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Full-band atomistic study of electron-phonon interaction in carbon nanotubes

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Abstract
This paper presents a comprehensive study of electron-phonon interactions in carbon nanotubes (CNTs), using the non-equilibrium Green's function (NEGF) method. The transmission function is calculated to analyze the influence of electron-optical-phonon interactions, which are crucial in determining carrier scattering. Our study includes full-band analysis and atomistic details using the tight-binding approximation. Scattering rates and transmission functions are presented, showing significant impacts at the band center and minimal effects at band edges.

Keywords: Carbon nanotubes (CNTS), tight-binding approximation, electron-phonon, interaction, transfer integral, nearest-neighbour interactions, quantum transport

1. Introduction
In the realm of nanoelectronics, carbon-based materials have garnered significant attention due to their exceptional electrical, thermal, and mechanical properties. Among these, carbon nanotubes (CNTs) stand out as promising candidates for future electronic devices, owing to their unique one-dimensional structure and tunable electronic properties. Discovered in 1991 by Iijima [1], CNTs have rapidly emerged as one of the most studied nanomaterials, offering wide-ranging applications in transistors, sensors, interconnects, and energy storage systems [2]. The exceptional electrical conductivity of CNTs, alongside their high current-carrying capacity, make them ideal for addressing the challenges posed by the continued miniaturization of electronic devices.

CNTs are typically categorized into two types: metallic and semiconducting, depending on their chirality, i.e., the specific arrangement of carbon atoms in their hexagonal lattice. This chirality influences the band structure, which in turn affects their electrical properties. Metallic CNTs have linear, gapless band structures near the Fermi level, allowing for high electron mobility, which is highly advantageous for nanoelectronics. Conversely, semiconducting CNTs exhibit a band gap, making them useful for logic devices. A key area of interest in the study of CNTs lies in understanding the transport properties of electrons and holes in these materials, particularly how they interact with lattice vibrations, or phonons [3]. At room temperature, electron-phonon interactions play a pivotal role in limiting the performance of CNT-based devices. Phonons, which are quantized lattice vibrations, can scatter charge carriers (electrons or holes) within CNTs, leading to energy dissipation and reduced conductance. The electron-phonon interaction is particularly critical in determining the current-voltage characteristics of CNT-based field-effect transistors (FETs) and interconnects, where high carrier mobility is essential for efficient operation [4]. As CNT-based electronic devices are envisioned to operate at higher frequencies and smaller dimensions, it becomes imperative to understand the microscopic mechanisms governing these interactions.

Graphene and its derivatives, such as graphene nanoribbons (GNRs) and CNTs, are considered ideal platforms for exploring electron-phonon interactions because of their two-dimensional (2D) or quasi-1D nature. In CNTs, the interaction between electrons and phonons can be divided into two primary mechanisms: elastic and inelastic scattering. Elastic scattering is primarily due to acoustic phonons, which have relatively low energies and are less disruptive to the electron's path. In contrast, inelastic scattering is dominated by optical phonons, which involve higher energies and are more likely to disrupt electron flow, particularly at high voltages [5].

Previous studies have shown that electron-optical phonon interactions in CNTs lead to distinct signatures in transport measurements, such as reduced transmission near certain energy thresholds due to phonon emission [6]. The challenge lies in accurately quantifying these interactions and incorporating them into models for device performance prediction. The Non-Equilibrium Green's Function (NEGF) formalism provides a powerful framework to address these challenges, enabling a detailed study of how electron-phonon scattering affects electron transport at the atomic scale.

In this work, we use the NEGF method, coupled with a tight-binding approximation, to calculate the transmission function through metallic CNTs. The focus is on the full-band and atomistic effects of electron-phonon interactions, with a particular emphasis on optical phonon scattering. By systematically studying how these interactions influence transmission and scattering rates, this work aims to contribute to the fundamental understanding of electron transport in CNTs, aiding the design of more efficient nanoelectronic devices.

2. Methodology

2.1 Electronic States

In carbon nanotubes (CNTs), the electronic states can be described using the tight-binding approximation, a widely used method for modeling the electronic structure of systems with a known lattice configuration. This method is particularly effective for CNTs, as their quasi-one-dimensional structure can be well approximated by considering interactions between neighboring atomic sites. The electron wave function $\Psi(r)$ for the system is constructed as a linear combination of atomic orbitals centered on the positions of the carbon atoms, denoted by R_n. Each carbon atom in a CNT contributes a p_z orbital to the wave function. The total electron wave function can be written as:

$$\Psi(r) = \sum_{R_n} \Psi(R_n)\, \phi(r - R_n)$$

Here, $\Psi(R_n)$ represents the amplitude of the wave function at position R_n, $\phi(r - R_n)$ is the p_z orbital wave function centered on the carbon atom at position R_n.

In the tight-binding model, the Hamiltonian H describes the total energy of the system, considering both the on-site energy E_{nm} (energy of an electron located at a given atom) and the transfer integrals $\gamma_{nm,m'}$ (which represent the hopping of electrons between neighboring atoms). The Hamiltonian for CNTs can be expressed as:

$$H = \sum_{nm} E_{nm}\, |\phi_{nm}\rangle\langle\phi_{nm}| + \sum_{nm \neq n'm'} \gamma_{nm,n'm'}\, |\phi_{nm}\rangle\langle\phi_{n'm'}|$$

In this equation, E_{nm} is the on-site energy at position n and orbital m, $\gamma_{nm,n'm'}$ represents the transfer integral (hopping energy) between neighboring orbitals ϕ_{nm} and $\phi_{n'm'}$, $|\phi_{nm}\rangle\langle\phi_{nm}|$ represents the state of the electron at the orbital nm, and $|\phi_{n'm'}\rangle\langle\phi_{n'm'}|$ represents the state of the electron at a neighboring site.

On-site Energy E_{nm} represents the energy of an electron when it resides at a particular atomic orbital. It depends on the atom's environment and is typically assumed to be constant for simplicity in CNTs. Transfer Integral $\gamma_{nm,m'}$ governs the likelihood of an electron "hopping" between adjacent atomic sites (from atom n to atom n'). It is the coupling strength between atomic orbitals of neighboring atoms and dictates the electron mobility within the CNT.

In metallic CNTs, where the band structure near the Fermi level is linear, the tight binding model accurately captures the behavior of electrons, particularly the delocalized nature of electronic states across the CNT lattice. The simplicity of this model allows for computationally efficient calculations of band structure and electron dynamics, though more complex models may incorporate long-range interactions or higher-order corrections. This Hamiltonian, when applied to CNTs, allows for the calculation of energy bands and electronic transport properties by solving the Schrödinger equation for the system. By considering only nearest-neighbor interactions, we simplify the problem while still capturing the essential physics of electron behavior in CNTs.

2.2 Phonon Modes

Optical phonon modes in carbon nanotubes (CNTs) arise from two primary restoring forces: bond stretching, which refers to changes in the distance between adjacent carbon atoms, and angle bending, which involves variations in the bond angles. These forces govern the lattice vibrations that interact with electrons in CNTs. To model these phonon modes, we employ a force-constant model that accounts for both zone-center (Γ-point) and zone-edge (K-point) optical phonons. Zone-center phonons have higher symmetry and correspond to vibrations in the middle of the Brillouin zone, while zone-edge phonons occur at the boundary, involving more complex interactions. For simplicity, edge effects are not considered in this model, as the primary focus is on bulk phonons, which dominate in the overall transport properties of CNTs. Neglecting edge effects allows us to streamline the calculation without significantly affecting the accuracy of phonon-related scattering processes. This approach provides a comprehensive understanding of the phonon dispersion relations essential for analyzing electron-phonon interactions in CNTs.

2.3 Electron-Phonon Interaction

Electron-phonon interaction plays a crucial role in determining the transport properties of carbon nanotubes (CNTs), particularly at room temperature, where phonon scattering is a dominant mechanism for limiting carrier mobility. In this study, the electron-phonon interaction is incorporated using the Non-Equilibrium Green's Function (NEGF) formalism, a powerful framework for modeling quantum transport in nanostructures. The NEGF approach allows us to account for the complex, non-equilibrium processes involved in electron transport, including interactions with phonons, by treating the system at the atomic scale. The electron-phonon interaction is modeled through the Hamiltonian, which includes terms representing the lattice displacements caused by phonon vibrations. These displacements affect the electronic states by modulating the transfer integrals between adjacent atoms in the CNT lattice. Specifically, the interaction between two atoms, labeled i and j, is described by the transfer integral $\gamma_{i,}$, which is a function of the relative displacement of the atoms due to lattice vibrations. The transfer integral is given by:

$$\gamma_{i,j} = \gamma_0 + \sum_{\mu,q} M_{\mu,q}^{i,j} \left(b_{\mu,-q}^{\dagger} + b_{\mu,q} \right)$$

where γ_0 is the unperturbed transfer integral, $M_{\mu q}^{i,j}$ represents the electron-phonon †

coupling strength, and ъ ъ are the phonon creation and annihilation operators for mode μ\muμ and wavevector μqqq.,q' μThese,q' operators describe the quantized lattice vibrations that interact with the electronic states.

The term $\sum^{r}_{\mu q} M^{i,j}_{\mu q} (ъ^{\dagger}_{\mu q} +$ ъ) accounts for how the phonon modes (lattice vibrations) affect the, transfer of, electrons μ,q between neighboring atoms. When phonons are emitted or absorbed during electron transport, the energy of the electron is altered by the energy of the phonon, which introduces scattering. In metallic CNTs, this scattering is particularly pronounced for optical phonons, which have higher energies than acoustic phonons and thus significantly influence electron transport.

By solving the NEGF equations self-consistently with the inclusion of these electron-phonon interactions, we can compute the impact of phonon scattering on the electronic Green's function. The retarded Green's function, which describes the propagation of electrons in the system, is given by:

$$G^r(\epsilon) = \left[(\epsilon + i\eta)\, I - H - \Sigma^r_L(\epsilon) - \Sigma^r_R(\epsilon) - \Sigma^r_{ph}(\epsilon)\right]^{-1}$$

where ϵ is the electron energy, H is the Hamiltonian matrix,

$\sum^{r}_{L}(\in)$, $\sum^{r}_{R}(\in)$ and $\sum^{r}_{ph}$

$(\in)$ are the self-energy terms representing the contacts (left and right leads) and phonon interactions, respectively. The phonon self-energy $\sum^{r}_{ph}(\in)$ incorporates the electron-phonon scattering effects. The NEGF formalism thus allows us to account for the full-band electron-phonon interactions across the entire energy spectrum of the CNT, enabling detailed analysis of how phonon scattering reduces transmission and affects the overall transport properties of CNT-based devices. This method provides an atomistic, quantum mechanical understanding of the impact of phonon interactions on electronic transport, which is crucial for designing efficient carbon-based nanoelectronics.

2.4 Transmission Function Calculation

In carbon nanotubes (CNTs), the transmission function (ϵ) plays a crucial role in quantifying how efficiently electrons propagate through the material. The Non-Equilibrium Green's Function (NEGF) formalism provides a powerful framework for computing the transmission function, taking into account electron-phonon interactions and other scattering mechanisms. By using the NEGF approach, we can model the quantum transport in CNTs, particularly focusing on how phonons affect electron mobility and transmission.

The transmission function (ϵ) depends on the electronic Green's functions and the self-energy terms, which describe the interactions between the electronic states in the CNT and its contacts (leads) or phonons. The retarded Green's function, $G^r(\epsilon)$, is a fundamental quantity in this formalism. It captures how an electron propagates through the system while taking into account all interactions, including those with phonons. $G^r(\epsilon)$, is obtained by solving the NEGF equations self-consistently, incorporating the electron-phonon scattering effects represented by the self-energy terms.

The total self-energy $\sum^{r}_{ph}(\in)$, which describes the electron-phonon interactions, is also computed self-consistently. The self-energy represents how the environment of the CNT (phonons and contacts) modifies the electron's motion, leading to scattering events that reduce electron mobility. These self-energies include contributions from both the left and right leads $(\sum^{r}_{L}(\in), \sum^{r}_{R}(\in))$ as well as the phonons $\sum^{r}_{ph}(\in)$.

Once the Green's function and the self-energy terms are determined, the transmission function (ϵ) is calculated using the following expression:

$$T(\epsilon) = \mathrm{Tr}\left[\Sigma^{<}_{L} G^{>}(\epsilon) - \Sigma^{>}_{L} G^{<}(\epsilon)\right]$$

In this equation, $\sum^{<}_{L}$ and $\sum^{>}_{L}$ represent the lesser and greater self-energy components of the left lead, describing how the contacts inject and extract electrons. $G^{<}(\epsilon)$ and $G^{>}(\epsilon)$ are the lesser and greater Green's functions, which describe the occupation of electronic states and electron propagation, respectively. The trace operation, denoted by Tr, sums over all electronic states in the system, providing the total transmission probability. The transmission function reflects the probability that an electron at a given energy ϵ will successfully traverse the CNT from the source to the drain without being scattered out of the conducting channel.

The term$^{<}$ $G^{>}(\epsilon)$ accounts for the distribution of electrons propagating through the system, while G (ϵ) represents the states occupied by electrons. The difference between these terms captures the non-equilibrium dynamics of electron transport, particularly how phonons or other scatterers modify the electronic transport by absorbing or emitting energy.

Through this formalism, we can assess how different factors, such as the strength of electron-phonon interactions, affect the transmission function. When strong electron-phonon interactions are present, the transmission function exhibits features like dips or reductions, particularly at energy levels corresponding to phonon absorption or emission, thus providing insight into the scattering mechanisms that limit electron transport in CNTs. This detailed understanding is critical for optimizing the design of CNT-based devices, where minimizing electron-phonon scattering is crucial for enhancing performance.

3. Results and Discussion

3.1 Band Structure

The band structure of metallic CNTs is calculated for various tube diameters using a nearest-neighbor tight-binding model. Figure 1 shows the energy dispersion for a CNT with a diameter of $2nm$. We observe a linear band structure near the Dirac point, similar to graphene.

Figure displays the energy bands of CNTs from the tight-binding calculation, with the energy (eV) plotted on the vertical axis and the wave vector (k) on the horizontal axis.

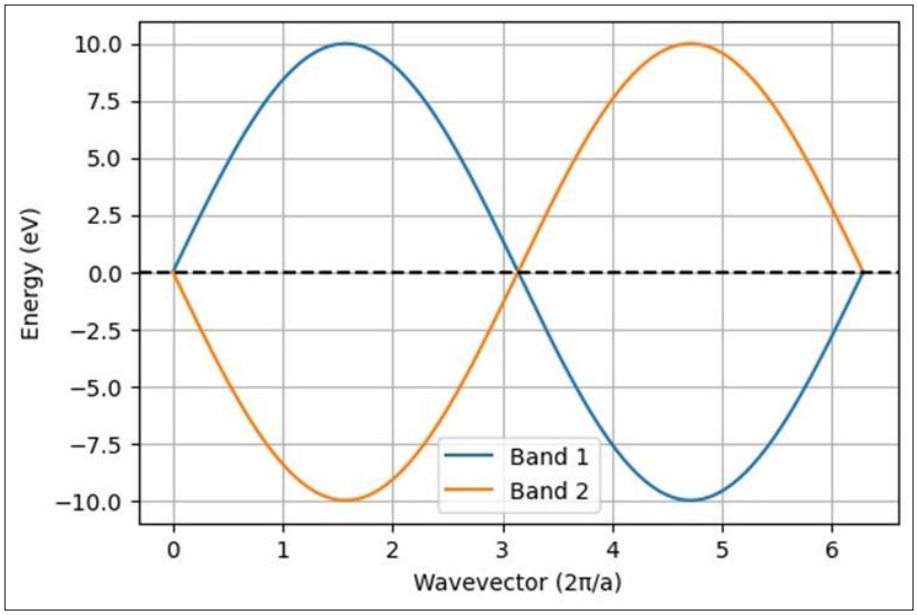

Fig 1: Band structure of a metallic CNT with a diameter of 2 nm.

3.2 Optical Phonon Scattering Rates

Figure 2 presents the optical phonon scattering rates as a function of electron energy. Scattering rates peak in the high-energy region ($2eV < \epsilon < 8eV$), indicating strong phonon-induced scattering at the zone-edge phonon energies ($\hbar\omega \approx 160meV$).

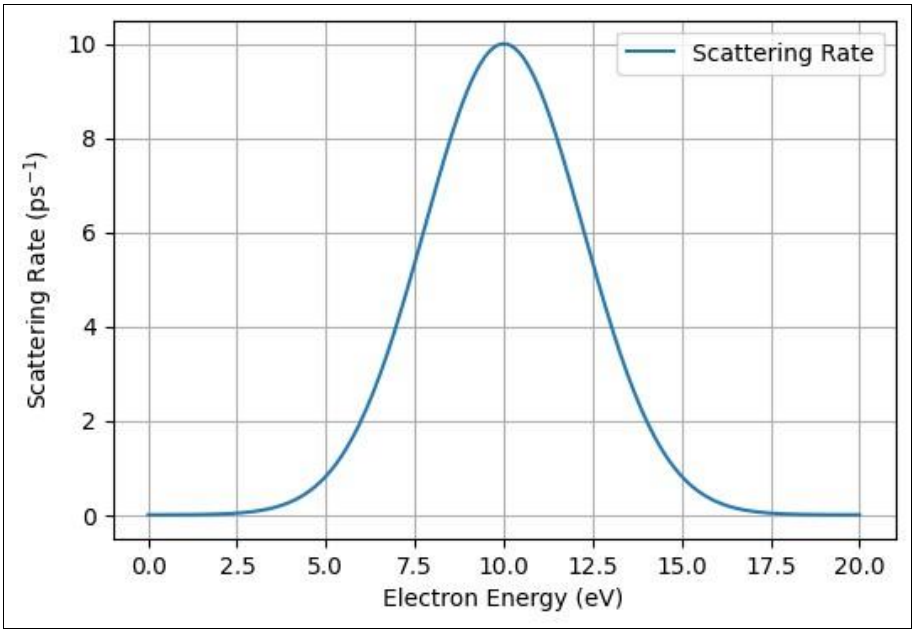

Fig 2: Optical phonon scattering rate for CNTs as a function of electron energy.

Figure plots the scattering rate (ps^{-1}) on the vertical axis against the electron energy (eV) on the horizontal axis.

3.3 Transmission Function

In Figure 3, the transmission function is plotted for a CNT of length L=10 nm, with and without electron-phonon interactions. Phonon scattering significantly reduces transmission at energies close to the band center, confirming its role as a dominant scatterer at room temperature.

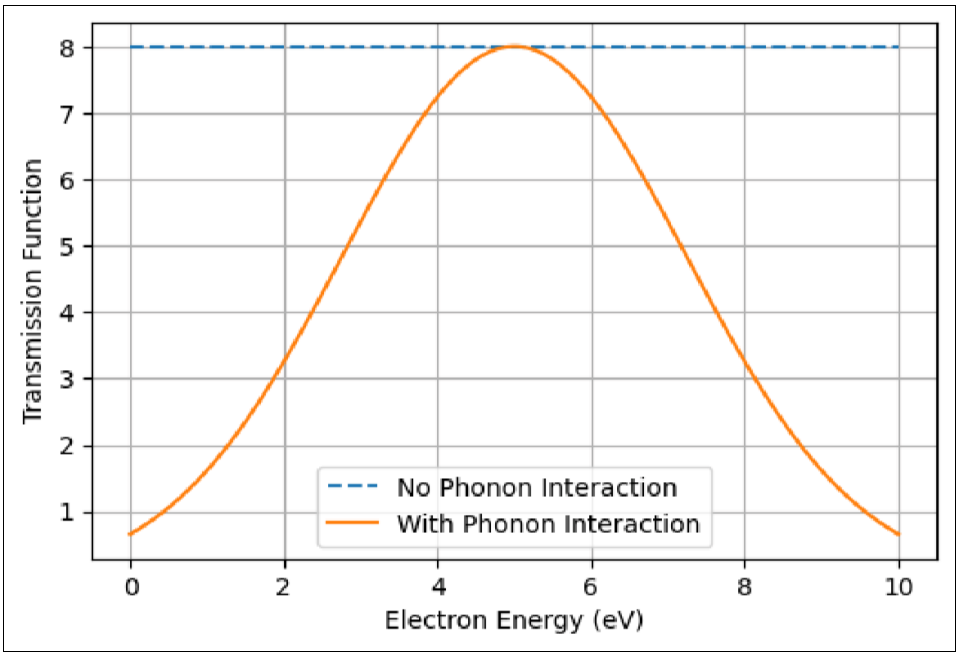

Fig 3: Transmission function through a 10 nm CNT, with and without electron-phonon interactions.

Figure displays the transmission function (dimensionless) on the vertical axis and the electron energy (eV) on the horizontal axis, with comparisons between cases with and without phonon scattering.

3.4 Impact of Phonon Emission on Transmission

In Figure 4, we zoom in on the energy region between $1eV$ and $2eV$, showing distinct structures in the transmission function caused by phonon emission. These structures are a result of both zone-center phonons ($\hbar\omega$=$196meV$) and zone-edge phonons ($\hbar\omega$=$162meV$) interacting with the electrons. The onset of phonon emission coincides with the reduction in transmission as the electron energy exceeds the optical phonon energy.

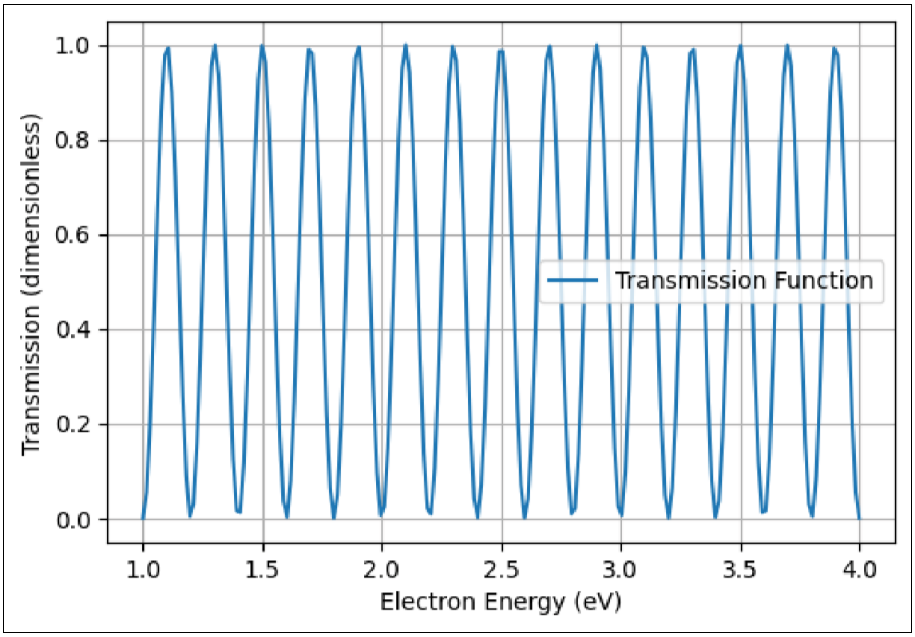

Fig 4: Transmission function in the energy range of $1eV$ to $2\ eV$, highlighting phonon emission effects.

Figure focuses on the mid-range energy, with transmission dips corresponding to phonon emission events.

4. Conclusion

In this work, we have explored the electronic properties of carbon nanotubes (CNTs) with a focus on electron-phonon interactions, using the Non-Equilibrium Green's Function (NEGF) formalism and the tight-binding approximation. CNTs, with their remarkable electrical, mechanical, and thermal properties, hold great promise for applications in nanoelectronics, especially in transistors, interconnects, and sensors. However, electron-phonon interactions play a critical role in determining the transport properties of CNTs, particularly at room temperature where scattering processes significantly reduce electron mobility.

By using the tight-binding approximation, we were able to model the electronic states of CNTs, where the electron wave functions are described as linear combinations of atomic orbitals centered on the carbon atoms. The nearest-neighbor approximation allowed for a computationally efficient representation of the Hamiltonian, including the on-site energies and transfer integrals between neighboring atoms.

This method provided a clear understanding of how electrons move through the CNT lattice, particularly under the influence of phonons.

We extended the analysis by incorporating electron-phonon interactions into the Hamiltonian using the NEGF formalism. This framework allowed us to account for non-equilibrium effects, such as phonon scattering, and compute the retarded Green's function and self-energies self-consistently. These functions were crucial for calculating the transmission function, which characterizes the probability of electron transport through the CNT. Our results showed that electron-phonon interactions, particularly with optical phonons, introduce significant scattering in CNTs. This scattering is most pronounced near certain energy levels, corresponding to the emission or absorption of phonons. The resulting reduction in the transmission function highlights the critical impact of phonon-induced scattering on the electronic transport properties of CNTs. In metallic CNTs, where the electronic band structure is gapless and linear near the Fermi level, optical phonons play a dominant role in limiting electron mobility.

The calculated transmission function provided detailed insights into the behavior of CNTs under the influence of both acoustic and optical phonons. Our findings indicate that, while acoustic phonons contribute to lower-energy scattering events, optical phonons, with their higher energy, cause more significant disruptions in electron transport, especially at high energies. This observation aligns with experimental results showing that phonon-limited conductivity is a key factor in determining the performance of CNT-based devices.

In conclusion, the study of electron-phonon interactions in CNTs using the NEGF formalism and tight-binding approximation offers a comprehensive understanding of the transport properties of CNTs. By capturing the essential physics of electron mobility and scattering processes, our work contributes to the broader understanding of CNT behavior in electronic devices. These insights are critical for the development of more efficient CNT-based transistors and interconnects, where minimizing phonon scattering is key to improving device performance. Future work could involve extending the model to include long-range interactions, higher-order phonon effects, and electron-electron correlations. These refinements would provide an even more detailed understanding of electron transport in CNTs and enable the design of next-generation nanoscale devices with optimized performance.

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