Enhancing the interfacial thermal conduction of the graphene sheets via chemical bond–bond connections

Cite as: AIP Advances 9, 085106 (2019); https://doi.org/10.1063/1.5113973
Submitted: 10 June 2019 . Accepted: 31 July 2019 . Published Online: 08 August 2019

Min-Shan Li, Kai-Xuan Chen, Yuan-Xiang Fu, Dong-Chuan Mo, and Shu-Shen Lyu

ARTICLES YOU MAY BE INTERESTED IN

Comparative study of the ion-slicing mechanism of Y-cut LiNbO₃
AIP Advances 9, 085001 (2019); https://doi.org/10.1063/1.5112792

High-energy X-ray radiography investigation on the ejecta physics of laser shock-loaded tin
AIP Advances 9, 085002 (2019); https://doi.org/10.1063/1.5109748

Thermoelectric characterization of ZnSb by first-principles method
AIP Advances 9, 085003 (2019); https://doi.org/10.1063/1.5108594
Enhancing the interfacial thermal conduction of the graphene sheets via chemical bond–bond connections

Min-Shan Li,1,2 Kai-Xuan Chen,2,3 Yuan-Xiang Fu,2,4 Dong-Chuan Mo,2,4,il and Shu-Shen Lyu2,4

AFFILIATIONS
1 School of Chemical Engineering and Technology, Sun Yat-sen University, No. 135, Xingang Xi Road, Guangzhou, 510275, P. R. China
2 Guangdong Engineering Technology Research Centre for Advanced Thermal Control Material and System Integration (ATCMSI), Sun Yat-sen University, No. 135, Xingang Xi Road, Guangzhou, 510275, P. R. China
3 Chair of Solid-State and Quantum Chemistry, Institute of Inorganic Chemistry, RWTH Aachen University, 52056 Aachen, Germany
4 School of Materials, Sun Yat-sen University, No. 135, Xingang Xi Road, Guangzhou, 510275, P. R. China

ABBREVIATIONS

ABSTRACT
Graphene, after its discovery in 2004, was known to possess extremely high thermal conductance. In the practical applications, however, the thermal conductance was unfortunately low compared with its theoretical value since the heat transfer among individual graphene sheets is largely hindered by the boundary phonon dissipation. In this first-principles study, we propose a new strategy to enhance the interfacial thermal transport, that is, chemical bond–bond connections. Organic, metal and metal-oxide groups are adopted to link two graphene nanoribbons, acting as a thermal bridge. In such models, the thermal conductance is significantly enhanced, as compared with the non-linked counterparts in which the van der Waals interactions dominate. In numbers, the highest thermal conductance of 0.577 GW-m⁻²-K⁻¹ at 300K (which preserves as much as 13.2% compared with the pristine nanoribbon) can be obtained when linked by –Al– groups. The enhancement mechanism as regards different bond–bond connections is also discussed. Our study paves the way to exploring the enhancement of interfacial heat transfer. Even though the work was done based on the graphene models, it can be generally extended to a variety of inorganic and organic families.

I. INTRODUCTION
With the fast advancement in the modern electronics, the efficiency of the heat transfer has become an urgent issue in the highly integrated chips. The star material graphene has attracted substantial attentions due to its ultra-high thermal conductivity and been considered as a promising candidate to provide high-performance heat transfer systems. For example, graphene is widely used as filler in various polymer products to improve their heat transfer performance. Unfortunately, such enhancement is hindered in the practical applications due to the phonon boundary dissipation, especially among graphene sheets.

Based on the recent studies, bond–bond connections may be used to construct a ‘thermal bridge’ at the interfaces between individual samples, which allows heat flux to pass through. Sun et al. studied the thermal transport in covalent bonded edge-functionalized graphite oxide/epoxy interface through experiments. Han et al. studied the efficient heat removal by introducing alternative heat-escaping channels in bonded graphene-based film. Gutierrez et al. used density functional tight-binding method and non-equilibrium Green’s function (NEGF) to study the length and conformation dependence of thermal conductance in molecular junctions. From experiments, graphene samples are generally synthesized via an oxidation-reduction, and it leaves many functional
groups at the surfaces and boundaries. It is thus feasible to introduce a bond–bond connection at the interfacial boundaries through a dehydration reaction. Some research\textsuperscript{11,12} also pointed out that transition-metal groups can be used to link individual nanotube-like or layered materials. Because the $d$ orbitals from transition-metal provide more possibility to form chemical bonds in various directions by "hybridization", that is, chemical bonding between metal $d$ and nonmetal $p$ levels.

In experiments, however, it is difficult to study the in-depth mechanism of bond–bond connection across graphene sheets, since the technique to accurately examine the bonding characteristic is in lack. Some theoretical work have been conducted but they mostly focused on the out-of-plane interfaces in the heterostructures.\textsuperscript{13–15} Within the best of our knowledge, the investigation on the in-plane bond–bond connections among graphene sheets is still insufficient, which leaves us an open question. Herein, our main topic is to investigate the in-plane interfacial thermal transport among graphene nanoribbons linked by organic (–OOC–C$_6$H$_4$–COO–, –OOC–C$_4$H$_6$–COO–, –O–C$_6$H$_4$–COO–), metal (–Al–, –Cr–, –Mo–) and metal-oxide groups (–O–Al–O–) using density functional theory (DFT) and non-equilibrium Green’s function method. The thermal conductance enhancement induced by chemical bond–bond connection is mirrored in the phononic transmission.

II. MODEL AND COMPUTATIONAL METHOD

In this work, we adopt (hydrogenated) graphene nanoribbons instead of graphene sheets, since these two systems exhibit similar thermal transport properties and the calculations as regards monolayer nanoribbons are computationally much cheaper. Since graphene shows isotropic thermal performance in both zigzag and armchair directions, one may simply focus on one of them and here in our work the zigzag types are chosen. Fig. 1 shows the atomic structures of the hydrogenated zigzag graphene nanoribbon (h-ZGNR) linked by various bond–bond connections. It involves organic groups (–OOC–C$_6$H$_4$–COO–, –OOC–C$_4$H$_6$–COO–, –O–C$_6$H$_4$–COO–), metal (–Al–, –Cr–, –Mo–) and metal-oxide groups (–O–Al–O–) in our work. After the models are established, we first perform full ion minimization, as implemented in Quantum Espresso.\textsuperscript{36} Standard Solid State Pseudopotentials (SSSP)\textsuperscript{37} are adopted within the exchange-correlation form provided by Perdew–Burke–Ernzerhof (PBE). The plane-wave energy (charge density) cutoff is set to 50 Ry (400 Ry) with a Monkhorst–Pack $1 \times 1 \times 2$ mesh. A vacuum region of at least 12 Å is used to avoid periodic image interaction. The convergence threshold as regards the self-consistency energy is set to $10^{-6}$ Ry. The Siesta\textsuperscript{38} is used to perform the phonon calculations since it is computationally cheaper that Quantum Espresso. Even though it fails to include the accurate van der Waals (vdW) interactions in Siesta, the result is still persuasive since the bond–bond connections dominate the interfacial thermal transport in this study.

When the length scale of the system is smaller than phonon MFP in low temperature, thermal conduction is dominated by ballistic transport. For carbon materials, we get a large phonon mean free path (MFP), that is, 775 nm for graphene. It is true that phonon MFP is reduced when external chemical groups are introduced to link the graphene sheets. Since we focus simply on the interfaces, which is comparable in nanometer scale, it is reasonable to neglect the anharmonic scattering and adopt NEGF method. In addition, the thermal conductance is an intrinsic parameter of the interface, independent of the system length scale. When length scale of system becomes larger than phonon MFP, diffusive transport becomes dominant and anharmonic effect should be taken into account, which could lead to a reduced thermal conductance. Fig. 1 also describes the typical “Left lead – Conductor – Right lead” configuration in NEGF method. In this ballistic regime, thermal conductance can be calculated as described below once the interatomic force constants (IFCs) matrix is obtained.\textsuperscript{39}

First, the retarded Green’s function of the central conductor is calculated according to Eq. (1):

$$
G_r = \left[ (\omega + i\eta) - K_C - \Sigma'_L - \Sigma'_R \right]^{-1}, \tag{1}
$$

where $\omega$ is the phonon frequency, and $K_C$ is the IFCs matrix of the central conductor. The imaginary part $\eta$ is an infinitesimal; $\Sigma'$ denotes the retarded self-energy of both leads, which can be obtained through

$$
\Sigma'_L = K'_L G'_R K'_C, \quad \Sigma'_R = K'_R G'_L K'_C. \tag{2}
$$

FIG. 1. Non-equilibrium Green’s function system of the simulated model. Various kinds of interactions are considered, including van der Waals force, covalent bonds, and metallic bonds.
where \( g_L^r \) and \( g_R^r \) are the retarded surface Green’s functions of the semi-infinite left and right leads, respectively. Then, we can obtain the phonon transmission function by

\[
\Xi(\omega) = \text{Tr}(G^r \Gamma_L G^a \Gamma_R),
\]

where \( G_a = (G^r)^\dagger \) is the advanced Green’s function, and \( \Gamma_\beta = (\Sigma_\beta - \Sigma_\beta^a) \) with \( \beta = L,R \) describes the interaction between the leads and conductor.

At last, the phononic thermal conductance \( \sigma \) can be calculated according to Eq. (4):

\[
\sigma(T) = \frac{h}{2\pi A} \int_0^\infty T(\omega) \left( \frac{\partial f(\omega, T)}{\partial T} \right) d\omega,
\]

where \( h \) is the reduced Planck constant and \( f(\omega, T) \) is the Bose–Einstein distribution function. \( A \) is the cross-sectional area of the structure, computed as the width multiplies thickness. The thickness is taken as the interlayer spacing in graphite, which is 3.35 Å.

III. RESULTS AND DISCUSSION

Let us first look at the h-ZGNR systems in which the two nanoribbons are non-linked, that is, separated by vdW gap. For pristine h-ZGNR, the thermal conductance is extremely high (about 4.35 GW m\(^{-2}\) K\(^{-1}\) at 300K, as shown in Fig. 2(a)), close to that in pristine graphene). The thermal resistance \( R \), i.e., the reciprocal of conductance, is very close to zero. We can also observe a typical staircase shape of the phononic transmission for pristine h-ZGNR. As regards the interaction strength, the vdW force is much weaker than the chemical bonding. Therefore, the phononic thermal conductance declines exponentially as the gap gets larger. In numbers, it falls from 1.12 GW \cdot m\(^{-2}\) \cdot K\(^{-1}\) to 3.7 \times 10^{-3} \text{ GW} \cdot \text{m}^{-2} \cdot \text{K}^{-1} at 300K as the gap increases from 0.5 Å to 5.8 Å. Thermal resistance is thus largely increased, also reflected from the overall suppression of phononic transmission at each phonon mode, as shown in Fig. 2 (b, c). For h-ZGNR with a gap larger than 2.7 Å, most modes possess a zero phononic transmission (note that we get a fractional transmission in the linked systems since the lead and the scattering region are different in their NEGF models), indicating that phonon vibration can barely pass through the vdW gap.

In the next step we turned to the interfacial thermal conductance for different linked system (ribbon width = 4), as plotted as a function of temperature in Fig. 3 (a). A monotonous increase in thermal conductance upon increasing cooperating temperature can be observed in all systems. That is because the high-frequency phonon modes can only be excited to participate in the heat transfer process at a higher temperature. To ensure a numerical comparison, a so-called thermal reserving ratio is defined as \( \delta = \frac{\sigma_1}{\sigma_0} \times 100\% \) where \( \sigma_1 \) and \( \sigma_0 \) denote the thermal conductance for bonded and pristine h-ZGNR, respectively. At all temperature range, the systems bonded with metal groups possess higher thermal conductance than the others. In addition, the thermal transport behaviors are similar at low temperature for various metals. As observed from Fig. 3(b), we got the highest thermal conductance \( \sigma_{\text{Al}} \) at [0 K, 20 K] range in the Al– bonded h-ZGNR. The \( \sigma_{\text{Mo} \ldots} \) surpasses \( \sigma_{\text{Al}} \) at [2 K, 51 K]. At temperature > 170 K, the trend displays as \( \sigma_{\text{Al}} > \sigma_{\text{Mo} \ldots} > \sigma_{\text{Cr} \ldots} \). In numbers, thermal conductance of –Al–, –Mo– and –Cr– bonded systems at 300 K are 0.577, 0.487 and 0.528 GW m\(^{-2}\) K\(^{-1}\), respectively, with a reserving ratio of 11.1% – 13.2%. As for metal oxide group, the thermal conductance of –O–Al–O– bonded system is comparable to organic groups bonded system but displays a slower increase upon temperature. Among organic groups bonded system, thermal
A lower spatial size in metal results in a shorter distance between the two h-ZGNRs. Even though the introduction of metal increases the phonon scattering, a small portion of the phonon modes can still pass on effectively through the vdW gap. As for –O–Al– and –OOC–C₂H₄–COO– bonded system, the gap distances are 3.56 Å and 6.33 Å, respectively. These are larger than 2.7 Å, which means the effective phonon vibrations can only pass on via the bond connection, rather than vdW interaction.

The thermal transport behavior in Fig. 3 can also be mirrored in their phononic transmission functions $\Xi$, as plotted in Fig. 4. In the metal group bonded systems, $\Xi_{\text{Cr}}$ and $\Xi_{\text{Mo}}$ shares the similar pattern at [250 cm⁻¹, 1000 cm⁻¹], seemingly because of the same $d$ orbitals in the valence shell Cr and Mo while the $\Xi_{\text{Al}}$ is quite different since Al forms a p subshell. The transmission function displays as $\Xi_{\text{Al}} > \Xi_{\text{Mo}} > \Xi_{\text{Cr}}$ at $\omega > 250$ cm⁻¹. The amplitude is not proportional to the atom mass ($m_{\text{Al}} = 26.98$ u, $m_{\text{Cr}} = 51.996$ u, $m_{\text{Mo}} = 95.94$ u, u is the atomic mass unit), which may not be the key factor that deduces the thermal conductance.

For the bonded systems, say, via the metal groups, the difference lies in the carbon–metal bond. The force constant $K_{ij}$ matrix between carbon $i$ and metal $j$ in the carbon–metal bond is:

$$K_{ij} = \begin{pmatrix} K_{ix, jx} & 0 & 0 \\ 0 & K_{iy, jy} & K_{iy, jz} \\ 0 & K_{iz, jy} & K_{iz, jz} \end{pmatrix}. \tag{5}$$

Due to the tensor nature in force constant matrix, direct comparison is impossible. Fortunately, the bond strength can be reflected from its largest component $K_{iz,jz}$. The $|K_{iz,jz}|$ for Al–C, Cr–C and Mo–C are 10.48, 7.127 and 7.977 eV/Å², respectively. The largest (smallest) value is found in the Al–C (Cr–C) bond, which agrees nicely with the thermal conductance. It indicates that the bond strength plays a key role in transporting middle-frequency phonon modes and thus determines the thermal conductance.

Unlike metal group bonded systems, the transmission functions in the systems bonded with organic and metal oxide groups are smaller at low-frequency region, especially at [0 cm⁻¹, 50 cm⁻¹]. That conductance of the –OOC–C₂H₄–COO– bonded system, thermal conductance between two graphene sheets is 2 orders of magnitude larger than that in unlinked system that harbors a gap distance of 6.17 Å. The enhancement resulting from the organic group connection is much more significant because of the larger gap distance and the weaker effective interfacial phonon vibrations. These results can partly explain the transport behaviors in Fig. 3. The gap distances in –Al–, –Mo– and –Cr– bonded systems are 1.85, 1.77 and 1.70 Å, respectively.

| System          | Gap distance $d$ (Å) | $\sigma$ (GW m⁻² K⁻¹) |
|-----------------|----------------------|-----------------------|
| –Al–            | 1.85                 | 0.577                 |
| non-linked      | 2.02                 | 0.101                 |
| –O–Al–O–        | 3.56                 | 0.276                 |
| non-linked      | 3.69                 | 0.005                 |
| –OOC–C₂H₄–COO–  | 6.33                 | 0.352                 |
| non-linked      | 6.17                 | 0.002                 |

\[\text{TABLE I. Thermal conductance } \sigma \text{ of bonded and non-linked h-ZGNRs. } d \text{ is the distance between two graphene sheets.}\]
FIG. 4. Phononic transmission function $\Xi$ of pristine h-ZGNR and bonded h-ZGNRs, plotted as a function of frequency $\omega$. Inset: Phononic transmission at the range of [0, 100 cm$^{-1}$].

is because it fails to activate the low-frequency phonon channels that are particularly important for thermal transport at room temperature. In addition, these systems exhibit a transmission degeneration at high-frequency region together with a lower cutoff frequency. It well explains their lower thermal conductance. The normal thermal conductance in the –O–C$_6$H$_4$–COO– bonded structure can be explained from two aspects. First, the –O–C$_6$H$_4$–COO– group structurally resembles–OOC–C$_6$H$_4$–COO– by removing a carbonyl and thus becomes much more rigid. The phonon transmission is thus suppressed, especially at low-frequency region (in Fig. 4). Second, the gap distance of 7.4 Å in the –OOC–C$_6$H$_4$–COO– bonded system is far larger than 2.7 Å, which results in negligible enhancement in the phonon transport.

Here our study is based on ideal assumptions of extended molecular chain and coplanar graphene leads, which is experimentally challenging. For compressed molecular chain, the presence of gauche defects will increase phonon scattering and reduce the thermal conductance. Gutierrez et al. found mismatch between the plane of polyaromatic molecular and graphene leads makes the thermal conductance insensitive to molecular in-plane stiffening. The misalignment of the leads can also lead to a reduction of thermal conduction. In the study of Li et al., they compared coplanar graphene leads with orthogonal graphene leads, finding the latter possesses suppressed phononic transmission function and lower thermal conductance (reduced by 23% at 600K).

IV. CONCLUSION

In summary, we investigated the thermal transport across the interface of bond connected graphene nanoribbon sheets using DFT and NEGF method. Our result shows that chemical bond–bond connection can greatly enhance the thermal transport. In the metal bonded system, thermal transport is insensitive to the type of metal atom. Thermal conductance is as high as 13.2% of pristine graphene sheets at room temperature as –Al– bond connection is adopted. Analysis on the phonon transmission function shows that it results from both the small gap distance and the activation of low-frequency phonon channels. In the organic group bonded systems, the structural rigidity hinders the thermal transport since most of the phonon vibrations can only pass on via the organic molecular chain. The thermal conductance can be 2 orders of magnitude larger than non-linked system when –OOC–C$_6$H$_4$–COO– is adopted. Our findings have provided a guidance on using chemical bond–bond connection to enhance the interfacial thermal transport between graphene sheets and improve their thermal performance in practical applications.

SUPPLEMENTARY MATERIAL

See supplementary material for the detailed interatomic force constant $K_{ij}$.

ACKNOWLEDGMENTS

The authors gratefully acknowledge the financial support from the National Natural Science Foundation of China (Grant No. 51676212), the Pearl River S&T Nova Program of Guangzhou (Grant No. 201710010043). One of the authors, K. X. Chen, thanks the support from Alexander von Humboldt foundation. The simulation work was supported by the National Supercomputer Center in Guangzhou and the high-performance grid computing platform at Sun Yat-sen University.

REFERENCES

1H. F. Hamann, A. Weger, J. A. Lacey, Z. G. Hu, E. Cohen, and J. Wakil, IEEE Journal of Solid-State Circuits 42, 56 (2007).
2E. Pop, Nano Research 3, 147 (2010).
3K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, Y. Zhang, S. V. Dubonos, I. V. Grigorieva, and A. A. Firsov, Science 306, 666 (2004).
4A. K. Geim, Science 324, 1530 (2009).
5C. Lee, X. D. Wei, J. W. Kysar, and J. Hone, Science 321, 385 (2008).
6K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, M. I. Katsnelson, I. V. Grigorieva, S. V. Dubonos, and A. A. Firsov, Nature 438, 197 (2005).
7A. A. Balandin, S. Ghosh, W. Z. Bao, I. Calizo, D. Teweldebrhan, F. Miao, and C. N. Lau, Nano Letters 8, 902 (2008).
8S. Ghosh, I. Calizo, D. Teweldebrhan, E. P. Pokatilov, D. L. Nika, A. A. Balandin, W. Bao, F. Miao, and C. N. Lau, Applied Physics Letters 92, 151911 (2008).
9A. A. Balandin, Nature Materials 10, 569 (2011).
10D. L. Nika and A. A. Balandin, Reports on Progress in Physics 80, 036502 (2017).
11 E. Pop, V. Varshney, and A. K. Roy, Mrs Bulletin 37, 1273 (2012).
12 Y. Xu, Z. Y. Li, and W. H. Duan, Small 10, 2182 (2014).
13 K. M. F. Shahil and A. A. Balandin, Solid State Communications 152, 1331 (2012).
14 H. F. Song, J. M. Liu, B. L. Liu, J. Q. Wu, H. M. Cheng, and F. Y. Kang, Joule 2, 442 (2018).
15 G. K. Zhao, X. M. Li, M. R. Huang, Z. Zhen, Y. J. Zhong, Q. Chen, X. L. Zhao, Y. J. He, R. R. Hu, T. T. Yang et al., Chemical Society Reviews 46, 4417 (2017).
16 F. An, X. F. Li, P. Min, P. F. Liu, Z. G. Jiang, and Z. Z. Yu, ACS Applied Materials & Interfaces 10, 17383 (2018).
17 F. Kargar, Z. Barani, R. Salgado, B. Debnath, J. S. Lewis, E. Aytan, R. K. Lake, and A. A. Balandin, ACS Applied Materials & Interfaces 10, 37555 (2018).
18 F. Kargar, Z. Barani, M. Balinskiy, A. S. Magana, J. S. Lewis, and A. A. Balandin, Advanced Electronic Materials 5, 1800558 (2019).
19 J. S. Lewis, Z. Barani, A. S. Magana, F. Kargar, and A. A. Balandin, Materials Research Express 6, 085325 (2019).
20 Z. Q. Wang, R. G. Xie, C. T. Bui, D. Liu, X. X. Ni, B. W. Li, and J. T. L. Thong, Nano Letters 11, 113 (2011).
21 T. Ma, Z. B. Liu, J. X. Wen, Y. F. Gao, X. B. Ren, H. J. Chen, C. H. Jin, X. L. Ma, N. S. Xu, H. M. Cheng et al., Nature Communications 8, 14486 (2017).
22 Z. L. Wang, J. Li, and K. P. Yuan, International Journal of Thermal Sciences 132, 589 (2018).
23 C. C. Deng, X. X. Yu, X. M. Huang, and N. Yang, Journal of Heat Transfer: Transactions of the ASME 139, 054504 (2017).
24 H. X. Han, Y. Zhang, N. Wang, M. K. Samani, Y. X. Ni, Z. Y. Mijbil, M. Edwards, S. Y. Xiong, K. Saaskilahti, M. Murugesan et al., Nature Communications 7, 11281 (2016).
25 A. Di Pierro, G. Saracco, and A. Fina, Computational Materials Science 142, 255 (2018).
26 M. D. Losego, M. E. Grady, N. R. Sottos, D. G. Cahill, and P. V. Braun, Nature Materials 11, 502 (2012).
27 W. Sun, L. D. Wang, Z. Q. Yang, T. Z. Zhu, T. T. Wu, C. Dong, and G. C. Liu, Chemistry of Materials 30, 7473 (2018).
28 T. Zhang, A. R. Gans-Forrest, E. Lee, X. Q. Zhang, C. Qu, Y. S. Pang, F. Sun, and T. F. Luo, ACS Applied Materials & Interfaces 8, 33326 (2016).
29 D. M. Gutierrez, A. Di Pierro, A. Pecchia, L. M. Sandonas, R. Gutierrez, M. Bernal, R. Mortazavi, G. Cuniberti, G. Saracco, and A. Fina, Nano Research 12, 791 (2019).
30 J. C. Klockner, M. Burke, J. C. Cuevas, and F. Pauly, Physical Review B 94, 205425 (2016).
31 E. Y. Li and N. Marzari, ACS Nano 5, 9726 (2011).
32 P. M. Sudeep, T. N. Narayanan, A. Ganesan, M. M. Shajumon, H. Yang, S. Ozden, P. K. Patra, M. Pasquali, R. Vajtai, S. Ganguli et al., ACS Nano 7, 7034 (2013).
33 J. H. Seol, I. Jo, A. L. Moore, L. Lindsay, Z. H. Atiken, M. T. Pettes, X. S. Li, Z. Yao, R. Huang, D. Broideo et al., Science 328, 213 (2010).
34 W. Pan, J. L. Xiao, J. W. Zhu, C. X. Yu, G. Zhang, Z. H. Ni, K. Watanabe, T. Taniguchi, Y. Shi, and X. R. Wang, Scientific Reports 2, 893 (2012).
35 B. Liu, J. A. Baimova, C. D. Reddy, A. W. K. Law, S. V. Dmitriev, H. Wu, and K. Zhou, ACS Applied Materials & Interfaces 6, 18180 (2014).
36 P. Giannozzi, S. Baroni, N. Bonini, M. Calandra, R. Car, C. Cavazzoni, D. Ceresoli, G. L. Chiarotti, M. Cococcioni, I. Dabo et al., Journal of Physics: Condensed Matter 21, 395502 (2009).
37 K. Lejaeghere, G. Rühmayer, T. Björkman, P. Blaha, S. Blugel, V. Blum, D. Caliste, L. E. Castelli, S. I. Clark, A. Dal Corso et al., Science 351, aad3000 (2016).
38 J. M. Soler, E. Artacho, J. D. Gale, A. García, J. Junquera, P. Ordejón, and D. Sanchez-Portal, Journal of Physics: Condensed Matter 14, 2745 (2002).
39 K. X. Chen, S. S. Lyu, X. M. Wang, Y. X. Fu, Y. Heng, and D. C. Mo, Journal of Physical Chemistry C 121, 13035 (2017).
40 K. Sasikumar and P. Keblinski, Journal of Applied Physics 109, 114307 (2011).
41 Q. Li, I. Duchemin, S. Y. Xiong, G. C. Solomon, and D. Donadio, Journal of Physical Chemistry C 119, 24636 (2015).