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Tunable thermal properties of the biphenylene and the lateral heterostructure formed with graphene: A molecular dynamics investigation

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Recently, biphenylene was successfully synthesized as a novel allotrope of carbon. In this investigation, non-equilibrium molecular dynamics calculations are conducted to explore the intrinsic thermal properties of biphenylene. The isotropic thermal conductivity of biphenylene is obtained, which is also sensitive to size and temperature. Furthermore, the graphene/biphenylene lateral heterostructure is constructed to possess an interfacial thermal conductance of about $2.84 \times 10^9 \text{ W K}^{-1} \text{ m}^{-2}$. The external tensile strain can induce a redshift of the vibrational density of states of pristine graphene and biphenylene, and the improved overlap also results in an enhanced heat flux in the biphenylene/graphene heterostructure. Our approach can provide theoretical guidance to design a thermal management device based on graphene and biphenylene.

KEYWORDS

biphenylene, thermal conductivity, biphenylene/graphene heterostructure, interfacial thermal conductance, strain effect

Introduction

After the graphene was prepared by the Geim using a mechanical stripping method [1]; two-dimensional (2D) materials attract extensive attention because of their novel performance and promising applications [2–8]. Specifically, transition metal dichalcogenides (TMDs) and transition metal carbides or carbonitrides (MXene) have also been proposed to rise rapidly [9–12]. Their unique layered structure endows unusual physical and chemical properties, such as high mechanical strength [13] and excellent thermal [14], magnetic [4], and optical performance [15]. For example, when GeC changes from an indirect band gap to a direct band gap, it can maintain structural stability under high pressure [16]. Interestingly, the band gap of arsenene can be changed under

the effect of stress. Research studies found a novel phenomenon, especially for folded arsenene: when 6% stress is applied, the gap of arsenene will be closed [17].

Thermal behaviors of 2D materials act as critical factors in heat dissipation when used as nano-devices, and the heat transport will directly determine the efficiency [18, 19]. Thus, research on the thermal properties of 2D materials has become a hotspot. For example, Balandin et al. measured the thermal conductivity of a suspended graphene monolayer in a room-temperature environment for the first time using the Raman method [20]. The measurement results show that its thermal conductivity is much higher than that of diamond and graphite block, reaching about 4,840–5,300 W m⁻¹ K⁻¹. Cai et al. obtained the thermal conductivity of the suspended graphene monolayer using the same method and simultaneously measured the Raman laser absorption of graphene using a laser power meter [21]. The results demonstrate that the thermal conductivity of the graphene monolayer grown by chemical vapor deposition (CVD) was about 2,500–3,100 W m⁻¹ K⁻¹ and 1,200–1,400 W m⁻¹ K⁻¹, at the temperatures 350 K and 500 K, respectively. Interestingly, when two different layered materials form a lateral heterostructure, the phonons can scatter when passing through the interface, resulting in interfacial thermal conductance [22]. For example, topological defects can improve the interfacial thermal conductance of graphene/h-BN from 6.42 × 10⁹ W K⁻¹ m⁻² to 7.09 × 10⁹ W K⁻¹ m⁻² [23]. The interfacial thermal conductance of the black phosphorene heterostructure can be reduced using a nanophononic structure [24]. In addition, the covalent interface of the lateral heterostructure can evidently induce a temperature drop, which is a critical factor for interfacial thermal conductance [25]. Recently, a novel non-benzenoid carbon allotrope was prepared [26], named biphenylene, which shows metallic characteristics [26]. It is an anti-aromatic compound and possesses tunable magnetic properties [27]. In addition, the maximum Young's modulus of biphenylene is obtained as 259.7 N/m, and its ultra-high melting point is up to 4,500 K, showing strong mechanical and high stability performance [28]. In addition, biphenylene has been reported to be a candidate material for fuel cells [29].

In this work, the thermal conductivity of biphenylene is addressed using molecular dynamics calculations. Then, the size and temperature dependence of the thermal conductivity of biphenylene are addressed. Importantly, the biphenylene/graphene heterostructure is constructed, and interfacial thermal conductance is investigated. In addition, the stain-tunable interfacial thermal conductance of the biphenylene/graphene heterostructure is studied, and the vibrational density of states is further explored.

Computational methods

In our simulations, the LAMMPS package was used for all the molecular dynamics (MD) calculations [30]. The interaction

between the C atoms was described by the Tersoff potential [3]. The time step was set as 0.5 fs and NPT (isothermal and isobaric), NVT, and NVE (isovolumetric and isoenergetic) ensembles were conducted for 500 ps in the MD simulations to obtain an equilibrium state for the system. Moreover, Newton's equations were reflected in the integrated velocity. The Verlet algorithm was used to show the atomic motion. The temperature and energy of the studied system were monitored, and they also present a convergence, further showing a steady state. In the calculations for the phonon spectra of the system, the density functional perturbation theory (DFPT) within the PHONOPY code was used [31, 32].

Results and discussion

In order to investigate the heat transfer characteristics along the x direction, the nanoribbon of the biphenylene monolayer is constructed along x , as shown in Figure 1. Two ends of biphenylene are fixed and hot and cold baths are used by Nosé–Hoover reservoirs next to the two ends. Thus, the heat current induced by such a temperature gradient is obtained along the x direction. The size dependence of thermal conductivity was considered by setting the width (in the y direction) of the biphenylene nanoribbon to about 50 Å, while the length (L , in the x direction) is variable by 411.1, 616.5, 822.8, 1,027.8, and 1,233.4 Å. Similarly, the thermal conductivity of the biphenylene monolayer along the y direction is also calculated using the nanoribbon with the width (in the x direction) of the biphenylene nanoribbon about 50 Å, while the length (in the y direction) is variable by 409.1, 614.0, 818.3, 1,022.8, and 1,227.0 Å.

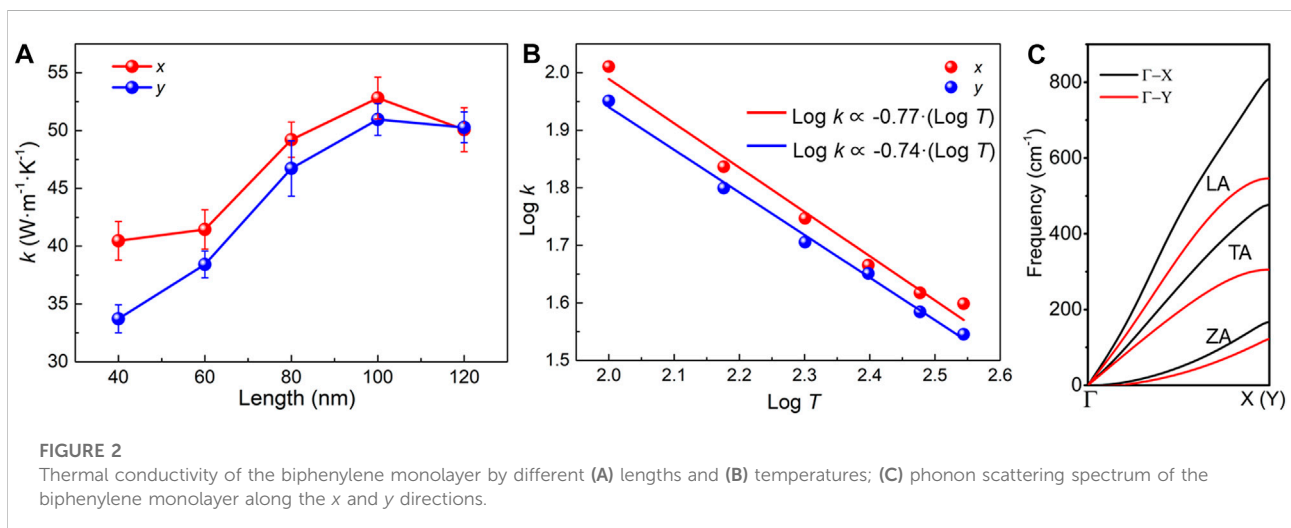
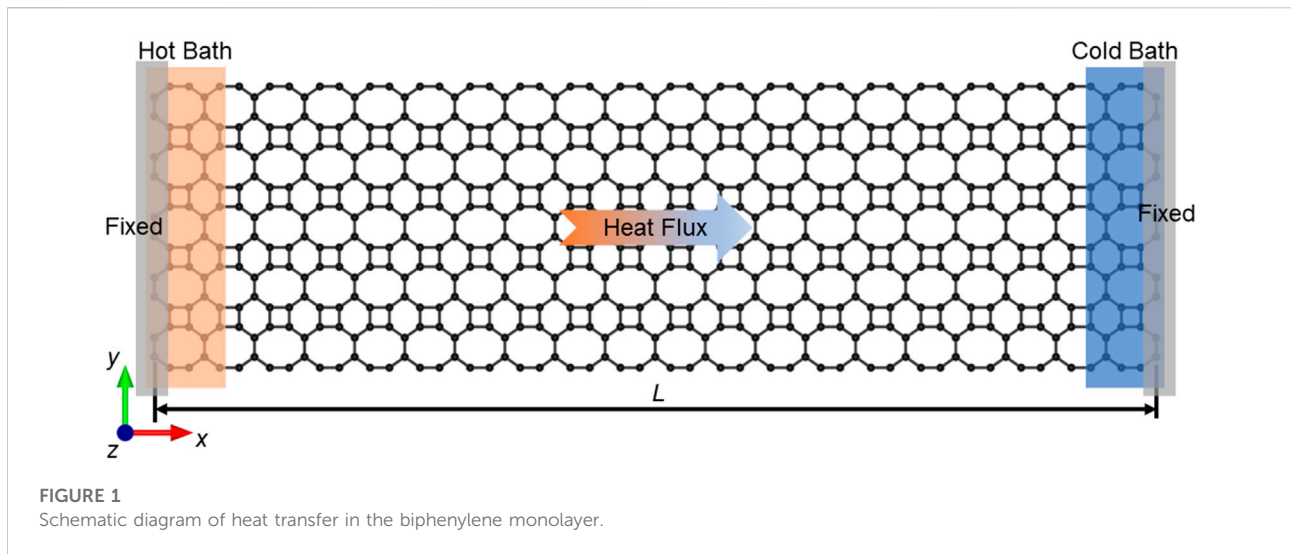
The thermal conductivity κ of pure biphenylene is obtained by Fourier's calculation of

$$\kappa = \frac{J}{S \cdot dT/dL}, \quad (1)$$

where J is the heat flux and T and S are the temperature and the cross-sectional area of the heat flux, respectively [33]. Importantly, dT/dL is obtained by the fitting of the linear region. In addition, we calculate the heat flux (J) using the non-equilibrium molecular dynamics (NEMD) method [30]:

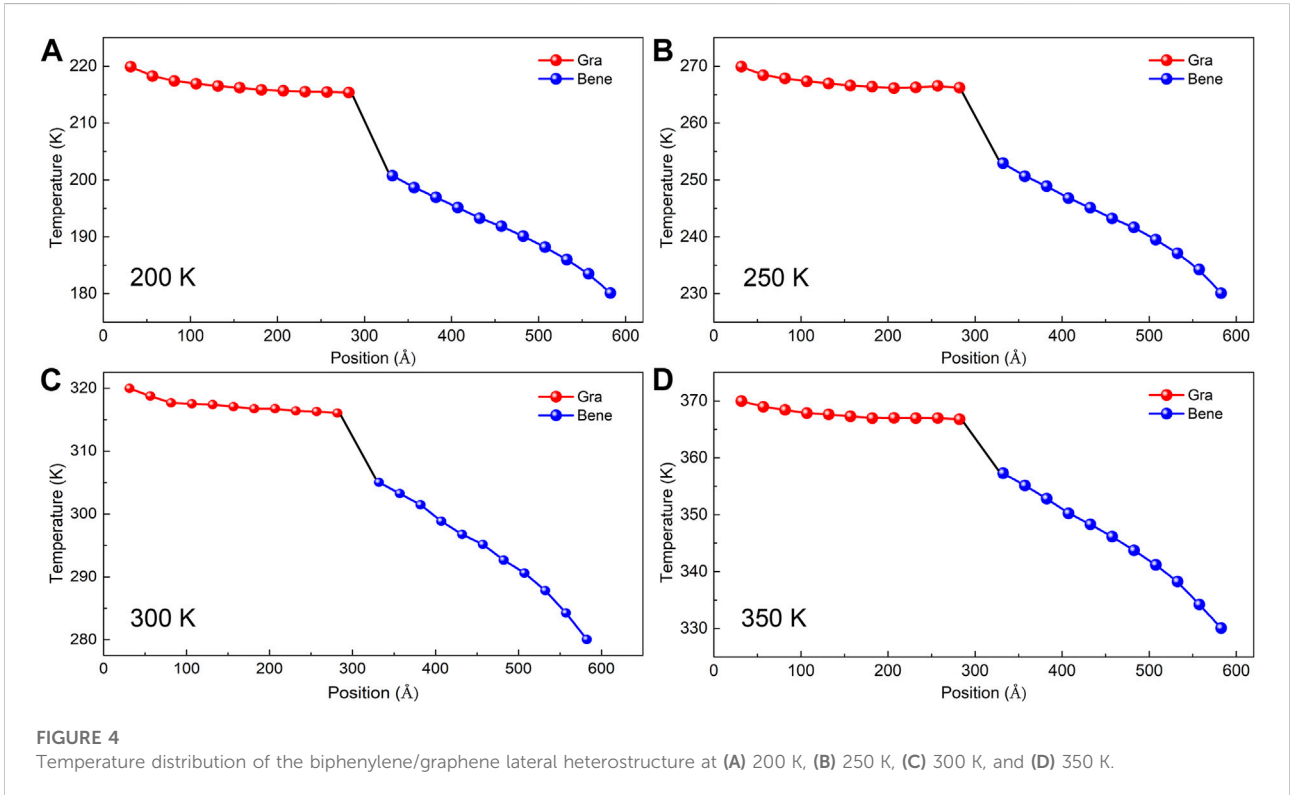
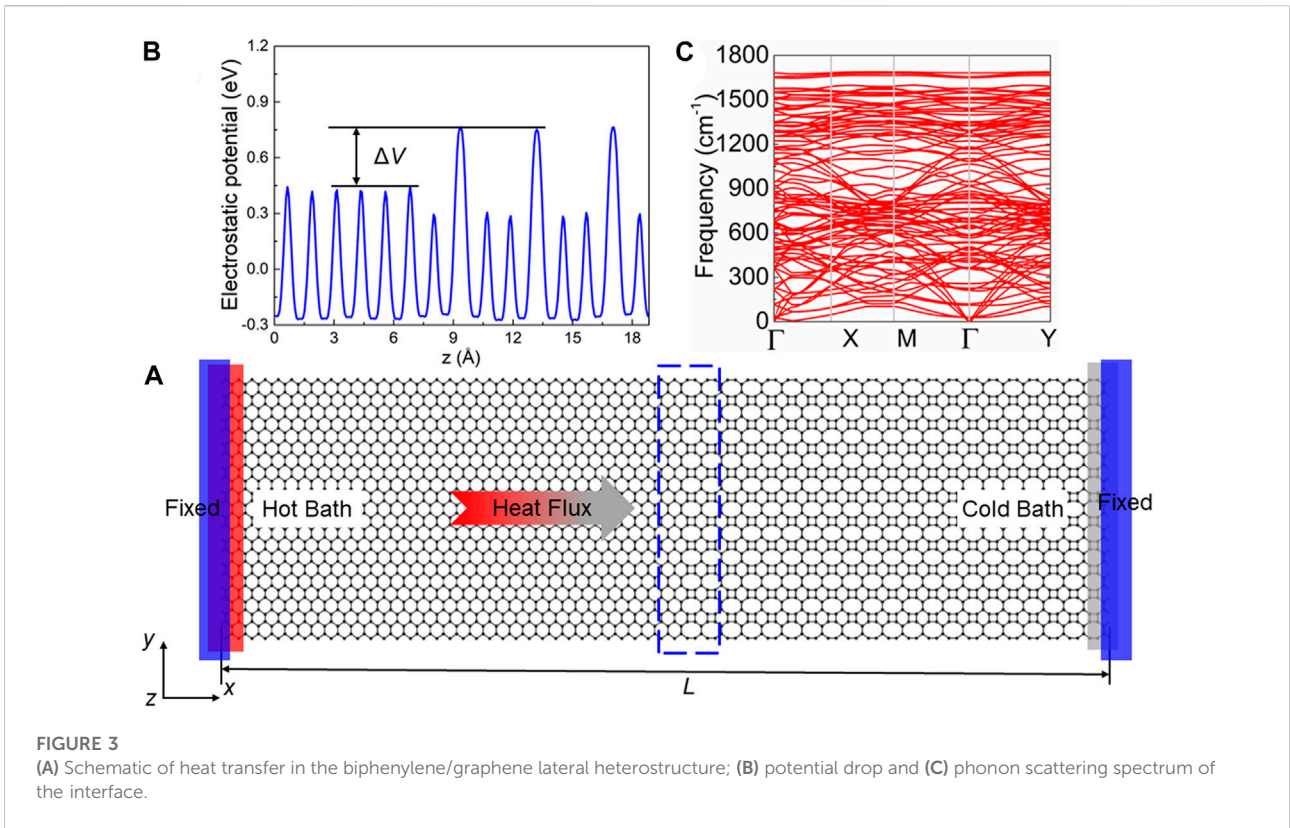
$$J = \frac{1}{V} \left[\sum_i^N \varepsilon_i v_i + \frac{1}{2} \sum_{ij,i \neq j}^N (F_{ij} \cdot v_i) r_{ij} + \frac{1}{6} \sum_{ijk,i \neq j \neq k}^N (F_{ijk} \cdot v_i) (r_{ij} + r_{jk}) \right], \quad (2)$$

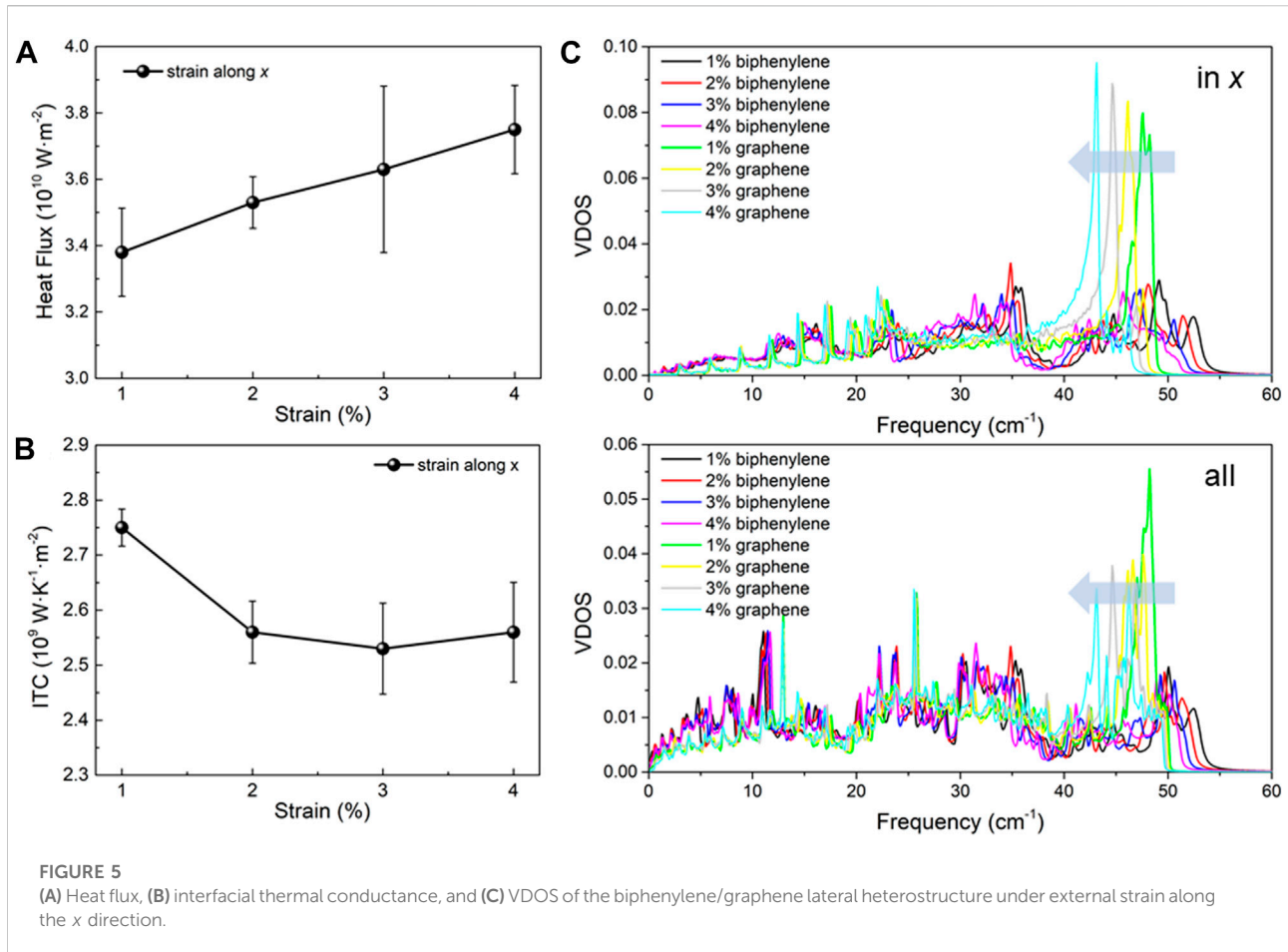
where ε_i is the energy of the atoms i , while v_i represents the velocity of the atom. r_{ij} is used to decide the distance between i and j . F_{ij} and F_{ijk} are the two-body and three-body forces, respectively. V is the volume of the studied system. The thermal conductivity of the biphenylene monolayer is shown



in Figure 2A with the length ranging from 40 nm to 120 nm at 300 K in the x and y directions. One can see that the biphenylene monolayer reveals isotropic thermal conductivity, which is enhanced as the length increases, but it will not increase at a certain length of about 100 nm. In addition, we obtain the maximum thermal conductivity of about $52.82 \text{ W m}^{-1} \text{ K}^{-1}$ and $50.97 \text{ W m}^{-1} \text{ K}^{-1}$ in the x and y directions, respectively. In contrast, the thermal conductivity of the biphenylene monolayer can be decreased by increasing the temperature, as shown in Figure 2B, in both x and y directions. In addition, there is a decent linear relationship between temperature and thermal conductivity. It is worth noting that the thermal conductivity of biphenylene in the x direction is higher than that in the y direction, which is contributed by the higher group velocity in the x direction because the acoustic branches in the x direction are steeper than those in the y direction, as shown in Figure 2C.

Then, we construct the lateral heterostructure by biphenylene and graphene with the length and width as 613.7 and 47.5 \AA , respectively, as shown in Figure 3A, where the interface is denoted by the blue dashed line. To investigate the interface properties of biphenylene and graphene, the potential drop (ΔV) is calculated as shown in Figure 3B. The obtained potential drop of the biphenylene/graphene interface is 0.326 eV , which is important to induce a built-in electric field enhancing the migration of the charges [10]. Then, the stability of the biphenylene/graphene lateral heterostructure is calculated by the phonon spectrum, as shown in Figure 3C. One can see that an imaginary frequency exists in the phonon spectrum of the biphenylene/graphene lateral heterostructure, suggesting the stability of the structure. To explore the thermal performance of the biphenylene/graphene lateral heterostructure, the NEMD method is also used to obtain the heat flux of the calculated





system. Similarly, hot and cold baths are fixed on biphenylene and graphene, respectively, by Nosé–Hoover reservoirs as shown in Figure 3A. Thus, the heat flux is transferred from graphene to biphenylene. After crossing the interface, the interfacial thermal conductance of the biphenylene/graphene lateral heterostructure is further explored by

$$\lambda = \frac{J}{\Delta T}, \quad (3)$$

where ΔT is the temperature difference across the biphenylene/graphene interface. In addition, a free boundary condition was set in the y -direction and z -direction to build such a nanoribbon structure for the biphenylene/graphene lateral heterostructure. The system temperature is decided by the average temperature of the hot and cold baths.

The temperature difference of the biphenylene/graphene lateral heterostructure under different temperatures is shown in Figure 4. Evidently, a large temperature difference is induced across the interface. The obtained temperature difference of the biphenylene/graphene lateral heterostructure at 300 K is about 11.02 K. In addition, the heat flux is calculated as $3.13 \times 10^{10} \text{ W m}^{-2}$; thus, the interfacial thermal conductance of the biphenylene/graphene

lateral heterostructure is about $2.84 \times 10^9 \text{ W K}^{-1} \text{ m}^{-2}$. Such a pronounced temperature drop resulted in phonon scattering across the interface. In addition, the calculated interfacial thermal conductance of the biphenylene/graphene heterostructure is higher than that of other graphene-based lateral heterostructures such as graphene/BN (about $1.2 \times 10^9 \text{ W K}^{-1} \text{ m}^{-2}$) [34], graphene/metal (about $2.50 \times 10^8 \text{ W K}^{-1} \text{ m}^{-2}$) [35], graphene/phosphorene (about $2.49 \times 10^8 \text{ W K}^{-1} \text{ m}^{-2}$) [36], and graphene/MoS₂ (about $2.49 \times 10^8 \text{ W K}^{-1} \text{ m}^{-2}$) [37].

Strain engineering is a popular method to tune the properties of the 2D materials, such as electronic [38], thermal [39], and thermoelectric [40] performances. In general, the thermal conductivity of 2D materials can be reduced because of the suppressed phonon group velocity and the improved anharmonicity under external tensile strain, which is reported by graphene [41, 42]. Thus, we further investigate the response of the thermal transport of the biphenylene/graphene lateral heterostructure on external tensile stress along the x direction. We can see that the heat flux of the biphenylene/graphene heterostructure is increased while the interfacial thermal conductance is decreased by the strain, as shown in Figure 5A and Figure 5B, respectively. To

clarify the intrinsic mechanism of the strain-dependent thermal transport in the biphenylene/graphene heterostructure, the vibrational density of states (VDOS) of pristine graphene and biphenylene is calculated, which is defined as follows [43]:

$$\text{VDOS}(\omega) = \frac{1}{\sqrt{2\pi}} \int_0^{\infty} e^{i\omega t} C(t) dt, \quad (4)$$

where ω and $C(t)$ demonstrate the angular frequency and the velocity auto-correlation function, respectively. In the calculations of the total VDOS, $C(t)$ is obtained by

$$C(t) = \left\langle \sum_{j=1}^N \vec{v}_j(0) \cdot \vec{v}_j(t) \right\rangle, \quad (5)$$

where $\vec{v}_j(t)$ represents the velocity of atom j , and the ensemble average is described by $\langle \rangle$. The obtained VDOS in the x direction and the total VDOS are shown in Figures 5C,D, respectively. It is worth emphasizing that the increase in strain can result in a redshift for both graphene and biphenylene. In addition, the calculated value of the overlap (S) of the total VDOS for graphene and biphenylene increases from 0.7062 to 0.8392 with strain from 1% to 4% along the x direction, which also explains the enhanced heat flow by the strain in the biphenylene/graphene heterostructure.

Conclusion

In conclusion, the non-equilibrium molecular dynamics calculations in this work demonstrate that biphenylene possesses isotropic thermal transport characteristics. The thermal conductivity of biphenylene can be improved by length along the heat flux but reduced by increasing the temperature. The graphene/biphenylene heterostructure presents interfacial thermal conductance of about $2.84 \times 10^9 \text{ W K}^{-1} \text{ m}^{-2}$. In addition, the interfacial thermal conductance of the biphenylene/graphene heterostructure is found to be dependent on strain, and the enhanced heat flux by the strain results from the larger overlap of the VDOS between graphene and biphenylene.

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Data availability statement

The original contributions presented in the study are included in the article/Supplementary Material; further inquiries can be directed to the corresponding author.

Author contributions

Conceptualization, QC; methodology, KR and RZ; software, JL; validation, KR; investigation, JL; writing—original draft preparation, QC, KR and RZ; writing—review and editing, JL; funding acquisition, QC and KR. All authors have read and agreed to the published version of the manuscript.

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Conflict of interest

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