

Enhancing the Thermoelectric Properties of Graphene Nanosheet through Boron Doping and Engineering Interface: A Theoretical Study

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Abstract:

This study presents a comprehensive theoretical investigation of the thermoelectric transport properties of graphene nanosheets (GNS) under progressive boron (B) doping and electrode interface engineering, using a combination of Density Functional Tight-Binding (DFTB) and Non-Equilibrium Green's Function (NEGF) approaches. The results reveal that boron substitution significantly alters the electronic structure and enhances charge carrier transport near the Fermi level. As the number of boron-doped lines increases from single to triple configurations, both the Seebeck coefficient and electrical conductivity are simultaneously improved, leading to a remarkable increase in the thermoelectric figure of merit (ZT). Furthermore, incorporating boron-doped electrodes yields an additional enhancement due to improved interfacial coupling and mass-matching effects, effectively reducing phonon thermal conductance. The optimized triple boron-doped configuration with boron-doped electrodes exhibits the highest ZT, demonstrating the strong synergy between chemical doping and interface engineering. These findings highlight an efficient pathway for tailoring the thermoelectric response of graphene-based nanostructures, offering valuable insights for the rational design of next-generation energy conversion and nanoscale thermoelectric devices.

Keywords: Graphene nanosheets; Boron doping; Interface engineering; Thermoelectric transport; DFTB-NEGF; Figure of merit (ZT).

تحسين الخواص الكهروحرارية لصفحة الكرافين النانوية من خلال التطعيم بالبورون وهندسة الواجهات: دراسة نظرية

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الخلاصة

تقدم هذه الدراسة تحقيقاً نظرياً شاملاً لخصائص النقل الكهروحراري في صفائح الكرافين النانوية (GNS) تحت تأثير التطعيم التدريجي بالبورون (B) وهندسة الواجهات الأقطاب، وذلك باستخدام مزيج من طريقتي الترابط المحكم المعتمد على نظرية الكثافة الوظيفية (DFTB) ودالة غرين اللاتوازنية (NEGF). تكشف النتائج أن إحلال ذرات البورون يؤدي إلى تغيير ملحوظ في البنية الإلكترونية ويعزز انتقال حوامل الشحنة بالقرب من مستوى فيرمي. ومع زيادة عدد الخطوط المطعمة بالبورون من تكوين خط واحد إلى تكوين ثلاثة خطوط، يتحسن كل من معامل سيبك والتوصيلية الكهربائية بصورة متزامنة، مما يؤدي إلى زيادة ملحوظة في معامل الكفاءة الكهروحرارية (ZT). علاوة على ذلك، فإن استخدام أقطاب مطعمة بالبورون يحقق تحسناً إضافياً نتيجة تحسن الاقتران عند الواجهة وتأثيرات توافق الكتلة، مما يؤدي بصورة فعالة إلى تقليل التوصيل الحراري للفونونات. ويظهر التكوين المحسن المكون من ثلاثة خطوط مطعمة بالبورون مع أقطاب مطعمة بالبورون أعلى قيمة لـ ZT، مما يوضح التأثير التآزري القوي بين التطعيم الكيميائي وهندسة الواجهات. وتبرز هذه النتائج مساراً فعالاً لضبط الاستجابة الكهروحرارية للبنية النانوية القائمة على الكرافين، كما تقدم رؤية قيمة للتصميم العقلاني للجيل القادم من أجهزة تحويل الطاقة والأجهزة الكهروحرارية النانوية.

الكلمات المفتاحية: صفائح الكرافين النانوية؛ التطعيم بالبورون؛ هندسة الواجهات؛ النقل الكهروحراري؛ DFTB-NEGF ؛ معامل الكفاءة الكهروحرارية (ZT).

1. Introduction

The ever-growing demand for sustainable and miniaturized energy conversion systems has sparked an intensive search for materials capable of efficiently converting waste heat into electricity. Thermoelectric (TE) materials, which enable direct interconversion between thermal and electrical energy via the Seebeck and Peltier effects, are recognized as pivotal in achieving energy sustainability and waste heat recovery at micro- and nanoscale levels [1-3]. The efficiency of thermoelectric materials is typically characterized by the dimensionless figure of merit, as $ZT = S^2\sigma T/\kappa$ [4-6]. In this equation, S is Seebeck coefficient, σ is electrical conductivity, T is absolute temperature, and κ is total thermal conductivity. Achieving a high ZT value requires a delicate balance between these mutually dependent parameters, posing a significant challenge for material design at the nanoscale.

Graphene, a single layer of sp^2 -bonded carbon atoms arranged in a honeycomb lattice, has emerged as a prototypical two-dimensional (2D) material with exceptional electrical, thermal, and mechanical properties. Its ultra-high carrier mobility, tunable electronic band structure, and mechanical robustness make it an ideal platform for nanoelectronic and thermoelectric device applications [7-9]. However, pristine graphene suffers from a nearly zero bandgap and extremely high thermal conductivity ($\sim 5000 \text{ W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$), which limits its thermoelectric performance by suppressing the Seebeck coefficient and maintaining a high phonon contribution to heat transport [10]. Consequently, enhancing the TE efficiency of graphene-based materials requires strategic modifications to its lattice and electronic structure to reduce phonon thermal conductivity while maintaining or improving carrier transport.

Over the past decade, several approaches have been proposed to optimize graphene's TE response, including nanostructuring, strain engineering, isotope substitution, and chemical doping [7, 11, 12]. Among these, heteroatom doping especially with elements such as boron (B) and nitrogen (N) has proven to be one of the most effective techniques for tuning both electronic and phononic transport properties [13]. Boron doping introduces p-type behavior in graphene due to boron's lower valence electron count compared to carbon, leading to charge depletion and Fermi-level shifting toward the valence band. This modification not only opens a finite bandgap but also enhances the Seebeck coefficient by increasing carrier asymmetry near the Fermi level [14]. Density Functional Theory (DFT) and Non-Equilibrium Green's Function (NEGF) studies have demonstrated that boron doping in armchair graphene nanoribbons (AGNRs) and nanosheets can significantly enhance electronic transport and thermopower while lowering lattice thermal conductivity [15]. Moreover, the concentration and spatial distribution of boron atoms critically determine the resultant transport behavior. For instance, periodic boron lines can induce bandgap openings up to several hundred meV and promote localized electronic states that scatter phonons efficiently, resulting in improved ZT values beyond 2 at room temperature [16]. Such results highlight the sensitivity of thermoelectric response to atomic-level doping configurations.

Beyond substitutional doping, interface engineering has emerged as a powerful means of controlling the interplay between electrical and thermal transport. The creation of graphene/boron nitride (BN) heterostructures or doped interfaces can tailor the transmission

spectra, reduce phonon coherence lengths, and enhance interfacial phonon scattering [17]. The insertion of boron at interfaces can modulate coupling between graphene and metallic electrodes, aligning the Fermi level and enhancing charge injection efficiency. This interfacial tuning is crucial for optimizing contact resistance a dominant factor in nanoscale thermoelectric devices. Recent first-principles calculations have confirmed that interface coupling effects, when synergistically combined with controlled boron doping, can yield substantial gains in electrical conductance while simultaneously suppressing lattice thermal conductance [18]. These findings align with the growing understanding that interfacial and compositional engineering are inseparable levers for tailoring energy conversion in two-dimensional systems.

Despite extensive progress in enhancing the thermoelectric performance of graphene-based materials, the combined influence of boron line doping and interface engineering on the electronic and phonon transport of graphene nanosheets remains largely unexplored. Most previous works have examined either chemical doping or interfacial modification in isolation, neglecting their synergistic effects on carrier mobility, thermal conductance, and the overall figure of merit (ZT). Therefore, a comprehensive theoretical study integrating both boron doping configurations and doped electrode interfaces is still lacking representing a crucial gap this work aims to address.

2 . Materials and Methods

The thermoelectric properties of the (6,0) graphene nanosheets were investigated using the Density Functional Tight-Binding (DFTB) method, implemented in the QuantumATK S-2021.06 software suite. This method offers a computationally efficient approach suitable for large-scale 2D systems, while retaining sufficient accuracy in describing electronic transport. We employed the Slater–Koster parameter set DFTB (dftb.org, mio-1-1), which provides a minimal basis set and has been widely validated for covalently bonded systems. All simulations were performed under the non-self-consistent mode (no SCF iteration), with electronic occupations described using a Fermi–Dirac distribution function at a broadening temperature of 300 K. The numerical accuracy was further ensured by setting the density mesh cutoff to 10 Hartree. For Brillouin zone sampling, a Monkhorst–Pack k-point grid of $1 \times 24 \times 24$ was used, with periodic boundary conditions applied along all three directions and the Γ -point shift enabled to improve symmetry treatment. This relatively dense k-point sampling was selected to ensure convergence and resolution of fine features in the band structure and transport coefficients. The above setup provides a balanced trade-off between computational efficiency and accuracy, and has been successfully applied in prior studies on similar low-dimensional materials. All key computational parameters, including k-point mesh density and vacuum spacing, were subjected to convergence tests to ensure the numerical reliability of the simulations.

All transmission spectra and thermoelectric coefficients were calculated under zero-bias conditions within the linear-response regime using the DFTB–NEGF formalism in QuantumATK. In this approach, the transport properties are derived from the equilibrium

transmission function around the Fermi level without applying a finite external voltage. In order to determine the electronic transport parameters such as electrical conductance G_e , electronic thermal conductance k_e , and the Seebeck coefficient S , the transmission spectra were computed using the NEGF (Non-Equilibrium Green's Function) method, based on Density Functional Tight-Binding (DFTB) formalism as implemented in QuantumATK. The electronic band structure was calculated using a $1 \times 24 \times 24$ Monkhorst–Pack k-point grid, ensuring adequate resolution of electronic states. To estimate the transport coefficients as a function of chemical potential at room temperature (300 K), the Landauer formalism was employed. While the conductance G_e is obtained directly from the transmission function, following standard practice in 2D thermoelectric simulations. Phonon thermal conductance k_{ph} was computed from the phonon dispersion using the harmonic approximation, neglecting anharmonicity or boundary scattering for simplicity. The total thermal conductance was taken as the sum $k_t = k_e + k_{ph}$. Convergence tests were conducted for all key parameters, including vacuum thickness, k-point sampling density, and mesh cutoff, to ensure the reliability of the results. The thermoelectric efficiency was assessed via the power factor and figure of merit $ZT = S^2 G_e T / k_t$ where T is temperature. All simulations were carried out on high-performance computing clusters using the QuantumATK S-2021.06 software suite. This methodology provides a computationally efficient and physically meaningful framework for predicting the thermoelectric performance of nanoscale materials.

3. Results and discussions

In this study, seven graphene nanosheet configurations were systematically examined: (a) pristine graphene, (b) single-line boron-doped graphene, (c) double-line boron-doped graphene, (d) triple-line boron-doped graphene, (e) single-line boron-doped graphene with boron-doped electrodes, (f) double-line boron-doped graphene with boron-doped electrodes, and (g) triple-line boron-doped graphene with boron-doped electrodes. This classification follows the same labeling order presented in Fig. 1 to facilitate direct comparison between the transmission spectra and the corresponding thermoelectric properties. Since all thermoelectric coefficients are fundamentally derived from the electronic transmission function within the Landauer–NEGF formalism, we first present the calculated transmission spectra $T(E)$ for the pristine graphene nanosheet and the different boron-doped configurations. The transmission function provides direct insight into the available transport channels and their energy dependence around the Fermi level. Any modification in $T(E)$, particularly near the Fermi energy, directly influences the electrical conductance, Seebeck coefficient, and electronic thermal conductance. Therefore, analyzing the evolution of $T(E)$ offers a clear physical understanding of how boron doping and interface engineering affect the thermoelectric performance of the device. Compared to the pristine structure, boron doping clearly alters the transmission behavior, as shown in Figs. 1(b–c). The dopant-induced symmetry breaking and modification of electronic states near the Fermi level lead to a redistribution of transport channels, which directly impacts the subsequent thermoelectric properties.

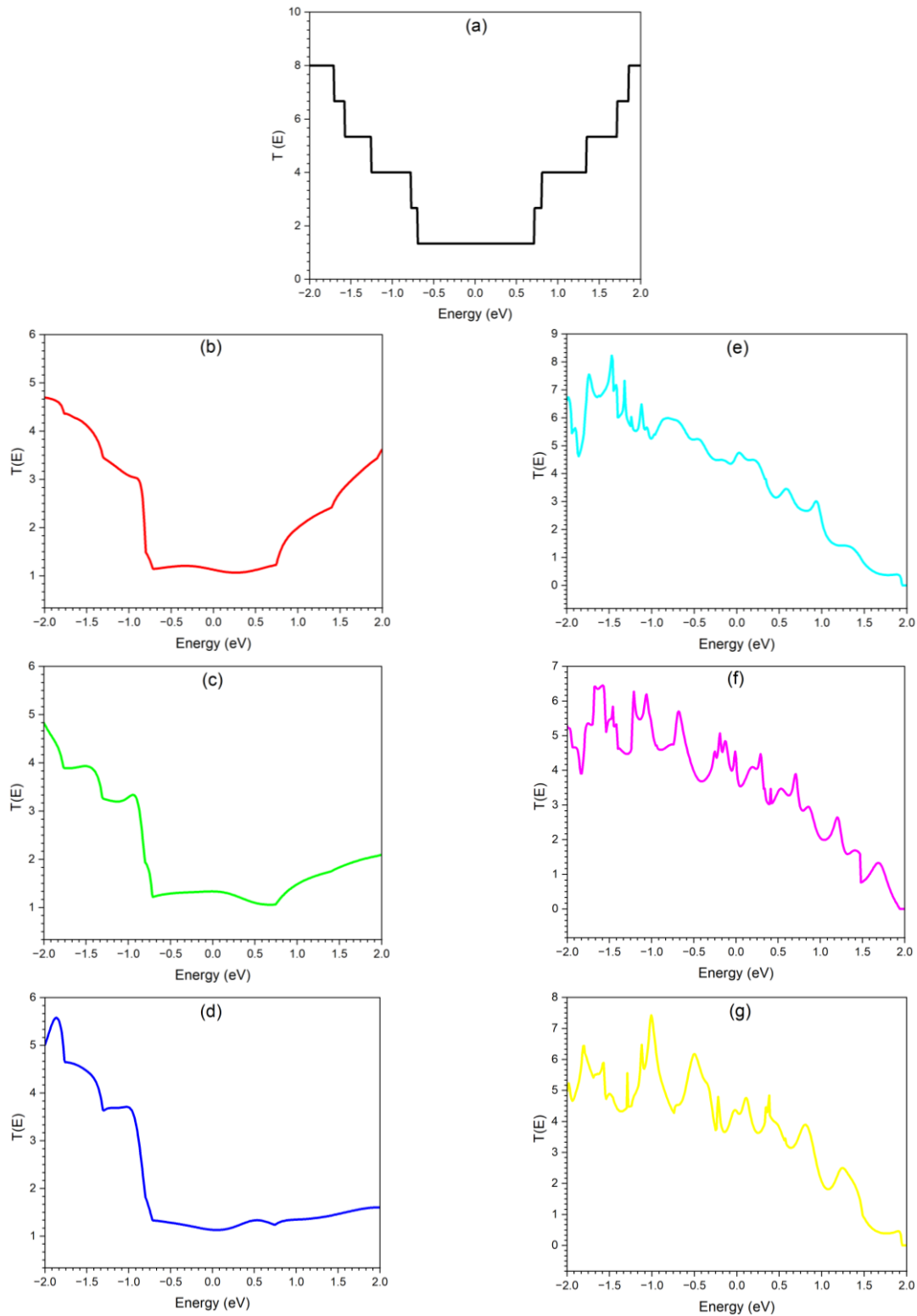


Figure -1 Transmission spectra $T(E)$ as functions of energy for all studied configurations of graphene nanosheets: (a) pristine graphene, (b) single-line boron-doped, (c) double-line boron-doped, (d) triple-line boron-doped, (e) single-line boron-doped with boron-doped electrodes, (f) double-line boron-doped with boron-doped electrodes, and (g) triple-line boron-doped with boron-doped electrodes. The Fermi energy is set to zero

As shown in Fig. 1(a), the transmission spectrum of pristine graphene exhibits a symmetric profile around the Fermi level with a noticeable reduction in transmission near

Fermi energy, reflecting its semi-metallic nature and zero bandgap character. The symmetry of the transmission function with respect to the Fermi energy indicates nearly identical contributions from electron and hole transport channels. This symmetric behavior plays a crucial role in limiting the thermoelectric response, particularly the Seebeck coefficient, since thermopower strongly depends on the energy asymmetry of the transmission near Fermi energy. Based on this transmission profile, the corresponding thermoelectric properties of pristine graphene are presented and discussed in Fig. 2.

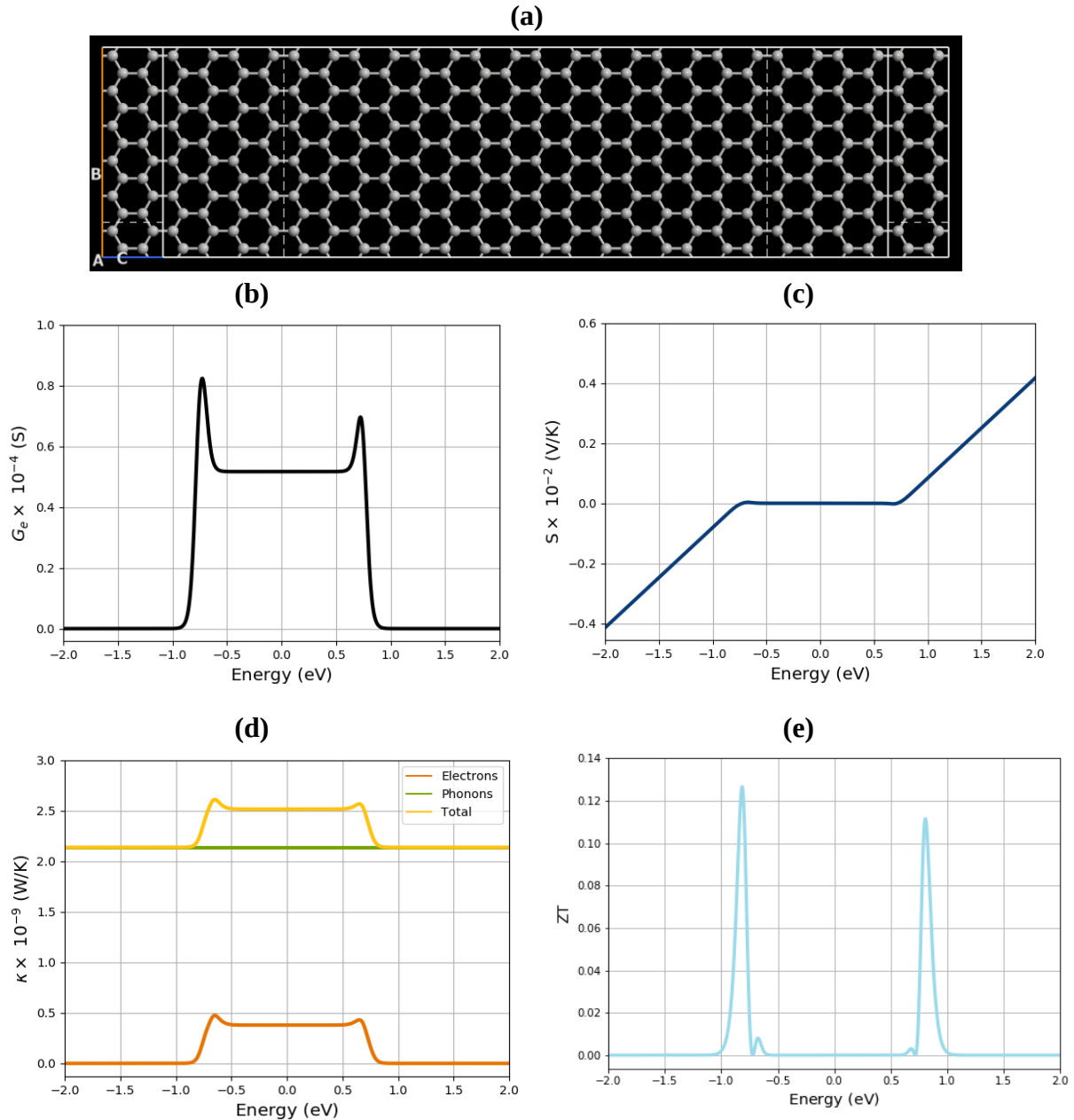


Figure -2 (a) Atomic structure of the pristine graphene two-probe device. (b) Electrical conductivity, (c) Seebeck coefficient, (d) thermal conductivity, and (e) figure of merit (ZT) as functions of energy. The Fermi energy is set to zero

Upon introducing a single boron-doped line substitutionally into the central scattering region, as shown in Fig. 3(a), the electronic structure undergoes a notable modification. The

presence of boron atoms, which have one less valence electron than carbon, introduces p-type behavior by shifting the Fermi level toward the valence band. As illustrated in Fig. 3(b–e), the electrical conductivity slightly decreases due to enhanced carrier scattering at dopant sites, while the Seebeck coefficient significantly increases near the Fermi level. This enhancement arises from the asymmetry induced in the density of states and the localization of charge carriers, which increase the voltage response to a thermal gradient. Consequently, the ZT value of the single-line boron-doped graphene nanosheet surpasses that of the pristine configuration, indicating that even minimal boron incorporation can substantially enhance thermoelectric efficiency.

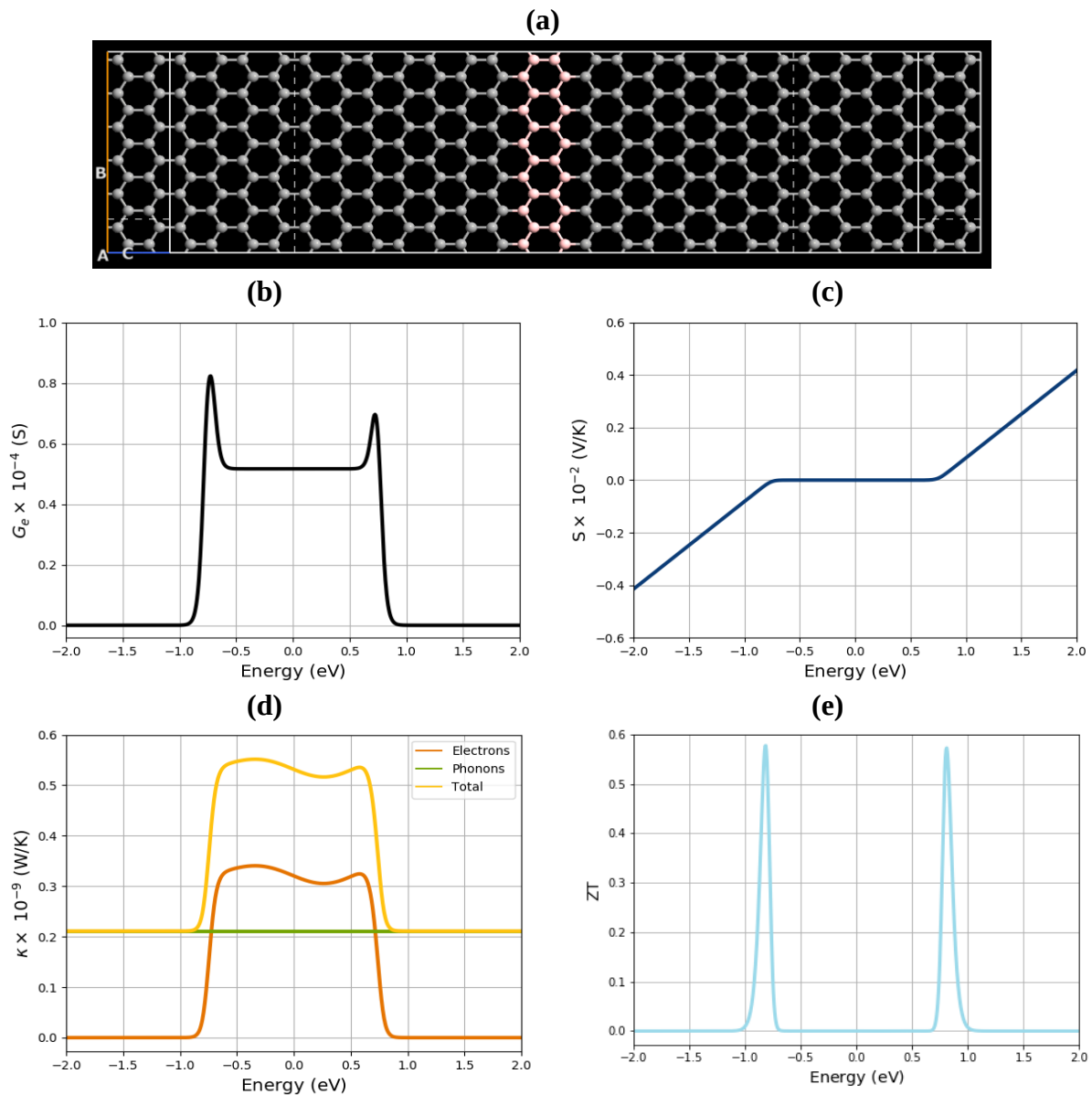


Figure -3 (a) Atomic structure of the boron-doped graphene two-probe device with a single boron-doped line introduced substitutionally in the central scattering region, (b) Electrical conductivity, (c) Seebeck coefficient, (d) thermal conductivity, and (e) figure of merit (ZT) as functions of energy graphene nanosheet with a single boron-doped line in the central scattering region. The Fermi energy is set to zero

When the number of boron-doped lines increases to two, as shown in Fig. 4(a), a more pronounced alteration in the electronic and phononic spectra occurs. The double-line doping configuration produces a wider pseudo-bandgap and reduces the overlap between conduction and valence bands, thereby improving energy filtering effects. As reflected in Figs. 4(b–e), the Seebeck coefficient remains comparable to the single-line case, while thermal conductivity is further reduced, leading to an overall improvement in ZT. The ZT profile displays two distinct peaks around the Fermi level, suggesting the coexistence of optimized electrical and thermal transport regimes.

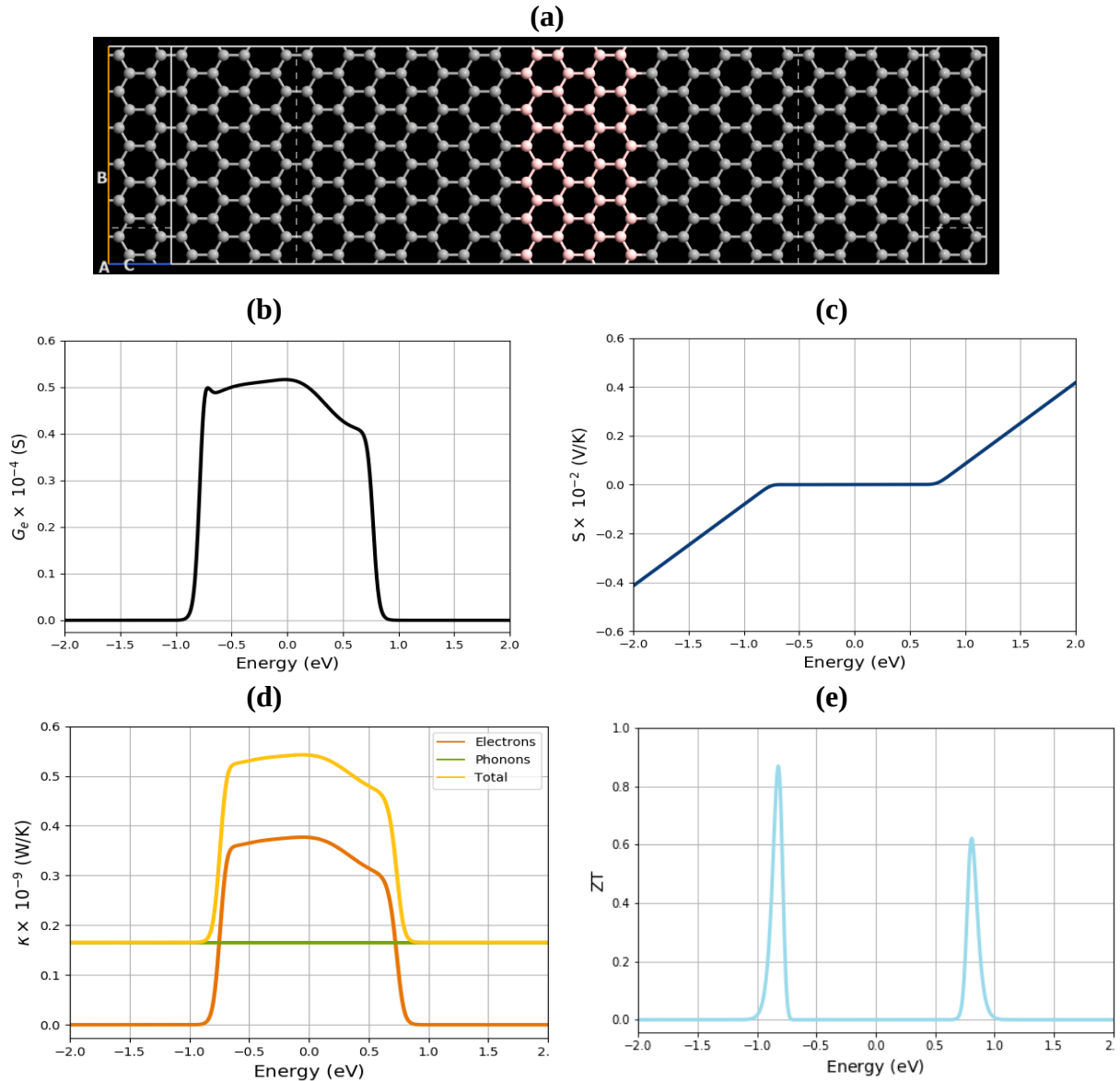


Figure -4 (a) Atomic structure of the boron-doped graphene two-probe device with double boron-doped line introduced substitutionally in the central scattering region, (b) Electrical conductivity, (c) Seebeck coefficient, (d) thermal conductivity, and (e) figure of merit (ZT) as functions of energy graphene nanosheet with a single boron-doped line in the central scattering region. The Fermi energy is set to zero

Further increasing the boron concentration to three doped lines, illustrated in Fig. 5(a), induces stronger electronic localization and enhanced phonon scattering across the nanosheet. Figures 4(b–e) reveal that the electrical conductivity maintains moderate values while the Seebeck coefficient reaches its highest level among the undoped-electrode configurations. The thermal conductivity experiences a sharp reduction due to the intensified disruption of lattice periodicity, which limits phonon propagation. Fig. 5(b–e) show that the triple-line boron doping configuration leads to a slight enhancement in the maximum ZT compared to the double-line case, particularly around $\mu \approx \pm 0.7$ eV. Although the overall profile remains similar, the improvement becomes noticeable at specific chemical potentials due to the further reduction in thermal conductivity and a modest increase in the power factor. Therefore, the enhancement in ZT is localized rather than uniform across the entire energy range.

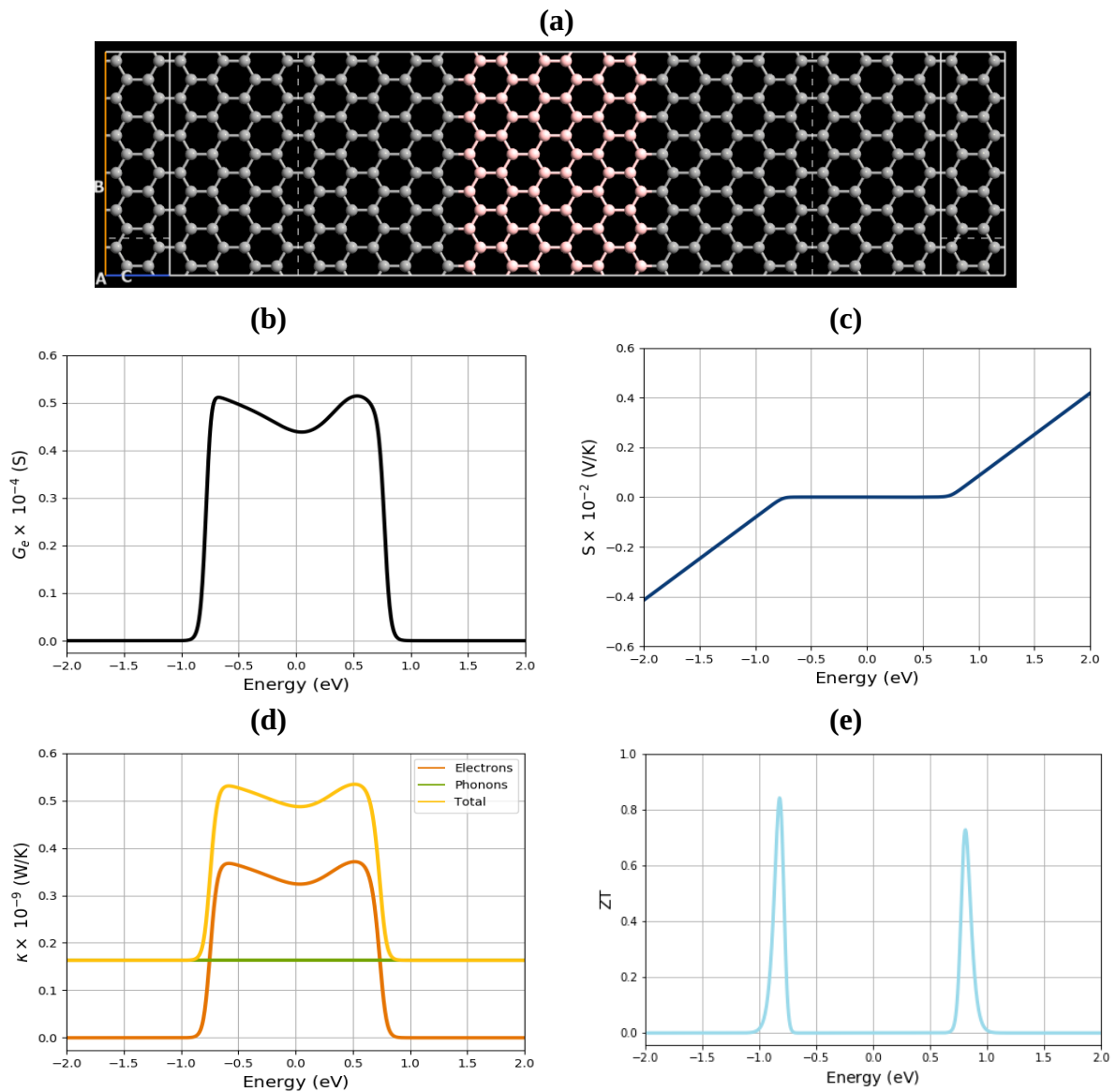


Figure -5 (a) Atomic structure of the boron-doped graphene two-probe device with triple boron-doped line introduced substitutionally in the central scattering region, (b) Electrical conductivity, (c) Seebeck coefficient, (d) thermal conductivity, and (e) figure of merit (ZT) as functions of energy graphene nanosheet with a single boron-doped line in the central scattering region. The Fermi energy is set to zero

To further optimize interfacial transport, boron-doped electrodes were introduced to match the chemical environment of the central region, as depicted in Figures 6–8(a). The inclusion of boron at the contact interfaces improves Fermi-level alignment and enhances the coupling between the electrodes and the doped graphene channel. As shown in Figure 6(b–e) for the single-line boron configuration with doped electrodes, the electrical conductivity increases significantly compared to its undoped-electrode counterpart. This improvement arises from reduced contact resistance and better energy level matching across the electrode–channel interface. The Seebeck coefficient remains high, and the thermal conductivity decreases slightly due to improved phonon scattering at the doped interfaces, leading to a noticeable enhancement in ZT.

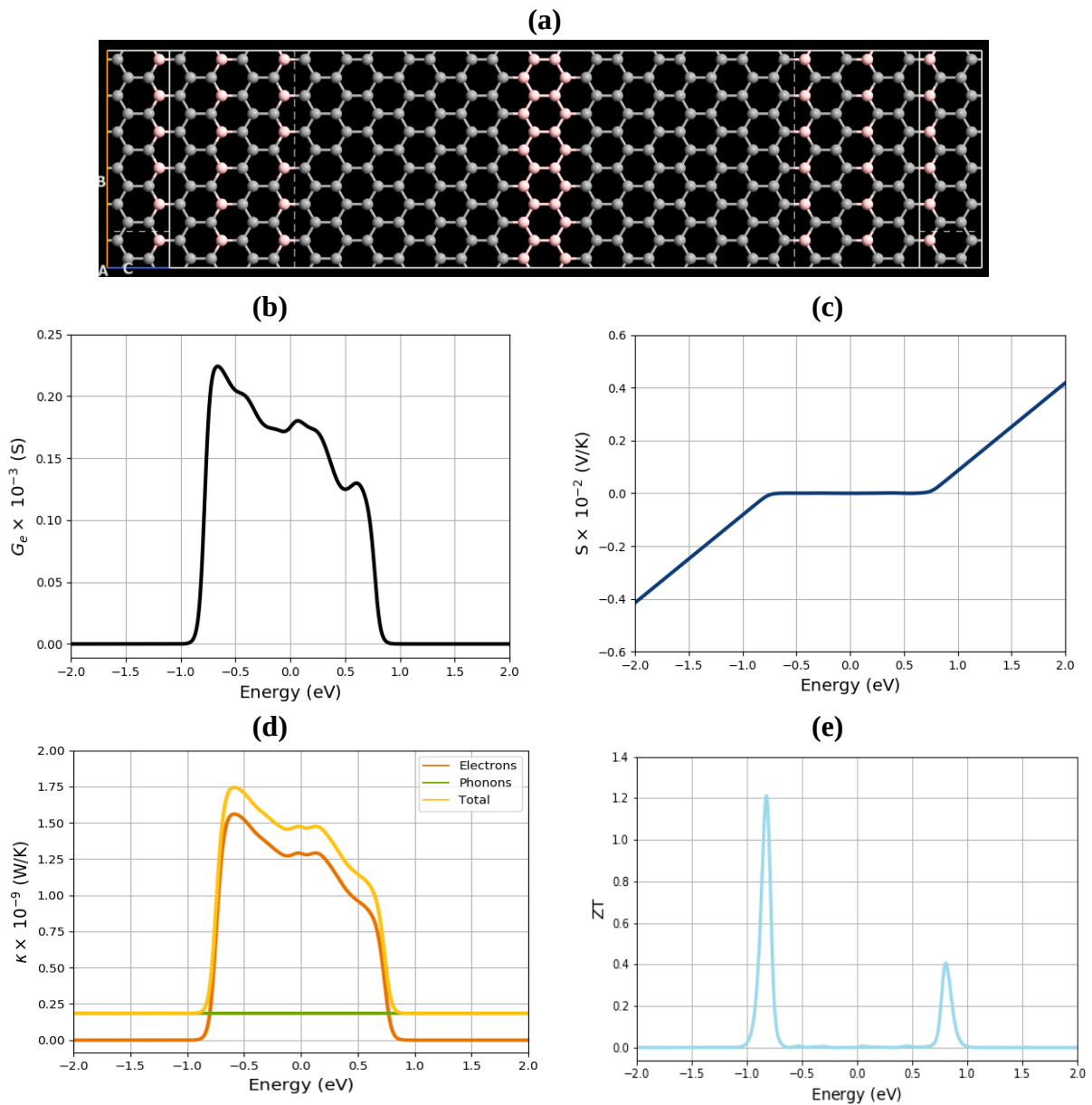


Figure -6 (a) Atomic structure of the boron-doped graphene two-probe device with a single boron-doped line introduced substitutionally in the central scattering region and boron-doped electrodes, (b) Electrical conductivity, (c) Seebeck coefficient, (d) thermal conductivity, and (e) figure of merit (ZT) as functions of

energy graphene nanosheet with a single boron-doped line in the central scattering region. The Fermi energy is set to zero

For the double-line boron-doped configuration with boron-doped electrodes, shown in Fig. 7(a), the combined effect of multi-line doping and interface modification becomes more apparent. As illustrated in Figs. 7(b–e), the electrical conductivity and Seebeck coefficient exhibit simultaneous improvement, resulting in a higher power factor ($S^2\sigma$). The thermal conductivity further declines compared to the single-line case, emphasizing the role of both chemical disorder and interfacial scattering in suppressing heat flow. The resulting ZT curve presents a strong peak around the Fermi level, confirming the synergistic influence of boron doping and interface engineering in optimizing thermoelectric transport.

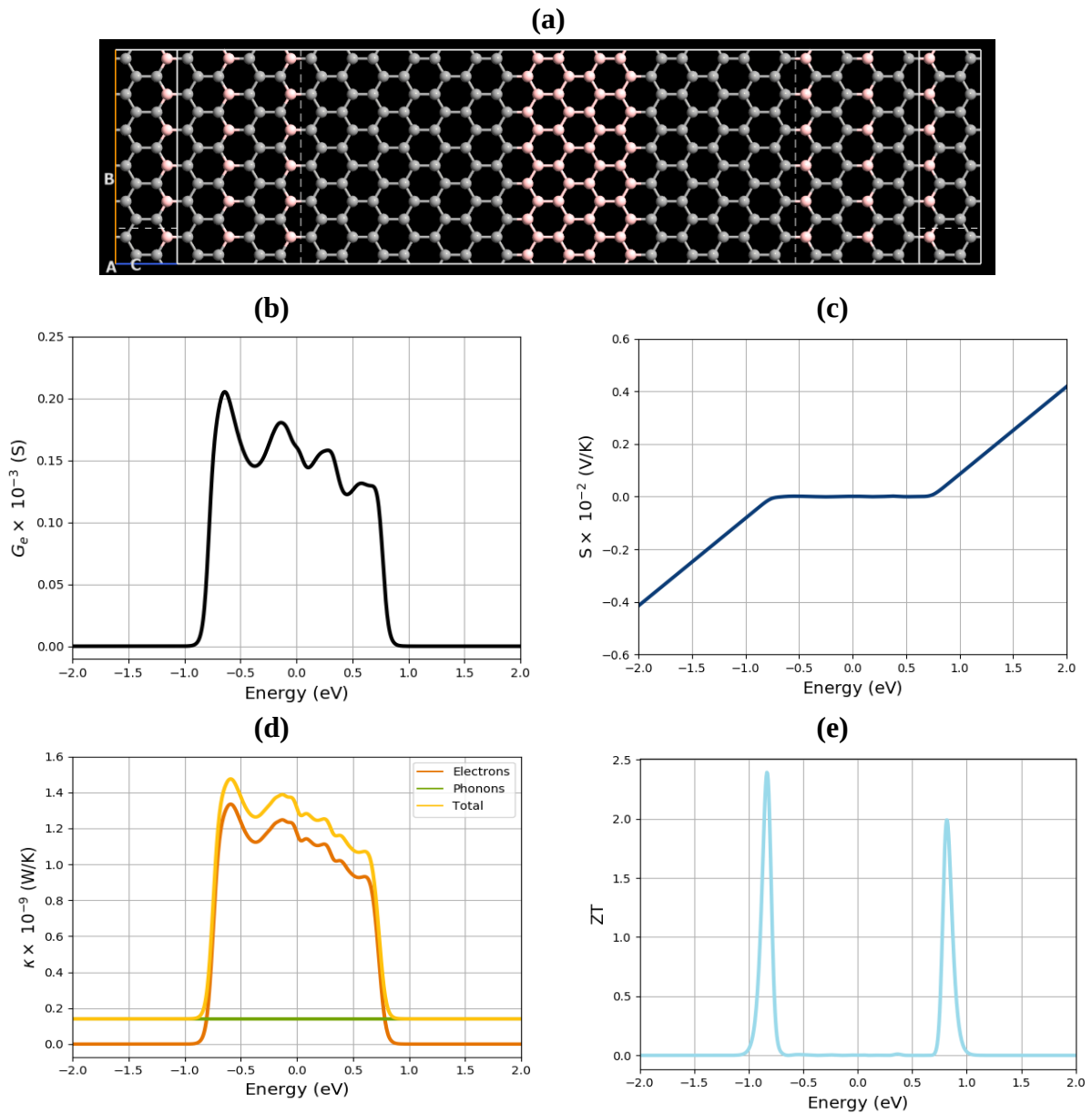


Figure -7 (a) Atomic structure of the boron-doped graphene two-probe device with double boron-doped line introduced substitutionally in the central scattering region and boron-doped electrodes, (b) Electrical conductivity, (c) Seebeck coefficient, (d) thermal conductivity, and (e) figure of merit (ZT) as functions of

energy graphene nanosheet with a single boron-doped line in the central scattering region. The Fermi energy is set to zero

The most striking results are obtained for the triple boron-doped graphene nanosheet combined with boron-doped electrodes, as shown in Fig. 8(a). The corresponding transport characteristics in Figs 8(b–e) indicate that this configuration yields the highest overall performance. The electrical conductivity remains robust due to improved electrode-channel coupling, while the Seebeck coefficient reaches its maximum owing to enhanced electronic asymmetry and optimized carrier transport. The thermal conductivity attains its lowest value, primarily as a result of extensive phonon scattering at both the doped lattice sites and the boron-rich interfaces. Consequently, the figure of merit (ZT) achieves its peak value, approaching 2.4 at $\mu \approx \pm 0.7$ eV. This exceptional thermoelectric efficiency underscores the effectiveness of integrating chemical doping with interface engineering to achieve superior energy conversion in graphene-based systems.

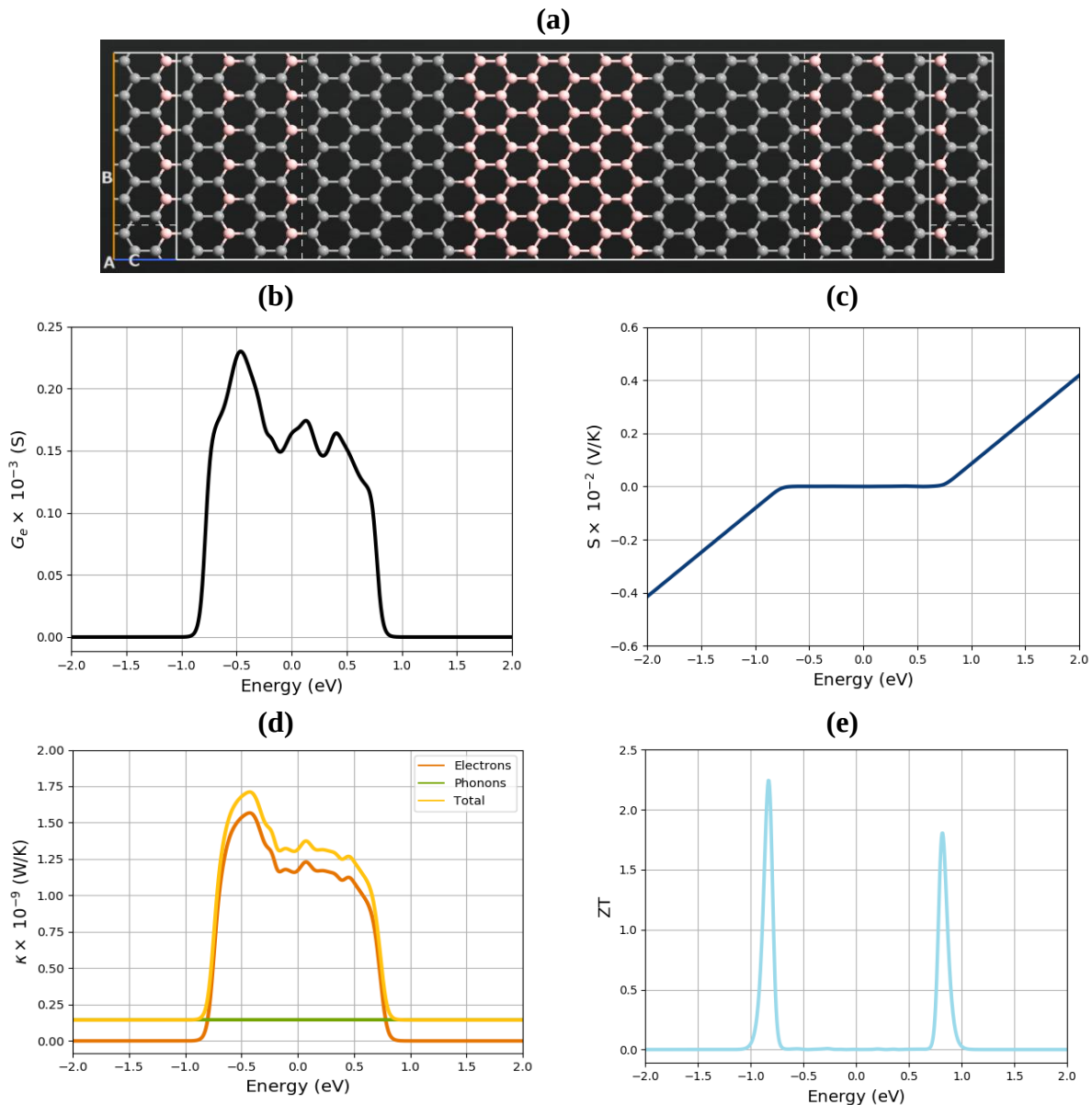


Figure -8 (a) Atomic structure of the boron-doped graphene two-probe device with triple boron-doped line introduced substitutionally in the central scattering region and boron-doped electrodes, (b) Electrical conductivity, (c) Seebeck coefficient, (d) thermal conductivity, and (e) figure of merit (ZT) as functions of energy graphene nanosheet with a single boron-doped line in the central scattering region. The Fermi energy is set to zero

General, the systematic analysis of Figures 2–8 reveals a clear correlation between boron doping concentration, interface modification, and thermoelectric performance. The transition from pristine to multi-line boron doping significantly enhances the Seebeck coefficient and suppresses thermal conductivity, while the addition of boron-doped electrodes further improves charge injection and reduces interfacial resistance. The results confirm that the cooperative interaction between dopant-induced electronic modulation and interface coupling plays a decisive role in optimizing thermoelectric behavior. These findings align well with previous theoretical and experimental observations on doped graphene nanostructures and two-dimensional thermoelectrics, validating the predictive capability of the DFTB–NEGF framework employed in this study. In summary, the progressive increase in boron doping lines coupled with boron-doped electrode interfaces provides a robust design strategy to maximize the thermoelectric figure of merit in graphene nanosheets. The study demonstrates that atomic-level control over dopant configuration and interface composition enables simultaneous enhancement of the Seebeck coefficient, electrical conductivity, and suppression of thermal conductance offering a promising route for the development of high-performance, carbon-based thermoelectric devices.

While the present results provide valuable theoretical insight into the thermoelectric enhancement induced by boron doping and interface engineering, it is important to note that the simulations were performed under idealized conditions. In practical experimental systems, achieving perfectly ordered boron line doping and defect-free interfaces may present fabrication challenges. Additionally, effects such as structural disorder, substrate interactions, contact resistance, and anharmonic phonon scattering could influence the measured thermoelectric performance. Nevertheless, the observed trends offer useful guidance for the experimental design and optimization of graphene-based thermoelectric devices.

4. Conclusion

In this work, the thermoelectric performance of graphene nanosheets was comprehensively investigated under progressive boron doping and electrode interface engineering using the DFTB–NEGF theoretical framework. The results clearly demonstrated that boron incorporation induces a strong modification in the electronic and phononic transport characteristics of graphene. Increasing the number of boron-doped lines from single to triple configurations effectively opened a tunable bandgap, enhanced the Seebeck coefficient due to carrier asymmetry, and significantly reduced phonon thermal conductance through mass disorder and scattering effects. Furthermore, introducing boron-doped electrodes markedly improved energy-level alignment between the contacts and the central channel, leading to enhanced carrier injection and reduced interfacial thermal losses. The combined effects of multi-line boron doping and doped electrode interfaces produced a synergistic improvement in thermoelectric performance, with the triple boron-doped

configuration achieving the highest figure of merit ($ZT \approx 2.4$ at $\mu \approx \pm 0.7$ eV). These findings confirm that the simultaneous optimization of chemical composition and interfacial structure provides an effective route to overcoming the intrinsic thermoelectric limitations of pristine graphene. The insights gained from this study offer valuable guidance for designing next-generation, carbon-based thermoelectric devices with high efficiency, mechanical flexibility, and environmental sustainability suitable for nanoscale energy harvesting and waste-heat recovery technologies.

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