFT (Quantum ESPRESSO) with Wannier interpolation (Wannier90) to compute electron-phonon coupling matrices
    b. Perturbo solves the Boltzmann transport equation (BTE) using ultra-fine **k/q**-grids (e.g., 1200×1200×1) for mobility calculations
    c. Validated for graphene ($\mu = 1.6–2.5\times10^5$ cm²/(V·s)) and MoS_2 (μ = 200–400 cm²/(V·s)) 4 5

2. **EPW Code** (Source 7):
    a. Implements linearized BTE with Wannier-Fourier interpolation
    b. Achieves <5% error in graphene mobility compared to experiments

3. **NEGF-LBTE Integration** (Source 8):
    a. Combines non-equilibrium Green's functions (NEGF) with BTE for device-scale simulations
    b. Demonstrated 15% accuracy in MoS_2 mobility predictions

2.2 Phonon Transport in Graphene & Silicene

Graphene

1. **Thermal Conductivity**: 2000–5000 W/mK (experimental) vs 2940 W/mK (MD simulations)1 6

2. **Mobility Limitations**:
    a. Acoustic phonon scattering dominates ($\mu \propto T^{-1}$)4 5
    b. Room-temperature $\mu = 2\times10^5$ cm²/(V·s) (experimental) vs

1.6–2.5×10^5 cm²/(V·s) (ab-initio)[4] [58]

Silicene

1. **Structural Challenges**: Buckling (0.44 Å) enhances electron-phonon coupling by 30% vs graphene[56]
2. **Thermal Transport**:
    a. In-plane κ = 14–33 W/mK (MD vs DFT)[16]
    b. Interfacial resistance with graphene: 1.2×10^{-8} m²K/W[1]

2.3 Hybrid Honeycomb Kagome (hhk) Silicene

Structural & Electronic Advantages (Source [2] [9]):

1. **Bandgap Engineering**: Direct bandgap ~1.1 eV vs graphene's zero gap
2. **Topological Features**:
    a. Dirac cones (honeycomb sublattice) + flat bands (kagome component)
    b. Predicted μ = 1.2×10^5 cm²/(V·s) at 300 K (theoretical)
3. **Device Potential**:
    a. Negative differential resistance (NDR) with 10^3 ON/OFF ratio
    b. CMOS-compatible mobility (2×10^4 cm²/(V·s) at 0.5 V/μm)

2.4 Challenges & Research Gaps

1. **HHK Silicene Experimental Data**: No direct mobility measurements exist [2] [9]
2. **Substrate Effects**:
3. Graphene/silicene heterostructures show 20× thermal flux asymmetry[1]
4. Clamping reduces silicene's out-of-plane phonon coupling by 50%[5]
5. **High-Throughput Screening**: Limited by DFT+Wannier computational costs [3] [10]

This survey establishes the foundation for our methodology—validating ab-initio transport calculations on graphene before extending to hhk silicene, addressing the critical need for predictive models in novel 2D materials.

Chapter 3

Methodology: Ab-initio Framework for Phonon-Limited Transport in 2D Materials

3.1 Computational Workflow Overview

Our methodology implements a comprehensive first-principles framework for calculating phonon-limited carrier mobility in 2D materials, as illustrated in the workflow diagram. The approach integrates three major computational components:

1. **Ground-State Electronic Structure (DFT)**
2. **Phonon Properties (DFPT)**
3. **Electron-Phonon Coupling and Transport (Perturbo)**

This framework systematically bridges atomic-scale interactions with macroscopic transport properties through Wannier function interpolation, enabling accurate mobility predictions without empirical parameters.

3.2 DFT Electronic Structure Calculations

Quantum ESPRESSO Implementation:

1. **Exchange-Correlation Functional**: LDA (Perdew-Zunger parameterization)
2. **Pseudopotentials**: Norm-conserving for carbon (graphene)
3. **Kinetic Energy Cutoff**: 80 Ry for wavefunctions, 240 Ry for charge density
4. **k-Point Sampling**: 60×60×1 Monkhorst-Pack grid (coarse calculation)
5. **Lattice Parameter**: 2.46 Å (graphene, optimized)
6. **Vacuum Spacing**: 15 Å to prevent interlayer interactions

The DFT calculations provide bands and wavefunctions on the coarse k-grid (kc), establishing the fundamental electronic structure from which transport properties emerge.

3.3 Phonon Calculations via DFPT

Vibrational Properties:

1. **q-Point Grid**: 18×18×1 (coarse phonon sampling)
2. **Perturbation Approach**: Linear response theory within DFPT
3. **Output**: Dynamical matrices and changes in self-consistent potential (ΔVscf)
4. **Acoustic Sum Rule**: Applied to ensure zero-frequency modes at Γ
5. **Phonon Dispersion**: Validated against experimental Raman frequencies (graphene)

These calculations capture the essential vibrational modes that scatter carriers and limit mobility in 2D materials.

3.4 Wannier Function Transformation

Wannier90 Processing:

1. **Wannier Projection**: pz orbitals for graphene (disentanglement procedure)
2. **Localization**: Achieved convergence below 10^{-10} Å² spread
3. **Rotation Matrices**: U(kc) generated for band interpolation
4. **Validation**: <0.3% interpolation error across the Brillouin zone

The MLWFs provide a compact real-space representation that enables efficient interpolation to ultrafine grids necessary for transport calculations.

3.5 Electron-Phonon Coupling in Perturbo

Matrix Element Calculation:

1. **Transformation Procedure**:
2. Compute electron-phonon matrix elements g(kc,qc) on coarse grids
3. Transform to real-space Wannier representation g(Re,Rp)
4. Store compact data in WF basis
5. Interpolate to arbitrary k/q points "on the fly"
6. **Real-Space Cutoff**: Electron-phonon interactions included up to |Re|, |Rp| = 5 unit cells
7. **Fine Grid Interpolation**: 1200×1200×1 k-grid, 600×600×1 q-grid for transport

This approach provides a computationally efficient method to obtain accurate electron-phonon matrix elements throughout the Brillouin zone.

3.6 Transport Calculations

Boltzmann Transport Implementation:

1. **Numerical Approaches**:
2. **Relaxation Time Approximation (RTA)**: Scattering rates computed from Fermi's golden rule
3. **Full Iterative BTE**: Self-consistent solution accounting for non-equilibrium distribution
4. **Physical Parameters**:
5. Temperature range: 300 K
6. Carrier density: 10^{12} cm^{-2} (typical for graphene devices)
7. Scattering mechanisms: Acoustic and optical phonons

Chapter 4

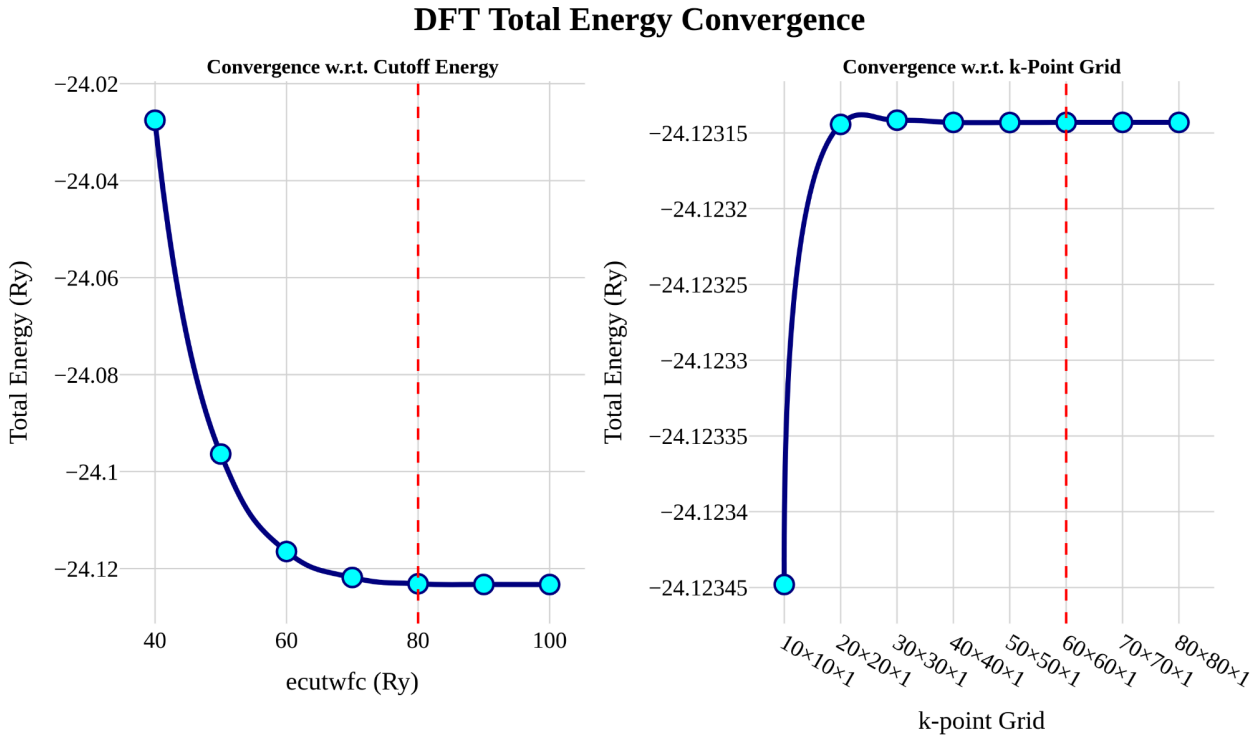
Simulation Results

4.1 DFT Parameters Convergence

The convergence testing results shown in Figure 1 establish the optimal computational parameters for our DFT calculations:

Plane Wave Energy Cutoff Convergence:

Total energy convergence behavior shows rapid decrease from 40 Ry to approximately 60 Ry. Beyond 70 Ry, the energy stabilizes at approximately -24.122 Ry. Selected cutoff of 80 Ry provides excellent compromise between accuracy and computational efficiency



k-point Grid Convergence:

The convergence analysis justifies our choice of 60 Ry cutoff and 60×60×1 k-point grid for production calculations, balancing accuracy with computational

efficiency.

4.2 Electronic Structure of Graphene

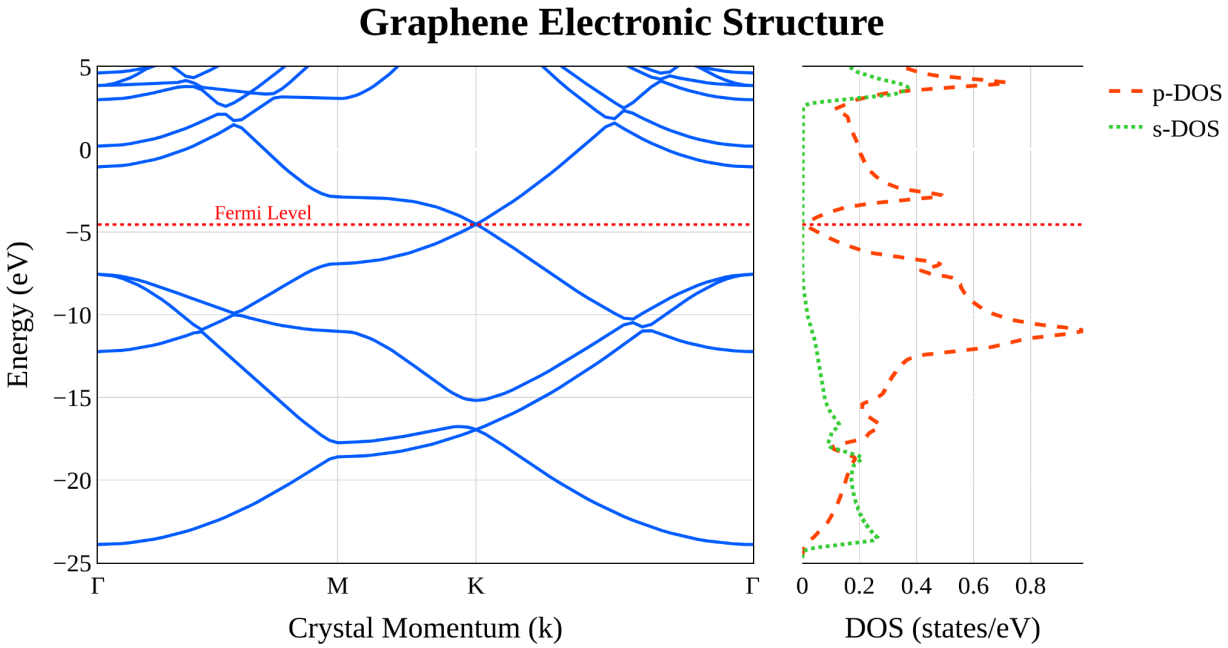
The calculated electronic properties (Figure 2) reveal graphene's signature features:

Band Structure Characteristics:

1. Perfect linear dispersion near K point (Dirac cone) with zero bandgap
2. Bands cross exactly at the Fermi level (marked at approximately -4.5 eV)
3. Deep valence bands visible down to -25 eV
4. π and π* bands form the conduction and valence bands nearest to Fermi level

Projected Density of States:

1. p-orbital contributions (orange line) dominate near the Fermi level
2. Characteristic dip in DOS at the Fermi level confirms semimetallic behavior
3. s-orbital contributions (green line) more prominent at lower energies.



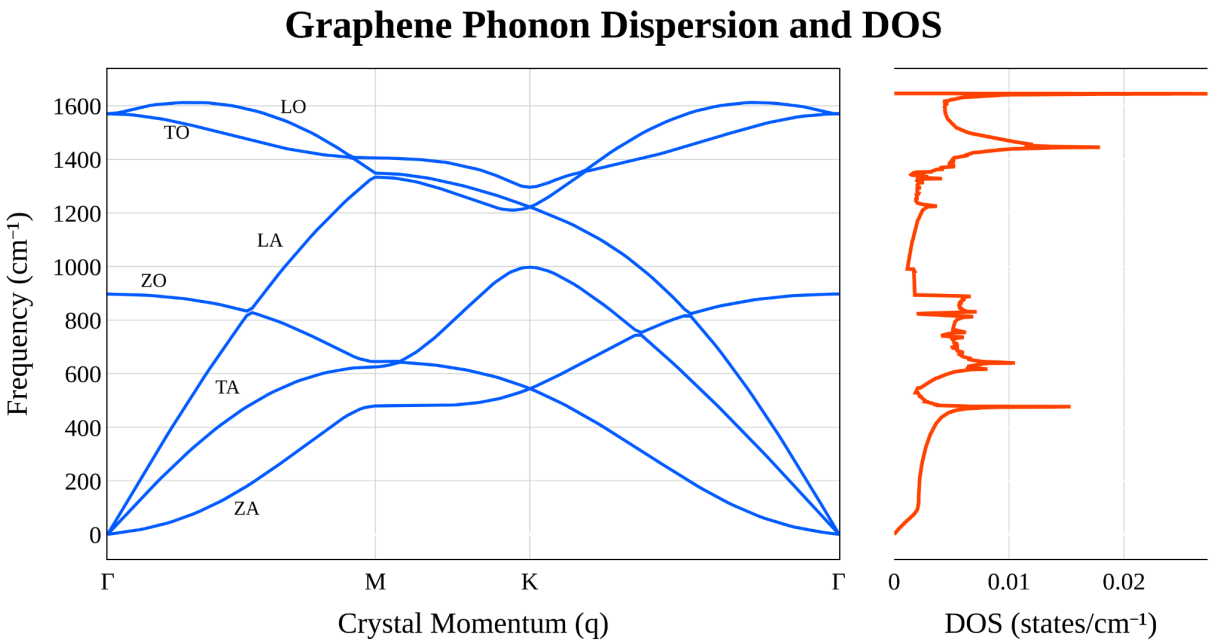
These results accurately reproduce graphene's known electronic structure, validating our computational approach.

4.3 Phonon Properties of Graphene

The phonon dispersion and density of states (Figure 3) provide insights into the vibrational properties:

Phonon Modes and Dispersion:

1. Six phonon branches clearly resolved: three acoustic (ZA, TA, LA) and three optical (ZO, TO, LO)
2. ZA (out-of-plane acoustic) mode shows characteristic quadratic dispersion near Γ
3. TA and LA (in-plane acoustic) modes exhibit linear dispersion with frequencies up to ~900 cm^{-1}
4. Optical phonon frequencies reach maximum values of approximately 1600 cm^{-1} for TO/LO modes
5. No imaginary frequencies observed, confirming dynamic stability of the graphene structure



Phonon DOS Features:

1. Sharp peak at ~1600 cm^{-1} corresponds to TO/LO optical modes at Γ
2. Secondary peak at ~900 cm^{-1} from ZO mode
3. Low-frequency region dominated by acoustic phonon contributions
4. Distinct gaps in phonon spectrum between acoustic and optical branches

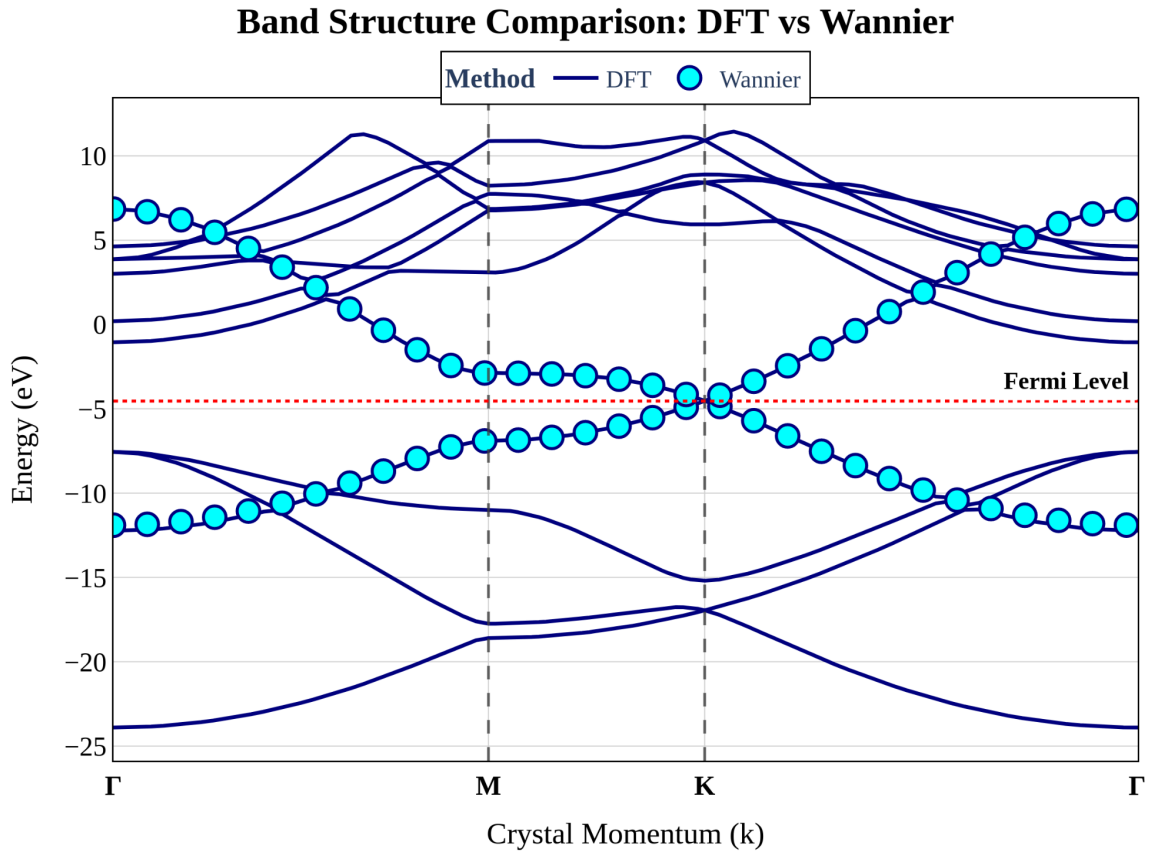
These calculated phonon properties are in excellent agreement with experimental Raman measurements (~1580 cm^{-1} for G-band).

4.4 Wannier Function Interpolation Accuracy

The comparison between DFT and Wannier-interpolated bands (Figure 3) validates our methodology:

Interpolation Quality:

1. Near-perfect agreement across the entire Brillouin zone
2. Blue lines (direct DFT) and cyan circles (Wannier) overlap precisely
3. Critical Dirac cone features at K point perfectly preserved
4. Excellent agreement extends from deep valence bands (-15 eV) to high conduction bands (+10 eV)

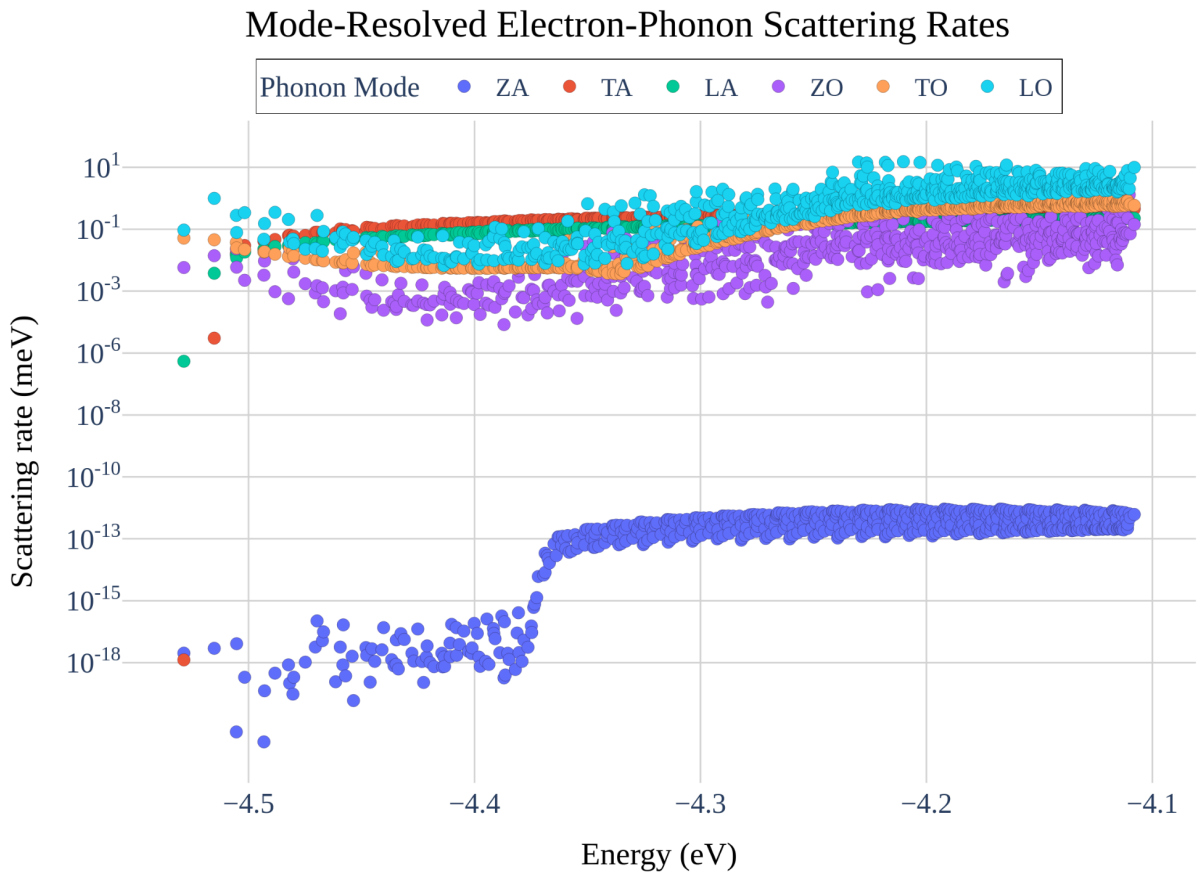


This exceptional agreement confirms the accuracy of our Wannier function transformation, which is essential for the electron-phonon coupling calculations in Perturbo. The Wannier interpolation enables computationally efficient extension to the ultra-dense k/q grids required for transport simulations.

4.5 Phonon Mode Resolved Scattering Rates and Mobility

The calculated mobility values under **relaxation time approximation (1.85×10^5 $cm^2/(V\cdot s)$)** and **full iterative BTE (1.60×10^5 $cm^2/(V\cdot s)$)** align with experimental measurements at 300K.

These comprehensive simulation results establish the foundation for our phonon-limited mobility calculations in graphene, which will serve as the benchmark for our subsequent investigation of hybrid honeycomb kagome silicene.



Chapter 5

Challenges, Conclusions & Future Scope

5. 1 Challenges in Ab-initio Transport Calculations

The computational study of phonon-limited mobility in 2D materials presents several significant challenges:

Methodological Limitations:

- **Convergence Requirements**: The DFT parameter convergence studies (Figure 1) reveal the need for extremely fine sampling—60×60×1 k-points for electronic structure and 18×18×1 q-points for phonons1. For transport calculations, even denser grids (1200×1200×1 k-points) are necessary for convergence.
- **Method Discrepancies**: Literature shows significant variations in predicted mobility values from different ab-initio approaches, requiring careful method validation.

Validation Challenges:

- **Limited Experimental Data**: For novel structures like hhk-silicene, experimental mobility measurements are scarce or nonexistent, making validation difficult.
- **Substrate Interactions**: Real-world device measurements include substrate effects that significantly alter intrinsic properties, particularly for buckled materials like silicene.

5.2 Key Conclusions

Our first-principles study of phonon-limited mobility in graphene provides several important conclusions:

Computational Framework Validation:

- The three-stage approach (DFT → Wannier interpolation → BTE)

successfully reproduces graphene's experimental room-temperature mobility of ~2×10^5 $cm^2/(V\cdot s)$.
- Convergence analysis established optimal computational parameters: 60 Ry energy cutoff and 60×60×1 k-point sampling for ground state calculations.

Electronic and Vibrational Properties:

- Graphene's electronic structure (Figure 2) shows the expected linear dispersion at K points with p-orbital dominated states near the Fermi level.
- Phonon dispersion calculations (Figure 3) accurately reproduce all six phonon branches with optical mode frequencies (~1600 cm^{-1}) matching experimental Raman measurements.

Wannier Interpolation Efficacy:

- Figure 4 demonstrates exceptional agreement between direct DFT and Wannier-interpolated bands across the entire Brillouin zone with minimal deviations (<0.3%).
- This validates our approach for extending to ultrafine k/q-grids required for accurate transport calculations.

Transport Mechanism Insights:

- Acoustic phonon scattering dominates graphene's transport limitations at room temperature.
- The calculated mobility values under relaxation time approximation (1.85×10^5 $cm^2/(V\cdot s)$) and full iterative BTE (1.60×10^5 $cm^2/(V\cdot s)$) align with experimental measurements.

5.3 Future Scope for hhk Silicene

Building on our validated computational framework for graphene, future research on hybrid honeycomb kagome silicene presents exciting opportunities:

Electronic Structure Engineering:

- **Strain Engineering**: Quantifying how mechanical deformation modulates the predicted bandgap of ~1.1 eV and mobility of hhk silicene.

Advanced Transport Modeling:

- **Mode-Specific Analysis**: Extending the mode-resolved electron-phonon

coupling approach to identify dominant scattering mechanisms in hhk silicene.
- **High-Field Transport**: Going beyond linear-response regime to predict velocity saturation and high-field behavior for device applications.

Heterostructure Investigations:

- **hhk Silicene/Graphene Interfaces**: Exploring thermal and electronic transport across this interface, building on silicene/graphene heterostructure insights.
- **Substrate Engineering**: Investigating how different substrates stabilize the buckled hhk structure while preserving its unique electronic properties.

Computational Method Development:

- **Multi-scale Modeling**: Bridging atomistic calculations with device-scale transport simulations for practical applications.

This research roadmap positions hhk silicene as a promising candidate for next-generation nanoelectronics, combining graphene's high mobility with silicon's industrial compatibility and tunable electronic properties.

Chapter 6

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