Electron-phonon coupling and superconductivity in LiB$_{1+x}$C$_{1-x}$

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Abstract – By means of the first-principles density-functional theory calculation and Wannier interpolation, electron-phonon coupling and superconductivity are systematically explored for boron-doped LiBC (i.e., LiB$_{1+x}$C$_{1-x}$), with $x$ between 0.1 and 0.9. Hole doping introduced by boron atoms is treated through virtual-crystal approximation. For the investigated doping concentrations, our calculations show that the optimal doping concentration corresponds to 0.8. By solving the anisotropic Eliashberg equations, we find that LiB$_{1.8}$C$_{0.2}$ is a two-gap superconductor, whose superconducting transition temperature, $T_c$, may exceed the experimentally observed value of MgB$_2$. Similar to MgB$_2$, the two-dimensional bond-stretching $E_{2g}$ phonon modes along the $\Gamma$-A line have the largest contribution to electron-phonon coupling. More importantly, we find that the first two acoustic phonon modes $B_1$ and $A_1$ around the midpoint of the $K$-$\Gamma$ line play a vital role for the rise of $T_c$ in LiB$_{1.8}$C$_{0.2}$. The origin of strong couplings in $B_1$ and $A_1$ modes can be attributed to enhanced electron-phonon coupling matrix elements and softened phonons. It is revealed that all these phonon modes couple strongly with $\sigma$-bonding electronic states.

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Introduction. – The discovery of 39 K superconductivity in MgB$_2$ [1] has aroused great interest in searching for new high-temperature superconductors whose pairing glue is electron-phonon coupling (EPC). Many compounds with atomic and/or electronic structures similar to MgB$_2$ have been extensively investigated, such as $MB_2$ ($M = Be$ [2–4], Na [5], Ca [3–7], Sc [3,5], Cu [8], Sr [4,5], Y [3,5], Zr [5,9], Ag [10], Ta [5,11], Os [12], and Au [10]), CaBeSi [2], LiBC [13], and MgB$_2$C$_2$ [4]. Among these compounds, the most fascinating one is Li-deficient Li$_x$BC, whose $T_c$ is predicted to be above 100 K for $x$ equal to 0.5.

In MgB$_2$, the underlying physics for high-$T_c$ superconductivity is the strong EPC between metallic covalent $\sigma$-bonding states and high-frequency $E_{2g}$ phonons associated with bond-stretching movements of boron atoms [14–18]. For semiconducting LiBC, the valence band maximum (VBM) locates on the $\Gamma$-A line, corresponding to the $\sigma$-bonding states between boron and carbon atoms. Rosner and coworkers suggested that the $\sigma$-bonding states can be rigidly lifted up to the Fermi level by removing some Li atoms [13], forming Li$_y$BC. Thus, the electronic structure of Li$_y$BC is reminiscent of that in MgB$_2$. And the high-$T_c$ superconductivity in Li$_y$BC seems natural. But evidence for superconductivity in Li$_x$BC is not available [19–21]. As a response to Li deficiency, the boron-carbon layer has drastic lattice distortions, which diminish the hope to metalize the boron-carbon $\sigma$-bonding states [22].

Considering the importance of Li atoms in holding the crystal structure, replacing a certain amount of carbon atoms by boron atoms is regarded as a feasible way to realize hole doping in LiBC. Miao et al. used virtual-crystal approximation (VCA) to study the EPC of LiB$_{1.4}$C$_{0.9}$, and suggested that the superconducting $T_c$ is about 36 K [23]. We proposed a new compound Li$_3$B$_4$C$_2$ (i.e., LiB$_{3.3}$C$_{0.67}$), whose $T_c$ is about 53.8 K, based on the Wannier interpolation technique [24]. Another material Li$_4$B$_4$C$_3$ (LiB$_{2.5}$C$_{0.75}$), which is obtained through the substitution of a BC$_2$ layer for one honeycomb B-C layer,

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47001-p1
layer in LiBC, is calculated to be superconducting under 16.8 K [25]. Although the superconductivity in LiBC under several hole doping concentrations has been explored, it is interesting to know how high $T_c$ can go and at which doping concentration the maximal $T_c$ can be obtained in LiB$_{1+x}$C$_{1-x}$ compounds.

In this work, we employ first-principles calculation and the Wannier interpolation technique to investigate the EPC and superconductivity in LiB$_{1+x}$C$_{1-x}$, with $x$ varying from 0.1 to 0.9 to determine the optimal doping concentration. Our calculation shows that the highest $T_c$ can be achieved in LiB$_{1.8}$C$_{0.2}$. By solving the anisotropic Eliashberg equations, it is found that LiB$_{1.8}$C$_{0.2}$ is a two-gap superconductor, whose $T_c$ may exceed the one of MgB$_2$ by a few kelvins. At low doping, two-dimensional bond-stretching $E_{2g}$ phonon modes at the $\Gamma$-point possess the largest contribution to EPC. For further increasing the hole doping concentration, $B_1$ and $A_1$ phonon modes at about $k\vec{F}$ contribute enormously to the EPC, due to enhanced EPC matrix element and phonon softening.

**Methods.** In our calculations the plane-wave basis method is used [26]. We adopt the local density approximation (LDA) of Perdew-Zunger as the exchange-correlation functions. The norm-conserving pseudopotentials [27] are employed to model the electron-phonon coupling potentials. The norm-conserving pseudopotentials [27] are employed to model the electron-phonon coupling potentials. The EPC matrix element is

$$\lambda = \frac{1}{N^q_{\nu}} \sum_{q} \lambda_{\nu q} = 2 \int \frac{\alpha^2 F(\omega)}{\omega} d\omega. \quad (1)$$

The EPC constant $\lambda_{\nu q}$ for mode $\nu$ at wave vector $q$ is defined by

$$\lambda_{\nu q} = \frac{2}{\hbar N(0) N_k} \sum_{i,j,k} \sum_{q} \left[ \frac{1}{\omega_{q}^{
u}} |g_{k,\nu}^{ij}|^2 (\epsilon_{k}^{\nu}) (\epsilon_{k+q}^{\nu}) \right]. \quad (2)$$

Here $N_{q}/N_k$ is the total number of $q/k$ points in the fine Brillouin-zone mesh. $N(0)$ is the electronic density of states (DOS) at the Fermi energy. $(i, j)$ and $\nu$ denote indices of energy bands and phonon modes, respectively. $\omega_{q}^\nu$ stands for the phonon frequency of the $\nu$-th phonon mode with wave vector $q$. $g_{k,\nu}^{ij}$ is the EPC matrix element. $\epsilon_{k}^{\nu}$ and $\epsilon_{k+q}^{\nu}$ are eigenvalues of Kohn-Sham states with respect to the Fermi energy at given bands and momenta. The Eliashberg spectral function can be expressed as

$$\alpha^2 F(\omega) = \frac{1}{2} \sum_{q} \delta(\omega - \omega_{q}^\nu) \lambda_{\nu q} \omega_{q}^\nu. \quad (3)$$

Finally, the superconducting transition temperature ($T_c$) is determined by utilizing the McMillian-Allen-Dynes formula [38],

$$T_c = \frac{\omega_{\log} + 1}{2} \exp \left[ \frac{-1.04(1 + \lambda)}{\lambda(1 - 0.62\mu^*) - \mu^*} \right]. \quad (4)$$

$\mu^*$ is the effective screened Coulomb repulsion constant, namely Coulomb pseudopotential. $\omega_{\log}$ is the logarithmic average frequency, which can be computed through

$$\frac{1}{2} \int \frac{\omega}{\log \omega} d\omega.$$ 

**Result and analysis.** Figure 1 contains the band structures of LiB$_{1+x}$C$_{1-x}$. As we see, LiB$_{1.8}$C$_{0.2}$ already becomes a metal. Namely, the $\sigma$-bonding states at the

| $x$ | $a$ (Å) | $c/a$ | $N(0)$ | $\omega_{E_{2g}}$ (meV) | $\lambda$ | $\omega_{\log}$ | $T_c$ (K) |
|-----|---------|-------|--------|---------------------|-------|-------------|--------|
| 0.1 | 2.750   | 2.602 | 0.07   | 76.9                | 0.69  | 75.0        | 28.9   |
| 0.2 | 2.767   | 2.587 | 0.11   | 86.2                | 0.68  | 64.5        | 24.5   |
| 0.3 | 2.786   | 2.567 | 0.13   | 87.5                | 0.75  | 52.6        | 25.0   |
| 0.4 | 2.806   | 2.547 | 0.13   | 80.5                | 0.77  | 56.7        | 28.1   |
| 0.5 | 2.825   | 2.530 | 0.11   | 82.8                | 0.81  | 59.4        | 33.5   |
| 0.6 | 2.846   | 2.507 | 0.11   | 99.3                | 0.81  | 58.5        | 33.0   |
| 0.7 | 2.871   | 2.473 | 0.11   | 92.0                | 0.93  | 51.4        | 36.7   |
| 0.8 | 2.895   | 2.446 | 0.11   | 82.1                | 1.05  | 45.3        | 39.3   |
| 0.9 | 2.919   | 2.423 | 0.11   | 84.7                | 1.04  | 43.8        | 37.5   |

Table 1: The optimized lattice constants, $N(0)$ (states/eV/atom/spin), frequency of $E_{2g}$ (meV), $\lambda$, $\omega_{\log}$ (meV) and $T_c$ (K) for different doping concentrations.
VBM have been successfully metallized. Thus, the hole cylinders around the Γ-A line are from σ-bonding bands (right panel of fig. 1(a)). By increasing hole doping concentration, the occupied energy bands almost move upward rigidly and the volumes enclosed by Fermi surfaces expand, while the location of empty energy bands is not affected by doping. As a consequence, the energy gap is gradually reduced, and close to zero for LiB_{1-x}C_{1-x}. The blue lines are calculated by the interpolation of first principles, the red circles are obtained through MLWFs interpolated from first principles. It is noted that the empty energy bands are not included in the Wannier interpolation. The Fermi energy is set to zero.

The phonon spectra weighted by $\lambda_{\nu q}$ are shown in fig. 2. For the selected doping interval, no imaginary phonon frequency is found, indicating the dynamical stability of LiB_{1-x}C_{1-x}. The strong EPC phonon modes, corresponding to the red lines along Γ-A, are $E_{2g}$ modes, whose frequencies are listed in table 1. Although the frequency of the $E_{2g}$ mode fluctuates with the increase of the doping concentration, an overall phonon softening is observed, especially the first two acoustic phonon modes $B_1$ and $A_1$ at about $\frac{\omega}{2}$ or $\frac{\omega}{4}$ in LiB_{1-x}C_{0.2} (see fig. 2(d)). The vibrational configurations of the $E_{2g}$ mode at Γ and $B_1$ mode at $\frac{\omega}{2}$ are shown schematically in fig. 2(e) and fig. 2(f), respectively. The vibration of $A_1$ resembles that of $B_1$, but with even smaller Li displacement. All these phonon modes mainly involve the two-dimensional movements of boron and virtual atoms.

Compared with other three doping conditions, there is a very sharp peak for the Eliashberg spectral function $\alpha^2F(\omega)$ in LiB_{1.0}C_{0.9} at about 80 meV associated with the strongly coupled $E_{2g}$ phonon modes (fig. 3(a)). Nevertheless, the spectral weight from the low-frequency region is almost zero. The amplitude of $\alpha^2F(\omega)$ is gradually reduced with rising doping concentration, but the low-frequency part of $\alpha^2F(\omega)$ becomes stronger and stronger (fig. 3(b)–(d)), consistent with the emergence of strong coupling $B_1$ and $A_1$ phonon modes in the phonon spectra (fig. 2).
The calculated EPC constant \( \lambda \), logarithmic average frequency \( \omega_{\log} \), and superconducting \( T_c \) are presented in fig. 4. For clarity, these quantities are also summarized in table 1. As we see, \( \lambda \) and \( T_c \) roughly display a monotonic increase vs. the doping concentration. \( \text{LiB}_{1+x}\text{C}_{0.9} \) possesses the maximal superconducting \( T_c \) of 39.3 K, slightly higher than that in \( \text{MgB}_2 \). In the determination of \( T_c \) for \( \text{LiB}_{1+x}\text{C}_{1-x} \), the Coulomb pseudopotential \( \mu^\ast \) is set to 0.1. As pointed out in ref. [39], an enhanced \( N(0) \) can lead to an enhanced Coulomb pseudopotential. For most doping concentrations, the \( N(0) \) of \( \text{LiB}_{1+x}\text{C}_{1-x} \) is around 0.11 states/eV/atom/spin (see table 1). Thus, the usage of a single \( \mu^\ast \), i.e., 0.1, for all the doping concentrations is reasonable. Interestingly, \( N(0) \) is also equal to 0.11 states/eV/atom/spin in \( \text{MgB}_2 \) from our Wannier interpolation.

Since \( \text{LiB}_{1.1}\text{C}_{0.9} \) has the largest \( \lambda_{\nu} \) from \( E_{2g} \) modes among these four doping situations along the \( \Gamma-A \) line (fig. 2(a)), it is surprising that the smallest \( \lambda \) is found in \( \text{LiB}_{1.1}\text{C}_{0.9} \). This suggests that there exist sizeable \( \lambda_{\nu} \)'s, which are not clearly reflected along the high-symmetry line in other three doping levels. To unambiguously confirm the above assumption, we plot \( \lambda(\mathbf{q}_{2D}) \), defined by \( \sum_{\mathbf{q},\nu} \lambda_{\nu} \), in the reduced two-dimensional (2D) Brillouin zone (fig. 5). Even though there is a big red spot around the \( \Gamma \)-point in \( \text{LiB}_{1.1}\text{C}_{0.9} \), \( \lambda(\mathbf{q}_{2D}) \) is close to zero in another area of the Brillouin zone (fig. 5(a)). In sharp contrast, considerable \( \lambda(\mathbf{q}_{2D}) \) emerges beside the \( \Gamma \)-point, especially for \( \text{LiB}_{1.8}\text{C}_{0.2} \) (fig. 5(d)), in which six bright spots obviously appear at \( \frac{2\pi}{a} \) and its equivalent points. These spots exactly come from the \( B_1 \) and \( A_1 \) phonon modes (fig. 2(d)), which thus have vital importance for the enhancement of \( \lambda \) and \( T_c \) upon the increase of hole doping.

In order to identify the origin of the strong EPC \( B_1 \) and \( A_1 \) phonon modes, we calculate \( \xi(\mathbf{q}) \) and \( \gamma(\mathbf{q}) \), which read

\[
\xi(\mathbf{q}) = \frac{1}{N_k} \sum_{ij} \delta(\epsilon^i_k)\delta(\epsilon^j_{k+\mathbf{q}})
\]

and

\[
\gamma(\mathbf{q}) = \frac{1}{N_k} \sum_{ij} |g^{ij}_{k\mathbf{q}}|^2 \delta(\epsilon^i_k)\delta(\epsilon^j_{k+\mathbf{q}}),
\]

respectively. \( \xi(\mathbf{q}) \) is the Fermi surface nesting function. \( \gamma(\mathbf{q}) \) is the summation of the EPC matrix element \( |g^{ij}_{k\mathbf{q}}|^2 \) around the Fermi level. \( \xi(\mathbf{q}) \) is almost the same with each other for the studied cases (fig. 6(a)). This indicates that the Fermi surface nesting function \( \xi(\mathbf{q}) \) is not a dominant factor for strong EPC in the \( B_1 \) and \( A_1 \) modes. We find that there are humps in \( \gamma(\mathbf{q}) \) at the middle point of \( K-\Gamma \) or \( H-A \) for the later three concentrations (fig. 6(b)), reflecting the aggrandizement of EPC matrix elements around the Fermi level. These humps are further amplified in \( \lambda(\mathbf{q}) \) by phonon softening (fig. 6(c) and fig. 2(d)). Thus, both enhanced EPC matrix element \( |g^{ij}_{k\mathbf{q}}|^2 \) and softened \( B_1 \) and \( A_1 \) phonon modes account for the occurrence of strong EPC.

Another important question should be addressed is which electrons strongly couple with the \( E_{2g} \) mode at \( \Gamma \) and the \( B_1/A_1 \) mode at \( \frac{2\pi}{a} \). Here we introduce a new quantity \( \lambda_{ki} \), which represents the EPC constant at a given momentum \( \mathbf{k} \) and band \( i \),

\[
\lambda_{ki} = \frac{2}{\hbar N(0)} \sum_{\mathbf{q},\nu} \frac{1}{\omega_{\nu\mathbf{q}}} |g^{ij}_{k\mathbf{q}}|^2 \delta(\epsilon^i_k)\delta(\epsilon^j_{k+\mathbf{q}}).
\]
Here $j$ is also the index of the electronic energy band. By specifying the phonon wave vector $\mathbf{q}$, one can explicitly determine the electronic states that have large coupling with phonon modes at this wave vector. To be specific, we calculate $\lambda_{\mathbf{k} \mathbf{q}}$ in LiB$_{1.8}$C$_{0.2}$ for $\mathbf{q}$ being $\Gamma$ and $\frac{\pi}{2\Gamma}$, respectively (fig. 7). It is found that the $E_{2\Gamma}$ phonon mode mainly couples with the cylinder-like hole Fermi surfaces around the $\Gamma$-$A$ line (fig. 7(a)–(d)). This is also the case for the $B_1$ and $A_1$ modes (fig. 7(e)–(h)). As we know, these cylindrical Fermi surfaces correspond to the B-X $\sigma$ bonding bands. So the high-$T_c$ superconductivity in LiB$_{1+x}$C$_{1-x}$ originates from strong coupling between phonon modes (i.e., $E_{2\Gamma}$ mode at $\Gamma$ and $B_1/A_1$ mode at $\frac{\pi}{2\Gamma}$) and B-X $\sigma$-bonding bands.

With respect to the semi-empirical McMillan-Allen-Dynes formula, superconducting $T_c$ can also be determined by solving the anisotropic Eliashberg equations. Besides $T_c$, this method can provide more information about the superconducting gap structure. For example, the two-gap structure in MgB$_2$ is clearly revealed by anisotropic Eliashberg calculations [40–43]. Bekker et al. further studied the novel superconducting gap resulted from the surface state in monolayer MgB$_2$ [44] or few-layer MgB$_2$ [45]. For the sake of making $T_c$ in LiB$_{1+x}$C$_{1-x}$ more reasonable, we solve the anisotropic Eliashberg equations along the imaginary axis for LiB$_{1.8}$C$_{0.2}$. The superconducting gaps are determined from the approximate Padé continuation, and the Coulomb potential is chosen to be 0.16. The reason for using 0.16 is to directly compare our result with that of MgB$_2$ given in refs. [36,40]. We can identify two distinct sets of superconducting gaps for LiB$_{1.8}$C$_{0.2}$ (fig. 8(a)), which are associated with the $\sigma$ and the $\pi$ sheets of the Fermi surface (fig. 8(b)). By taking the Fermi surface averages, these gaps are $\Delta_{\pi} = 2.8$ meV and $\Delta_{\sigma} = 9.5$ meV at 10 K, which are about 12% and 5.6% larger than that in MgB$_2$ [36], respectively. The two superconducting gaps vanish at 58 K, which is 7 K higher than the value of MgB$_2$ obtained by ref. [36] with the same calculation method. It is noteworthy that the anharmonic effect of phonons should be taken into consideration to reconcile the theoretically calculated $T_c$ with the experimentally observed one for MgB$_2$ [42,43,46]. But the investigation of the anharmonic effect in LiB$_{1+x}$C$_{1-x}$ is not the purpose of this work. The hot zones of anisotropic electron-phonon coupling strength $\lambda$ are mainly distributed on the $\sigma$ Fermi sheets (fig. 8(b)). This further confirms the results presented in fig. 7.

**Discussion and conclusion.** – The sampling points contained in our fine k-mesh for electrons and q-mesh for phonons are 42 times more than those used in previous simulations of LiB$_{1.1}$C$_{0.9}$ [23]. Thus, our $T_c$ of LiB$_{1.1}$C$_{0.9}$ should be more reliable. It is noted that superconducting $T_c$ of Li$_3$B$_4$C$_2$ [24] or Li$_4$B$_5$C$_3$ [25] is different from the trend determined in our calculations. The reasons for this inconsistency are twofold. Firstly, the distribution of boron and carbon atoms in LiB$_{1+x}$C$_{1-x}$ is not included in the VCA. Different distributions will result in different electronic states, phonons, and $T_c$. Secondly, the crystal structures used by Li$_3$B$_4$C$_2$ and Li$_4$B$_5$C$_3$ may be not the ground-state structures at corresponding stoichiometry.
Considering that several intelligent crystal structure prediction methods have been developed, such as random sampling method [47], particle-swarm optimization [48], and evolutionary technique [49], the ground-state structure of LiB$_{1.5}$C$_{0.5}$ is called for to verify our prediction.

In conclusion, we have extensively studied the EPC and phonon-mediated superconductivity for boron-doped LiBC, utilizing the first-principles calculations and evolutionary technique [49], the ground-state structure methods have been developed, such as random sampling method [47], particle-swarm optimization [48], and evolutionary technique [49], the ground-state structure of LiB$_{1.5}$C$_{0.5}$ is called for to verify our prediction.

Since the reliability of Wannier interpolation strongly depends on the localizations of the electronic Hamiltonian, the dynamical matrix, and the EPC matrix element in the Wannier representation, we have carefully examined the above quantities, which demonstrate excellent exponential decay (fig. 9). Three sets of fine k-meshes (i.e., $48 \times 48$, $60 \times 60 \times 40$, and $72 \times 72 \times 48$) are used to check at which smearing $\sigma$ the $\lambda$ is convergent (fig. 10). As $\sigma$ approaches the zero limit, the curves of $\lambda$ calculated by the two denser k-meshes begin to bifurcate for $\sigma$ being 125 meV (fig. 10(c)). Thus, we regard the EPC properties gained at 125 meV as the convergent ones, which have been presented in the main text. It is noted that the convergence of k-dependent superconducting gap $\Delta_{ki}$ is more challenging than for $\lambda$. As shown by Margine et al., the energy distribution of the $\sigma$ gap changes from 2.5 meV to 1.5 meV when increasing the fine $q$-mesh from 20$^3$ to 40$^3$, but the value of $\lambda$ is not affected [40]. Here, careful examination of the convergence of $\Delta_{ki}$ is not actualized, we adopt directly the convergent parameters for $\lambda$ to calculate the superconducting gap (fig. 8).

**REFERENCES**

[1] Nagamatsu J. et al., Nature (London), 410 (2001) 63.
[2] Satta G., Profeta G., Bernardini F., Continenza A. and Massidda S., Phys. Rev. B, 64 (2001) 104507.
[3] Medvedeva N. I., Ivanovskii A. L., Medvedeva J. E. and Freeman A. J., Phys. Rev. B, 64 (2001) 020502(R).
[4] Ravindran P., Vajeeston P., Vidya R., Kjekshus A. and Fjellvåg H., Phys. Rev. B, 64 (2001) 224509.
[5] Oguchi T., J. Phys. Soc. Jpn., 71 (2002) 1495.
[6] Medvedeva N. I., Medvedeva J. E., Ivanovskii A. L., Zubkov V. G. and Freeman A. J., JETP Lett., 73 (2001) 336.
[7] Choi H. J., Louie S. G. and Cohen M. L., Phys. Rev. B, 80 (2009) 064503.

47001-p6
Electron-phonon coupling and superconductivity in LiB$_{1+2}C_{1-x}$

[8] Mehl M. J., Papaconstantopoulos D. A. and Singh D. J., Phys. Rev. B, 64 (2001) 140509(R).
[9] Gasparov V. A., Sidorov N. S., Zverkova I. I. and Kulakov M. P., JETP Lett., 73 (2001) 532.
[10] Kwon S. K., Youn S. J., Kim K. S. and Min B. I., arXiv:cond-mat/0106483.
[11] Rosner H., Pickett W. E., Drechsler S.-L., Handstein A., Behr G., Fuchs G., Nenkov K., Miller K.-H. and Eschrig H., Phys. Rev. B, 64 (2001) 144516.
[12] Singh Y., Niazi A., Vannette M. D., Prozorov R. and Johnston D. C., Phys. Rev. B, 76 (2007) 214510.
[13] Rosner H., Kitaigorodsky A. and Pickett W. E., Phys. Rev. Lett., 88 (2002) 127001.
[14] An J. M. and Pickett W. E., Phys. Rev. Lett., 86 (2001) 4366.
[15] Kong Y., Dolgov O. V., Jepsen O. and Andersen O. K., Phys. Rev. B, 64 (2001) 020501(R).
[16] Yildirim T. et al., Phys. Rev. Lett., 87 (2001) 037001.
[17] Choi H. J., Roundy D., Sun H., Cohen M. L. and Louie S. G., Phys. Rev. B, 66 (2002) 020513.
[18] Choi H. J., Roundy D., Sun H., Cohen M. L. and Louie S. G., Nature, 418 (2002) 758.
[19] Bharathi A. et al., Solid State Commun., 124 (2002) 423.
[20] Soutpela D., Hessaini B., Behra G., Lösera W. and Geibel C., Solid State Commun., 125 (2003) 17.
[21] Fogg A. M., Chalker P. R., Claridge J. B., Darling G. R. and Rosseinsky M. J., Phys. Rev. B, 67 (2003) 245106.
[22] Fogg A. M., Meldrum J., Darling G. R., Claridge J. B. and Rosseinsky M. J., J. Am. Chem. Soc., 128 (2006) 10043.
[23] Miao R. et al., J. Appl. Phys., 113 (2013) 133910.
[24] Gao M., Lu Z.-Y. and Xiang T., Phys. Rev. B, 91 (2015) 045132.
[25] Bazihiro T., Sakai Y., Saito S. and Cohen M. L., Phys. Rev. B, 89 (2014) 045136.
[26] Giannozzi P. et al., J. Phys.: Condens. Matter, 21 (2009) 205502.
[27] Troullier N. and Martins J. L., Phys. Rev. B, 43 (1991) 1993.
[28] Methfessel M. and Paxton A. T., Phys. Rev. B, 40 (1989) 3616.
[29] Giustino F., Cohen M. L. and Louie S. G., Phys. Rev. B, 76 (2007) 165108.
[30] Baroni S., Giannozzi P. and Corso A. D., Rev. Mod. Phys., 73 (2001) 515.
[31] Marzari N. and Vanderbilt D., Phys. Rev. B, 56 (1997) 12847.
[32] Souza I., Marzari N. and Vanderbilt D., Phys. Rev. B, 65 (2001) 035109.
[33] Mostofi A. A., Yates J. R., Lee Y.-S., Souza I., Vanderbilt D. and Marzari N., Comput. Phys. Commun., 178 (2008) 685.
[34] Mostofi A. A., Yates J. R., Pizzi G., Lee Y.-S., Souza I., Vanderbilt D. and Marzari N., Comput. Phys. Commun., 185 (2014) 2309.
[35] Noffsinger J., Giustino F., Malone B. D., Park C.-H., Louie S. G. and Cohen M. L., Comput. Phys. Commun., 181 (2010) 2140.
[36] Poncè S., Margine E. R., Verdi C. and Giustino F., Comput. Phys. Commun., 209 (2016) 116.
[37] Allen P. B., Phys. Rev. B, 6 (1972) 2577.
[38] Allen P. B. and Dynes R. C., Phys. Rev. B, 12 (1975) 905.
[39] Jin Y.-G. and Chang K. J., Phys. Rev. B, 57 (1998) 14684.
[40] Margine E. R. and Giustino F., Phys. Rev. B, 87 (2013) 024505.
[41] Aperis A., Maldonado P. and Oppeneer P. M., Phys. Rev. B, 92 (2015) 054516.
[42] Choi H. J., Roundy D., Sun H., Cohen M. L. and Louie S. G., Phys. Rev. B, 66 (2002) 020513(R).
[43] Choi H. J., Roundy D., Sun H., Cohen M. L. and Louie S. G., Nature, 418 (2002) 758.
[44] Bekker J., Aperis A., Partoens B., Oppeneer P. M. and Milošević M. V., Phys. Rev. B, 96 (2017) 094510.
[45] Bekker J. et al., Sci. Rep., 7 (2017) 14458.
[46] Yildirim T. et al., Phys. Rev. Lett., 87 (2001) 037001.
[47] Pickard C. J. and Needs R., J. Phys.: Condens. Matter, 23 (2011) 053201.
[48] Wang Y., Lv J., Zhu L. and Ma Y., Phys. Rev. B, 82 (2010) 094116.
[49] Oganov A. R. and Glass C. W., J. Chem. Phys., 124 (2006) 244704.