Nanoscale thermal cloaking in graphene via chemical functionalization

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Macro-thermal cloaking is typically produced by coordinate transformations, but this method is unsuitable for nanostructures. We designed a graphene-based nanoscale thermal cloak using a novel mechanism of phonon localization. The nanocloak in graphene was produced via the chemical functionalization of hydrogen, methyl and hydroxyl using molecular dynamics simulations. The cloaking performance was quantified by the ratio of thermal cloaking (RTC). We found that the RTC correlated with the functionalization fraction and it has a local maximum at a certain width, since the heat flux reduction in the exterior and the protected region reversed if the width was excessive. The atomic mass of the functional group also correlated with the RTC. Our simulations determined that phonon localization occurred due to sp₂-to-sp³ bonding transitions, which caused the heat flux to avoid the transition region. Finally, the extent of phonon localization was related to the cloaking performance.

1. Introduction

Growing interest in the manipulation of heat flux led researchers to design metamaterials,¹–⁷ with certain properties. In thermal science, metamaterials known as “thermal crystals,”⁸ are used in thermal devices such as thermal diodes,⁹–¹¹ heat concentrators,¹² and thermal camouflage and thermal cloaks.¹³–¹⁹ However, most of these devices are still in the early stages of development. A thermal cloak is a device that redirects the heat flow around an object and renders it thermally invisible, making it seem invisible for heat flow.²⁰ Cloaking is different than isolation. Isolation affects other parts of the object, while cloaking makes the object seem invisible. Cloaking was first achieved by Pendry et al.,²¹ who used transformation optics to obtain an electromagnetic cloak. Subsequently, other types of cloaks were²²–²⁶ proposed. Thermal cloaking is a fascinating device that may be used in the future for thermal control and management.

Numerous studies on thermal cloaking have emerged since the pioneering theoretical work of Fan et al.,¹ who first discovered heat invisibility and reversed heat flux using the theory of coordinate transformation. Yang et al.¹⁴ further developed the scheme of arbitrary-shaped thermal cloaks. He et al.¹ designed an open cloak with finite material parameters. These early devices typically required anisotropic and inhomogeneous thermal conductivities, which made their fabrication difficult. Therefore, a simplified scheme known as “multilayered metamaterials” was proposed,⁵,¹⁵,²⁷ which discretized the inhomogeneous materials into a series of homogeneous materials. Experimental thermal cloaks used two materials with different thermal properties to form multilayered structures.¹³,²⁰,²⁸–³⁰ Narayana et al.²⁸ fabricated a micro-structured thermal cloak based on polyamide/copper multilayered structures. Xu et al.²⁰ designed an ultrathin three-dimensional thermal cloak. Dang et al.¹³ reported an active and controllable thermal cloaking device that was more intelligent and flexible. In general, most existing studies are based on the coordinate transformation approach and require inhomogeneous structures. In practice, inhomogeneous structures are reduced to homogeneous multilayered structures. However, this simplification is unsuitable for nanoscale structures for two reasons. First, particle size effects and interfacial thermal resistance cannot be neglected for nanoscale structures,³¹ and multilayers allow additional thermal resistance and damage to their mechanical properties. Second, the system size is close to the phonon mean free paths in the nanoscale structures, which suggests that the heat transport is nonlocal. Consequently, we cannot apply Fourier’s law to define the thermal properties of the local region in the nanoscale structures.³² To date, no studies have reported on nanoscale thermal cloaking. However, growing interest in heat transfer at the nanoscale level, such as for large-scale integrated circuits, calls for more research in nanoscale thermal cloaks for the thermal protection of nanocomponents.

We developed a graphene-based thermal cloak via chemical functionalization using a novel mechanism. Graphene,³³ one of the most important and popular nanomaterials, is a promising material in nanoelectronics because of its excellent thermal, mechanical and electrical properties. In addition, its thermal properties can be controlled by changing its edge, size, and
chemical functionalization.\textsuperscript{34–39} We used partial chemical functionalization, including hydrogen, methyl and hydroxyl on graphene to form a thermal cloak. Molecular dynamics (MD) simulations were used to investigate thermal cloaking effects caused by chemical functionalization on graphene. We focused on the influence of the size fractions of functional groups, cloaking sizes, and functionalization types. Further, we used a novel mechanism based on phonon localization theory to explain the thermal cloaking effects.

2. Molecular dynamics

The MD simulations were conducted using the LAMMPS packages.\textsuperscript{40} We used an adaptive intermolecular reactive bond order (AIREBO) potential to describe the C–C and C–H bonding interactions,\textsuperscript{41–43} whose expression is

\begin{equation}
E = \frac{1}{2} \sum_{i=1}^{N} \sum_{j \neq i} \left[ E_{ij}^{\text{REBO}} + E_{ij}^{\text{LJ}} + \sum_{k \neq i,j \neq i,j} E_{ijkl}^{\text{TORSION}} \right],
\end{equation}

where \( E \) denotes the whole potential energy, and where the first term on the right side of the equation is the hydrocarbon REBO potential,\textsuperscript{42} the second term is the Lennard-Jones potential, and the third term is an explicit four-body potential caused by various dihedral angle preferences in the hydrocarbon configurations. In addition, the C–O, C–O and O–H bonds were defined by an OPLS-aa potential model.\textsuperscript{43} Fig. 1 shows the schematic of graphene with a thermal cloak generated by hydrogen, methyl and hydroxyl. To maintain structural stability, the functional groups were evenly distributed on both surfaces of the graphene. The protected region was the center circle. The most popular design of the macroscale thermal cloak is a spheroid/cylinder shell.\textsuperscript{1,2,8} As such, the shape of this two dimensional cloak was designed as a ring, and the heat flux in the center of the circle was squeezed into the ring structure.

We used the nonequilibrium MD (NEMD) method to simulate the system under a temperature gradient. The temperature profile and heat flux field were recorded to visualize the thermal cloaking effect, upon which we performed a quantitative analysis of the thermal cloaking. The system was separated into three regions: the fixed region, the thermostat region and the free region. The \( X \) direction was applied a fixed boundary condition, and the atoms of the two ends were fixed. The \( Y \) and \( Z \) directions were free boundary conditions. Next to the fixed region was the thermostat region, with high and low temperatures on each side and with atoms calculated by Nosé–Hoover thermostats as follows:\textsuperscript{44}

\begin{align*}
\frac{d}{dt} p_i &= F_i - \gamma p_i, \\
\frac{d}{dt} T_i &= \frac{1}{\tau} \left[ T(t) - \frac{1}{N} \sum_{i} p_i^2 \right]. \\
T(t) &= \frac{2}{3Nk_B} \sum \frac{p_i^2}{m_i},
\end{align*}

where, \( p_i, F_i \) and \( m_i \) are the momentum, force and mass of atom \( i \), \( \gamma \) and \( \tau \) are the dynamic parameters and relaxation times of the thermostat, \( k_B \) is the Boltzmann constant, and \( N \) is the atomic number of the thermostats. The middle section, called the free region, was our primary focus, and the heat flux of each atom was calculated by

\begin{equation}
J_i = eSV_i - S\dot{V}_i,
\end{equation}

in which, \( J_i \) is the heat flux of atom \( i \); \( e \) is the total energy, including both kinetic and potential energies, \( V \) is the velocity vector, and \( S \) is the stress tensor for each atom, which had nine components: \( xx, yy, zz, xy, yx, zx, xz, yz, \) and \( zy \). Therefore, the heat flux of three directions for each atom was expressed as

\begin{align*}
J_x &= ev_x - (S_{xx}v_x + S_{yx}v_y + S_{zx}v_z), \\
J_y &= ev_y - (S_{xy}v_x + S_{yy}v_y + S_{zy}v_z), \\
J_z &= ev_z - (S_{xz}v_x + S_{yz}v_y + S_{zz}v_z).
\end{align*}

For convenience, the subscript “\( i \)” was omitted. The time step was set at 0.5 fs. The system was first relaxed in the \( NVT \) ensemble for 500 000 steps, and then in the \( NVE \) ensemble for another 500 000 steps. Finally, the NEMD method was used for 1 000 000 steps, during which the heat flux of each atom in the free region was recorded. The system size was 24.5 nm \( \times \) 21.2 nm. The cloaking region was placed in the center of the graphene sheet with a diameter of 6 nm. The high temperature thermostat was 350 K, and the low temperature thermostat was 250 K.

3. Results and discussion

First, we used a hydrogenated cloak to demonstrate the thermal cloaking in the nanostructures. For ease of description, it is called “hydrogenated graphene.” The cloak had a width of 1 nm and closely surrounded the cloaking region. To better
illustrate the efficiency of our cloak, three specific conditions were considered as references: perfect graphene, defective graphene, and hollow graphene. The perfect graphene was pristine graphene without a thermal cloak. For the defective graphene, the cloak was generated with vacancy defects in which twenty carbon atoms around the cloaking region were removed. For the hollow graphene, the cloaking region was entirely removed, which equaled absolute isolation. Fig. 2(a–d) show the temperature profiles of the four samples. To better visualize the temperature profiles, the temperature of each atom was the average of 200,000 steps. Overall, the temperature profiles of these graphene sheets were not as regular as those of macro materials. In particular, the isotherms were less notable. We made three observations. First, we noticed a subtle outline of the cloaking region in the defective graphene, in which the atom temperature was relatively uniform, indicating the occurrence of thermal cloaking.

Fig. 2  Temperature profiles of (a) perfect graphene, (b) defective graphene, (c) hollow graphene and (d) hydrogenated graphene; (e) the energy accumulation applied to the thermostats of the four conditions, $\eta_v$ is the normalized thermal conductivity.
Second, for the hydrogenated graphene, the outline was more significant than that of the defective graphene, and the temperature profile of the exterior region was slightly affected. Third, the hollow graphene was equivalent to thermal isolation, and the temperature profile was strongly influenced by the central hollow region, which should be avoided. Luo et al.\textsuperscript{45} use the standard deviation (STD) of the temperature difference of each small lattice to examine the thermal cloaking effectiveness of layered engineering materials, the equation is

\[
\Delta T(i) = T(i) - T_{Pendry}(i),
\]

\[
\text{STD} = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (\Delta T(i))^2},
\]

in which, \(T_{Pendry}\) refers to the theoretical temperature based on the transformation optics method. We separate the system into 80 \(\times\) 80 lattices, and calculate the temperature difference of each lattice. The results are shown in Table 1. Apparently, it is difficult to preserve the exterior temperature profile, but the defective graphene and hydrogenated graphene perform much better than hollow graphene in this respect.

Fig. 2(e) shows the energy accumulation applied to the thermostats of each graphene sample. The slope reflects the relative values of thermal conductivity, and shows that the ranking order of thermal conductivity is perfect > defective > hydrogenated > hollow. So the hydrogenation can reduce the thermal conductivity of graphene, it agrees well with the literature.\textsuperscript{46} It is reported that the defect in the interface may enhance thermal conductance,\textsuperscript{37} but our case has a different mechanism. The introduction of hydrogen can lead to the red shift in the phonon spectra, so the thermal conductivity decreases significantly.\textsuperscript{46} The thermal conductivities of the defective and hydrogenated graphene samples were almost the same, but the hydrogenated sample had remarkable superiority in thermal cloaking. Generally, the cloaks negatively impacted the thermal conductivities, but were still acceptable.

Fig. 3(a–d) show the heat flux fields of the four samples. The heat flux of each atom was the average value of 200 000 steps. As shown in Fig. 3(b), we focused on the middle section, which was separated into three typical regions. Considering the longitudinal symmetry, we focused on region A and region B. The heat flux field of graphene was almost uniform, and its orientation was parallel to the temperature gradient. For the defective graphene, the heat flux of region B was much less than that of region A, suggesting that the heat flux avoided the cloaking region. In addition, the heat flux field in region A was slightly heterogeneous, suggesting that it was affected by the cloak. An ideal thermal cloak should have little impact on other regions. As such, the defective graphene was not an acceptable thermal cloak. The heat flux field was the standard of thermal isolation for the hollow graphene, and showed that the heat flux of region A was considerably larger than that of the other regions because of the isolation in the center. In addition, the region near the inner ring where the direction of the heat flux that had a significant change was strongly influenced by the cloak. For the hydrogenated graphene, the orientation in region A was very smooth. Moreover, the heat flux of region B in hydrogenated graphene was smaller than that of the defective graphene. Therefore, we arrived at a similar conclusion: the performance of hydrogenated graphene was better than that of defective graphene.

We defined a new concept to quantify the performance of thermal cloaking, which was called the ratio of thermal cloaking (RTC),

\[
\eta = \frac{|HF_A|}{|HF_B|},
\]

where \(HF_A\) and \(HF_B\) is the mean heat flux in region A and region B. For a perfect cloak, there should be no heat flux in region B, such that \(HF_B = 0\), \(\eta\) is infinity, while \(\eta = 1\) indicates no thermal cloaking. RTC was an index of cloaking performance, namely, the higher the \(\eta\), the better the cloaking performance. Table 2 gives the RTC of perfect, defective and hydrogenated graphene. It shows that the RTC of hydrogenated graphene is 65% higher than that of defective graphene. It should be emphasized that our scheme is not a perfect thermal cloak, but it achieves heat flow manipulation in some sense. So we still call it “thermal cloak”.

Next, we investigated the influence of cloak width and hydrogen fractions. Fig. 4 shows the heat flux profiles of cloaks with different widths ranging from 0.5 nm to 2 nm. First, in each of the four samples, the central region had yellow and gray arrows, indicating a relatively low heat flux. Second, as the thermal cloak increased in size, the blue region gradually increased and became more homogeneous, which indicated that the heat flux moved to the bottom and top regions. The middle section was blocked by the cloak. Third, as shown in Fig. 4(d), the orange arrows for the 2 nm cloak increased significantly in the central region, indicating an increase of heat flux, but did not decline monotonously as the thermal cloak increased. Although the thicker cloak had a stronger impact on the heat flux profile, it did not result in a better cloaking performance.

Besides the cloak width, the hydrogen fraction was another important factor that affected the cloaking performance. Hydrogenated graphene is called graphane, and was first synthesized in 2009 by Elias et al.\textsuperscript{48} Pure graphene does not exist because current hydrogenation methods cannot completely hydrogenate graphene. Thus, it is necessary to study the influence of the hydrogen fraction. Because of the stability of the structure, we obtained only three stable states: 100%, 25% and 12.5%. Fig. 5 shows the heat flux profiles of the 12.5% and 25% cloaks, in which the width is 2 nm. Fig. 4(d) shows that, for the 100% cloak, as the hydrogen fraction decreased, a growing number of orange arrows appeared in the cloaking region, which indicated that the heat flux of the cloaking region was enhanced as the hydrogen fraction decreased, and that the cloaking performance declined.

| Table 1 STD of perfect, defective, hollow and hydrogenated graphene |
|-----------------|---------|-------|---------|---------|
| Perfect         | Defective | Hollow | Hydrogenated |
| STD, K          | 0       | 5.9    | 7.8      | 6.3      |

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Secondly, more blue arrows appeared in the top and bottom regions as the fraction increased, which showed that additional flow flux avoided the cloak.

The RTCs of different widths and hydrogen fractions are shown in Fig. 6. The results agreed with the above analyses. For the fraction, RTC increased monotonously. For the cloak width, the RTC reached a maximum at 1.0 nm, but above 1.0 nm, thicker or thinner cloaks both had negative effects on the cloaking performance. The presence of a thermal cloak reduced the heat flux of the whole system. The increased cloak width not only reduced the heat flux of the protected region, but also reduced the heat flux of the entire system. If the extent of the latter is greater than that of the former, RTC will decrease with the increasing width, otherwise, it will increase monotonously. Therefore, the RTC reached a maximum at a certain value that was dependent on the system size and the protected region size.

Besides hydrogenation, we used other functional groups to develop thermal cloaks, such as methyl and hydroxyl. Our early simulations suggested that the mass of the functional group had a positive impact on the cloaking performance. The relative atomic mass of methyl is 15 and of hydroxyl is 17, both of which are far greater than that of hydrogen. Therefore, we replaced hydrogen with methyl and hydroxyl to obtain enhanced thermal cloaking. We named the samples the methylic cloak and the hydroxy cloak. It should be noted that atoms of the functional groups will interfere with each other if the fraction is too high of methyl and hydroxyl. After several attempts, we obtained a stable structure while the fraction was 12.5%. Fig. 7 shows that the enhanced thermal cloaks generated by methyl and hydroxyl, in which the cloak width was 2 nm and the fraction was 12.5%. The hydrogenated cloak with the same parameters is shown in Fig. 5(a). By comparison, we found that the cloaking performance of methylic and hydroxy cloaks was significantly improved compared to that of hydrogenated cloak. In addition, the heat flux of the central region in the hydroxy cloak was lower than that in the methylic cloak, so the methylic cloak was superior to the hydroxy cloak. Then, we calculated the RTCs based on eqn (6), which were 1.714 for the methylic cloak and 2.36 for the hydroxy cloak. The RTC of the hydrogenated cloak with the same parameters was only 1.47, so the RTC increased 16.5% and 60.5% with the methylic and hydroxy cloaks. We observed that the RTC of the hydroxy cloak was even higher than that of the 100% hydrogenated cloak, though the fraction of the hydroxyl was only 12.5%. Hydroxyl greatly improved the

*Fig. 3*  Heat flux fields of (a) perfect graphene, (b) defective graphene, (c) hollow graphene and (d) hydrogenated graphene.

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<th>Table 2</th>
<th>RTC of perfect, defective and hydrogenated graphene</th>
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<td>Perfect graphene</td>
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cloaking performance compared to that of the methyl and hydrogen.

Prior studies that focused on the effect of hydrogenation on thermal conductivity of graphene found that the deterioration of thermal conductivity was due to the sp2-to-sp3 bonding transition, which softened the G-band phonon modes. Based on this finding, we investigated the changes in the phonon properties in chemical functionalized graphene to determine the underlying mechanism of the thermal cloak. The phonon density of states (DOS) is the most representative property that can characterize the phonon states. The DOS was calculated by the Fourier transform of the velocity autocorrelation function,

$$\text{DOS}(\omega) = \int e^{-i\omega t} \langle v(0)v(t) \rangle dt,$$  

where $\omega$ is the phonon frequency. Fig. 8 shows the four types of typical DOS of carbon atoms in the cloak, including the normal sp2 carbon, the affected sp2 carbon, the normal sp3 carbon and

Fig. 4  Heat flux fields of hydrogenated graphene with a cloak width of (a) 0.5 nm, (b) 1 nm, (c) 1.5 nm and (d) 2 nm.

Fig. 5  Heat flux fields of the cloaks with hydrogen fraction of (a) 12.5% and (b) 25%. The cloak width is 2 nm.
the affected sp3 carbon. The atoms in graphene are sp2 carbon atoms, but some will become sp3 atoms after chemical functionalization. Thus, both sp2 and sp3 carbon atoms existed in our samples. Fig. 8(a) shows the DOS of a normal sp2 carbon. A primary peak was observed at 48 THz, which was consistent with that of perfect graphene, and thus we concluded that these atoms were not affected by the cloak. Fig. 8(b) shows the DOS of sp2 carbon atoms near the cloak. Compared to Fig. 8(a), two notable changes are depicted in Fig. 8(b). First, the peak at 48 THz disappeared and was replaced by several small peaks, suggesting that high frequency states significantly decreased. This resulted from the atoms in the cloak having lower vibration frequencies, which affected the neighboring atoms. Second, the main peak shifted to 24 THz from 48 THz, so the cloak caused the phonon spectra to shift to a low frequency region. The same types of atoms had different DOS values, which indicated that the phonon localization occurred near the cloak. A similar situation occurred in Fig. 8(c) and (d). Fig. 8(c) shows the DOS of normal sp3 atoms. Both atoms were similar in structure to a diamond, and displayed a main peak at 37 THz. For Fig. 8(d), the DOS had a slight change, in which the main peak shifted to 30 THz. In general, the phonon localization phenomenon occurred in this system, and was more significant for sp2 atoms. Therefore, the phonon localization of sp2 was our primary focus in determining the underlying mechanism of the thermal cloak.

The phonon localization can be visualized by the spatial distribution of phonon modes. The spatial distribution was equivalent to the weight distribution of the specific modes. For the ith atom, the weight of a specific range (Δ) of phonon modes on the whole spectral range was expressed as

\[ p_{i,\Delta} = \frac{\int_{\Delta} DOS_i d\omega}{\int_0^{\infty} DOS_i d\omega} \]  

(8)

Since the changes of the sp2 atoms in the high frequency region were more significant, we showed the phonon (46 to 50 THz) spatial distribution of sp2 atoms in Fig. 9. We used the 12.5% hydrogenated cloak and the 12.5% hydroxy cloak to display the differences in phonon localization. Fig. 9(a) and (b) refer to the 12.5% hydrogenated and the 12.5% hydroxy cloak. The red spheres indicated the highest spatial distribution, then the yellow spheres with less spatial distribution, and finally the blue spheres with the lowest spatial distribution. We made three observations. First, the edge atoms usually had a low spatial distribution. The phonon spectra of the edge atoms shifted to low frequencies because of the interaction between sp3 and sp2 atoms, so the high frequency phonons had relatively low distributions at the edge. Second, more blue spheres appeared in Fig. 9(b) than in Fig. 9(a). This indicated that the extent of phonon localization was more prominent for the hydroxy cloak, because the atomic mass of hydroxyl was much larger than that of hydrogen, and therefore it had a larger impact on its connected sp3 carbon atoms and indirectly affected the neighbor sp2 carbon atoms. Third, the top and bottom atoms usually had lower distributions. According to the heat flux profiles, the top and bottom regions had the highest heat flux, indicating that the interactions in this region were more vigorous, and the phonon localization was more significant because of the stronger interactions.
To quantify the extent of the localization, Table 3 shows the average phonon (46 to 50 THz) spatial distribution of the edge atoms. As a comparison, the distribution of a perfect graphene is also given in Table 2. For the perfect graphene, high frequency phonons (46 to 50 THz) occupy almost 30% of the phonon states, but for the listed cloaks in Table 2, it decreased to different extents. The 100% hydrogenated cloak reduced the most, to 13.7%, and the 12.5% hydrogenated cloak declined the least, to 17.8%. Generally, phonon localization occurs due to the sp2-to-sp3 bonding transition, which has a great effect on the heat flux field. The heat flux automatically avoids the transition region, so the central section is protected from the heat flux. Our results also showed that the extent of phonon localization was positively associated with the fraction and the mass of the functional group, and correlated with the cloaking performance. Thus, we concluded that phonon localization induced the thermal cloaking phenomenon.

4. Conclusions

In summary, we proposed a novel nanoscale thermal cloak and underlying mechanism. Partial chemical functionalization on graphene was used to form a heat flux channel that avoided the specific region. MD simulations were used to determine the thermal cloaking effect caused by chemical functionalization on graphene. First, we compared perfect graphene, defective graphene and hollow graphene, and found that hydrogenated graphene had a better cloaking performance than that of

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<th>Table 3</th>
<th>Average phonon (46 to 50 THz) spatial distribution of the edge atoms</th>
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<td>100% H</td>
<td>25% H</td>
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<td>13.7%</td>
<td>15.9%</td>
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Fig. 8 Four kinds of typical DOS of carbon atoms in the cloak, (a) normal sp2 carbon atom, (b) affected sp2 carbon atom, (c) normal sp3 carbon atom, and (d) affected sp3 carbon atom.

Fig. 9 Phonon spatial distribution of (a) 12.5% hydrogenated cloak and (b) 12.5% hydroxy cloak.
defective and hollow graphenes. This result indicated that hydrogenated graphene could cloak a subject and maintain the original temperature field as long as possible. Hydrogenated graphene also had a slight influence on the mechanical and thermal properties of the system. Second, we investigated the influence of the chemical functionalization fraction and the cloak width. The cloaking performance was quantified by the RTC. A higher RTC indicated a better thermal cloaking performance. The results showed that the RTC was positively associated with the functional group fraction. For the 100% hydrogenated cloak, the RTC was 2.35, while it reduced to 1.45 for the 12.5% hydrogenated cloak. The RTC reached a local maximum when the cloak width was 1.0 nm, because the presence of the thermal cloak reduced the heat flux of both the exterior and the protected regions. The decreased extent reversed at a certain value, depending on the system size, indicating that the RTC reached its maximum. Third, we used functional groups, methyl and hydroxyl, with higher atomic masses to enhance the thermal cloaks. Although the fraction was only 12.5%, we still observed a dramatic improvement of the cloaking performance by 16.5% and 60.5%, as compared to 12.5% with the hydrogenated cloak. The 12.5% hydroxyl cloak equaled the 100% hydrogenated cloak. Finally, we found the mechanism of the thermal cloak based on the phonon localization theory. The connection between the thermal cloak and phonon localization was identified by the simulations. The introduction of chemical functional groups on graphene led to a sp2-to-sp3 bonding transition, which further increased phonon localization. The heat flux automatically avoided the transition region because of phonon localization, and the center section was protected from the heat flux. Considering the popularity of graphene, our research not only has great potential applications for the thermal protection of graphene-based devices, but also has profound significance for the development of other nanoelectric devices.

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