Temperature dependent elastic constants and thermodynamic properties of BAs: an ab-initio investigation.

Cristiano Malica\textsuperscript{1,*} and Andrea Dal Corso\textsuperscript{1,2}

\textsuperscript{1}International School for Advanced Studies (SISSA), Via Bonomea 265, 34136 Trieste (Italy).
\textsuperscript{2}IOM-CNR 34136 Trieste (Italy).

(Dated: 22 June 2020)

We present an ab-initio study of the temperature dependent elastic constants of boron arsenide (BAs), a semiconductor that exhibits ultra-high thermal conductivity and is under investigation for thermal management in electronics. We test the consistency of our predictions by computing the temperature dependent sound velocity of the longitudinal acoustic mode along the [111] direction and comparing with experiment. Furthermore, as a byproduct, we present the room temperature phonon dispersions, and the temperature dependent thermal expansion, isobaric heat capacity, and average Grüneisen parameter comparing with the most updated experiments and previous calculations when available. Finally, we present the theoretical estimate of the temperature dependent mean square atomic displacements.

I. INTRODUCTION

Boron arsenide (BAs) is a promising semiconductor for its high thermal conductivity at room temperature (RT) that makes it a possible candidate for applications in electronics and photonics that require efficient heat dissipation from hot spots in devices. Although the growth of BAs was reported since 1950s, only recently high-quality samples have been synthesized with the measurement of an ultrahigh thermal conductivity up to 1300 W m$^{-1}$K$^{-1}$\textsuperscript{11}. These measurements spurred the interest for this material so that many experiments and theoretical calculations have been carried out to investigate its physical properties. BAs has a zinc-blende cubic structure and belongs to the space group $F\bar{4}3m$\textsuperscript{24}. Recent measurements, supported by ab-initio calculations, range from the lattice constant and thermal expansion (TE), to the band gap and refractive index, to the elastic constants (EC) and the bulk modulus\textsuperscript{5,6,8–12}. The EC are important quantities to describe the mechanical and thermodynamic properties of materials since they allow the check of the crystal stability, determine the speeds of sound, and can be used to compute the TE and the thermal stresses. At $T=0$ K the ECs of BAs have been computed in several works by means of density functional theory (DFT) using several exchange and correlation functionals\textsuperscript{568–12}. However, in literature, the information about the effect of temperature on the ECs is rather indirect. Kang et al.\textsuperscript{6} reported the measured speed of sound of the longitudinal acoustic mode along the [111] direction from $T=80$ K to $T=500$ K showing a decrease of about 2.4 %, but no theoretical calculation is available to support this measurement and in general to estimate the temperature dependent elastic constants (TDECs) of BAs.

We have recently implemented in the thermo\_pw code\textsuperscript{13} the calculation of the TDECs both isothermal and adiabatic. The TDECs can be computed from second derivatives of the Helmholtz free-energy within the quasi-harmonic approximation (QHA) by means of density functional theory (DFT) and density functional perturbation theory (DFPT). In this paper we apply the calculation of TDECs to BAs. We found that in the range of temperature $0 – 1800$ K the percentage softening of adiabatic ECs is $\approx 11$ % for $C_{11}$, $\approx 9$ % for $C_{12}$ and $\approx 13$ % for $C_{44}$. In the range of temperature $0 – 800$ K the softening is comparable but slightly smaller than the one of silicon.

As a byproduct of our calculation we report the RT phonon dispersions of BAs comparing with the inelastic X-ray scattering measurements and the temperature dependence of several other thermodynamic quantities such as the TE, the isobaric heat capacity, the average Grüneisen parameter, and the atomic B-factors (BFs). We compare these quantities with experimental data and previous calculations when available. In general, the agreement is quite good.

II. THEORY

The calculation of the TDECs within the QHA is explained in detail in our recent work\textsuperscript{13}. In this section we limit ourselves to a summary of the most important formulas in order to make the paper self-contained.

The isothermal ECs are obtained from the derivatives of the Helmholtz free-energy $F$ with respect to strain $\varepsilon$:

$$\tilde{C}_{ijkl}^T = \frac{1}{\Omega} \left( \frac{\partial^2 F}{\partial \varepsilon_{ij} \partial \varepsilon_{kl}} \right)_{\varepsilon=0}. \quad (1)$$

Since we are usually interested in the ECs obtained from the stress-strain relationship ($C_{ijkl}^T$) we correct the $\tilde{C}_{ijkl}^T$ when the system is under a pressure $p$ as:

$$C_{ijkl}^T = \tilde{C}_{ijkl}^T + 12p \left( 2\delta_{ij}\delta_{kl} - \delta_{ik}\delta_{jl} - \delta_{il}\delta_{jk} \right). \quad (2)$$

The Helmholtz free-energy of Eq.\textsuperscript{11} is obtained as the sum of the DFT total energy $U$ and the vibrational free energy (neglecting the electronic contribution): $F = U + F_{vib}$. The latter is given by:

$$F_{vib}(\varepsilon, T) = \frac{1}{2N} \sum_{\vec{q}\eta} \hbar \omega_{\eta}(\vec{q}, \varepsilon) + \frac{k_B T}{N} \sum_{\vec{q}\eta} \ln \left[ 1 - \exp \left( -\frac{\hbar \omega_{\eta}(\vec{q}, \varepsilon)}{k_B T} \right) \right], \quad (3)$$

\textsuperscript{*}Electronic mail: cmalica@sissa.it

\textsuperscript{13}arXiv:2006.11143v1 [cond-mat.mtrl-sci] 19 Jun 2020
where $N$ is the number of cells in the crystal, $\omega_\eta(\mathbf{q}, \varepsilon)$ is the phonon angular frequency of the mode $\eta$ with wave-vector $\mathbf{q}$ computed in the system with a strain $\varepsilon$. Cubic solids have three independent ECs that in Voigt notations are $C_{11}$, $C_{12}$, and $C_{44}$. The QHA calculation of the ECs, Eq. [1] is performed on a grid of reference geometries by varying the lattice constant $a_0$. Phonon dispersions are computed in the same grid in order to evaluate the free-energy as a function of the volume, minimize it and obtain the temperature dependent crystal parameter $a(T)$ [13,10]. Then, at each temperature $T$, the TDECs as a function of $a_0$ are interpolated and evaluated at $a(T)$. The calculation requires phonon dispersions in all the strained configurations for all the reference geometries, in addition to the phonon dispersions used to compute $a(T)$.

The temperature dependent lattice parameter $a(T)$ can be used to derive the TE $\alpha$ as:

$$\alpha = \frac{1}{a(T)} \frac{da(T)}{dT}. \quad (4)$$

The isochoric heat capacity within the harmonic approximation is given by:

$$C_V = \frac{k_B}{N} \sum_{\mathbf{q}, \eta} \left( \frac{\hbar \omega_\eta(\mathbf{q})}{k_B T} \right)^2 \frac{\exp(\hbar \omega_\eta(\mathbf{q})/k_B T)}{[\exp(\hbar \omega_\eta(\mathbf{q})/k_B T) - 1]^2}. \quad (5)$$

It is computed for each reference geometry and it is interpolated at $a(T)$. The knowledge of $\alpha$ and $C_V$ allows to compute the isobaric heat capacity $C_P$ and the average Grüneisen parameter $\gamma$:

$$C_P = C_V + T \Omega \beta^2 B^T, \quad (6)$$

$$\gamma = \frac{\Omega \beta B^T}{C_V}, \quad (7)$$

where $\Omega$ is the volume of one unit cell at the temperature $T$, $\beta = 3\alpha$ is the volume TE and $B^T$ is the isothermal bulk modulus calculated from the ECs as:

$$B^T = \frac{1}{3} \left( C^T_{11} + 2C^T_{12} \right). \quad (8)$$

The adiabatic ECs $C_{i \eta \eta}^S$ are obtained from the isothermal ones with the relation:

$$C_{i \eta \eta}^S = C^T_{i \eta \eta} + T \Omega b_{i \eta} b_{\eta i}/C_V, \quad (9)$$

where the $b_{i \eta}$ are the thermal stresses obtained from:

$$b_{i \eta} = -\sum_{kl} C^T_{i \eta \eta} a_{kl}. \quad (10)$$

The adiabatic bulk modulus $B^S$ is computed as in Eq. [8] in terms of the adiabatic ECs.

The atomic BF is calculated as explained in a previous work [11]. Calling $B_{a \beta}(s)$ the mean-square displacement matrix of the atom $s$ we have:

$$B_{a \beta}(s) = \frac{\hbar}{2NM_s} \sum_{\mathbf{q}, \eta} \coth \left[ \frac{\hbar \omega_\eta(\mathbf{q})}{2k_B T} \right] \frac{u_{a \eta}(\mathbf{q}) u_{\beta \eta}(\mathbf{q})}{\omega_\eta(\mathbf{q})}, \quad (11)$$

where $M_s$ is the mass of $s$-th atom. $u_{a \eta}(\mathbf{q})$ is the $s\alpha$-th component of the dynamical matrix eigenvector of the mode $\eta$ with wave-vector $\mathbf{q}$. The BF is defined as $8\pi^2 B_{a \beta}(s)$ [17]. In order to include anharmonic effects, BFs are computed in the same reference geometries used for elastic constants and interpolated at each temperature at the $a(T)$.

III. METHOD

The calculations presented in this work were carried out using DFT as implemented in the Quantum ESPRESSO package [18,19]. Thermodynamic properties have been computed using the thermo_pw package [20]. The exchange and correlation functional was approximated by the local density approximation (LDA) which gives the best agreement between experimental and theoretical quantities especially for the $T = 0$ K ECs. We employed the projector augmented wave (PAW) method and a plane wave basis set with pseudopotentials [21,22] from pslibrary [23,24]. The pseudopotentials B.pz-n-kjpaw.psl.1.0.0.UPF and As.pz-n-kjpaw.psl.1.1.0.0.UPF have been used for boron and arsenic, respectively. The wave functions (charge density) were expanded in a plane waves basis with a kinetic energy cut-off of 60 Ry (400 Ry), and a $16 \times 16 \times 16$ mesh of $k$-points has been used for the Brillouin zone integration. Density functional perturbation theory (DFPT) [25,26] was used to calculate the dynamical matrices on a $4 \times 4 \times 4$ $q$-points grid. The dynamical matrices have been Fourier interpolated on a $200 \times 200 \times 200$ $q$-points mesh to evaluate the free-energy. The grid of the reference geometries was centered at the $T = 0$ K lattice constant reported in Table I. The number of reference geometries were 9 with lattice constants separated from each other by $\Delta a = 0.05$ a.u.. In the ECs calculation the number of strained configuration was 6 for each type of strain with an interval of strains between two strained geometries of 0.005. In total we computed phonon dispersions for 162 geometries (in addition to the 9 phonon dispersions used for the $a(T)$ calculation). A second degree polynomial has been used to fit the energy (for the ECs at $T = 0$ K) or the free-energy (for the QHA TDECs) as a function of strain, while a fourth degree polynomial was used to fit at each temperature all the other quantities computed at the various reference geometries versus $a(T)$.

IV. APPLICATIONS

In Table I we report the computed equilibrium lattice constant $a_0$ at $T = 0$ K both with and without the zero point energy (ZPE) and the RT value: the differences among them are of the order of hundreds of angstroms. The computed RT $a_0$ is in good agreement with the RT experiment [27] (the difference is smaller than $\approx 0.02$ Å). The comparison with other computed $a_0$ is also reported: the LDA values agree within $\approx 1$%. This small differences depend primarily on the computational parameters chosen for the calculation and from the different pseudopotentials. The PBE values of $a_0$ are slightly larger.
than the LDA ones as usually found with the functionals that use the generalized gradient approximation (GGA).

In Table I we report the calculated values of the elastic constants together with other theoretical estimates available in the literature and the experimental values. The LDA values are closer to experiment, while the PBE (Perdew Burke Ernzerhof) calculations give smaller ECs, as usually found with the GGA functionals. At \( T = 0 \) K, the softening due to the ZPE is \( \approx 2.4 \) % for \( C_{11} \), \( \approx 1.2 \) % for \( C_{12} \) and \( \approx 2.4 \) % in \( C_{44} \). In our calculation we relax the ionic positions for each strained configuration so the ECs are relaxed-ions results. This is relevant only for \( C_{44} \) while for \( C_{11} \) and \( C_{12} \) the ionic positions are determined by symmetry. The frozen-ions results, obtained by a uniform strain of the atomic positions but no further relaxation, are also shown in Table I: \( C_{44} \) is \( \approx 14 \) % larger than the relaxed-ions value. Our theoretical \( T = 300 \) K values are in good agreement with experiment: \( C_{11} \) is smaller of \( \approx 1.5 \) %, \( C_{12} \) is smaller of \( \approx 5.1 \) % and \( C_{44} \) is larger of \( \approx 1 \) %.

In Figure 1 the TDECs and the bulk modulus are reported. The red lines are the adiabatic ECs (or bulk modulus), while the blue lines are the isothermal ECs. Evaluating the percentage softening of ECs due to temperature as:

\[
C_{ij}(T = 0K) - C_{ij}(T = 1800K) \times 100\%\text{ }C_{ij}(T = 0K)
\]  
(12)

where the ZPE is included in \( C_{ij}(T = 0K) \) we find: \( \approx 11 \) % (adiabatic) and \( \approx 13 \) % (isothermal) for \( C_{11} \), \( \approx 9 \) % (adiabatic) and \( \approx 15 \) % (isothermal) for \( C_{12} \) and \( \approx 13 \) % for \( C_{44} \).

As far as we know, presently no experimental measurement of the TDECs is available to compare directly with our result, but recently the temperature dependence of the longitudinal sound velocity along the [111] direction was measured till \( \approx 500 \) K. Using the adiabatic TDECs and the density \( \rho \) this sound velocity can be written as:

\[
V_{long} = \left( \frac{C_{11} + 2C_{12} + 4C_{44}}{3\rho} \right)^{\frac{1}{2}}
\]  
(13)

and in Fig. 2 we compare our theoretical estimate with experiment. We take into account the temperature dependence of the density due to TE effect. The use of a temperature independent density in Eq. 13 (for instance the density at \( T = 0 \) K or \( T = 300 \) K) leads to an appreciably lower sound velocity above the RT (for instance at \( T = 1500 \) K the difference is \( \approx 90 \) m/s). The theoretical values of the sound velocity as a function of temperature is in reasonable agreement with experiment in the analyzed range, but the experimental slope of the curve at low temperatures is not reproduced. The comparison improves above RT. The difference between theory and experiment at RT (0.9%) is compatible with the errors in the elastic constants and in the density, while the difference at the lowest measured temperature (2.3%) is larger.

We can also compare the TDECs of BAs with those of silicon that we have calculated by using LDA. Silicon ECs are smaller, the \( T = 0 \) K values (with ZPE) are: \( C_{11} = 1580 \) kbar, \( C_{12} = 639 \) kbar and \( C_{44} = 746 \) kbar. In the range of temperature calculated for silicon (0 – 800 K) \( C_{11} \) and \( C_{12} \) decrease of about 7 % and \( C_{44} \) of 5 % (for both isothermal and adiabatic). In the same range of temperature the decrease of the ECs of BAs is slightly smaller: 3.8 % (adiabatic) and 4.5 % (isothermal) for \( C_{11} \), 3.2 % (adiabatic) and 5.7 % (isothermal) for \( C_{12} \) and 4.5 % for \( C_{44} \).

We now present several other thermodynamic properties of BAs that have been calculated together with the TDECs. The TE and the temperature dependence of the lattice constant \( a(T) \) are shown in Figure 3 in the range of temperature 0 – 1100 K. We compare our numerical result (black line) with two recent measurements in the temperature range 300 – 773 K (red points) and 321 – 773 K (blue points). The experimental \( a(T) \) is higher than the theoretical one by approximately 0.02 Å, but the temperature dependence is reproduced correctly as visible in the TE plot reported in the same figure. In the experimental temperature range, the experimental \( a(T) \) are both linear with \( T \) but the slope of the red points is slightly larger and more in agreement with our
calculation. This behavior is reflected in the TE: the TE of Chen et al.\textsuperscript{7} agrees with ours within experimental uncertainties while the TE of Kang et al.\textsuperscript{6} has slightly smaller values (although within the error bar of the former\textsuperscript{3}). In particular the RT TE is $4.0 \times 10^{-6} \text{K}^{-1}$ (this work), $(4.2 \pm 0.4) \times 10^{-6} \text{K}^{-1}$ (Chen et al.\textsuperscript{7}) and $3.85 \times 10^{-6} \text{K}^{-1}$ (Kang et al.\textsuperscript{6}). Other DFT-LDA estimates are: $4.0 \times 10^{-6} \text{K}^{-1}$ (Chen et al.\textsuperscript{7}), and $3.04 \times 10^{-6} \text{K}^{-1}$ (Broido et al.\textsuperscript{28}). Molecular dynamic simulations\textsuperscript{29} produced the result $4.1 \times 10^{-6}$. A much larger value has appeared recently\textsuperscript{30} $10.9 \times 10^{-6} \text{K}^{-1}$ by using DFT method within the GGA, quite far from experiment. The phonon frequencies computed at the different geometries are interpolated at $T = 300 \text{ K}$ and the result is shown in Figure 3b (colored lines). The phonons are compared with RT measurements obtained from inelastic X-ray scattering\textsuperscript{25} and Raman spectroscopy\textsuperscript{26} (points). As already found in previous references\textsuperscript{25,28} the agreement between theory and experiment is quite good. The difference between RT and $T = 0 \text{ K}$ phonons (black lines) is only barely visible in the optical branches.

The isobaric heat capacity is shown in Figure 3c. The points indicate the temperature dependence of experimental data below RT\textsuperscript{7} that we extrapolated from the plot. The agreement is very good, consistently with the fact that also the calculated Debye temperature ($\Theta_D = 668 \text{ K}$, obtained from the $T = 0 \text{ K}$+ ZPE EEs) is in good agreement with the experimental value\textsuperscript{27} ($\Theta_D = 681 \text{ K}$).
The temperature dependence of the average Grüneisen parameter is reported in Figure 3. We also report the RT experimental values of Kang et al. (blue point) and Chen et al. (orange point). The experimental uncertainty of the first point is not known, but it is very close to our curve. The second point is in agreement with our estimate within the experimental error bar.

Finally in Figure 4 we show our estimate of the BF for boron (red) and arsenic (blue). The BF of boron is $0.35 \text{ Å}^2$ at $T = 300 \text{ K}$ and grows up to $0.74 \text{ Å}^2$ at $T = 800 \text{ K}$. The BF of arsenic is smaller because of the larger mass: $0.25 \text{ Å}^2$ at $T = 300 \text{ K}$ and $0.64 \text{ Å}^2$ at $T = 800 \text{ K}$. They are smaller than the BFs of silicon [13] which has $0.52 \text{ Å}^2$ at $T = 300 \text{ K}$ and $1.29 \text{ Å}^2$ at $T = 800 \text{ K}$.

V. CONCLUSIONS

We studied TDECs of BAs by means of ab-initio simulation by using the recent tools implemented in the thermo_pw code within the QHA. The values of the adiabatic ECs at $T = 300 \text{ K}$ are $C_{11} = 2807 \text{ kbar}$, $C_{12} = 754 \text{ kbar}$, $C_{44} = 1507 \text{ kbar}$. We found that in the range of temperature $0 - 1800 \text{ K}$ the percentage softening of the adiabatic ECs is $\approx 11 \%$ for $C_{11}$, $\approx 9 \%$ for $C_{12}$ and $\approx 13 \%$ for $C_{44}$. The order of magnitude of the softening is consistent with the temperature variation of the longitudinal sound velocity measured along the [111] direction [6]. The slope of the curves are different below RT and similar for larger temperatures. The softening computed in BAs is slightly smaller than that calculated for silicon in the temperature range $0 - 800 \text{ K}$ [13]. We also computed thermodynamic properties of BAs such as the TE, the heat capacity, and the average Grüneisen parameter finding good agreement with experiments. Finally we presented the calculated atomic BFs as a function of the temperature for which no information, neither experimental nor theoretical, was available so far.
Temperature dependent elastic constants of BAs

FIG. 4. Temperature dependent atomic B-factor for the cubic BAs: boron (red), arsenic (blue).

ACKNOWLEDGMENTS

Computational facilities have been provided by SISSA through its Linux Cluster and ITCS and by CINECA through the SISSA-CINECA 2019-2020 Agreement.

1 J. S. Kang, H. Wu, and Y. Hu, Nano Lett. 17, 7507 (2017).
2 J. S. Kang, M. Li, H. Wu, H. Nguyen, and Y. Hu, Science 361, 575 (2018).
3 S. Li, Q. Zheng, Y. Lv, X. Liu, X. Wang, P. Y. Huang, D. G. Cahill, and B. Lv, Science 361, 579 (2018).
4 F. Tian, B. Song, X. Chen, N. K. Ravichandran, Y. Lv, K. Chen, S. Sullivan, and J. Kim, Science 361, 582 (2018).
5 F. Tian, K. Luo, C. Xie, B. Liu, X. Liang, L. Wang, G. A. Gamache, H. Sun, H. Ziyaee, J. Sun, Z. Zhao, B. Xu, G. Gao, X.-F. Zhou, and Z. Ren, Acta Crystallographica Section A 75, 624 (2019).
6 F. Giannozzi, S. Baroni, N. Bonini, M. Calandra, R. Car, C. Cavazzoni, D. Ceresoli, G. L. Chiarotti, M. Cococcioni, I. Dabo, A. Dal Corso, S. De Gironcoli, S. Fabris, G. Fratesi, U. G. Ralph Gebauer, C. Gougoussis, A. Kokalj, M. Lazzeri, L. Martin-Samos, N. Marzari, F. Mauri, R. Mazzarello, S. Paolini, A. Pasquarello, L. Paulatto, C. Sbraccia, S. Scandolo, G. Schlueter, A. P. Seitsonen, A. Smogunov, P. Umari, and R. M. Wentzcovitch, J. Phys.: Condens. Matter 21, 395501 (2009).
7 F. Giannozzi, O. Andreussi, T. Brumme, O. Bunau, M. B. Nardelli, M. Calandra, R. Car, C. Cavazzoni, D. Ceresoli, M. Cococcioni, N. Colonna, I. C. Carmineo, A. Dal Corso, S. De Gironcoli, P. Delugas, R. A. DiStasio, A. Ferretti, A. Floris, G. Fratesi, G. Fugallo, R. Gebauer, U. Gerstmann, F. Giustino, T. Gorni, J. Jia, M. Kamawura, H.-Y. Ko, A. Kokalj, E. Kucukbenli, M. Lazzeri, M. Marsili, N. Marzari, F. Mauri, N. L. Nguyen, H.-Y. Nguyen, A. O. de-la Roza, L. Paulatto, P. Poncè, D. Rocca, R. Sabatini, B. Santra, M. Schlip, A. P. Seitsonen, A. Smogunov, I. Timrov, T. Tomanhaus, P. Umari, N. Vast, X. Wu, and S. Baroni, “Advanced capabilities for materials modelling with quantum ESPRESSO,” Journal of Physics: Condensed Matter 29, 465901 (2017).
8 P. Giannozzi, O. Andreussi, T. Brumme, O. Bunau, M. B. Nardelli, M. Calandra, R. Car, C. Cavazzoni, D. Ceresoli, M. Cococcioni, N. Colonna, I. Carmineo, A. Dal Corso, S. De Gironcoli, P. Delugas, R. A. DiStasio, A. Ferretti, A. Floris, G. Fratesi, G. Fugallo, R. Gebauer, U. Gerstmann, F. Giustino, T. Gorni, J. Jia, M. Kamawura, H.-Y. Ko, A. Kokalj, E. Kucukbenli, M. Lazzeri, M. Marsili, N. Marzari, F. Mauri, N. L. Nguyen, H.-Y. Nguyen, A. O. de-la Roza, L. Paulatto, P. Poncè, D. Rocca, R. Sabatini, B. Santra, M. Schlip, A. P. Seitsonen, A. Smogunov, I. Timrov, T. Tomanhaus, P. Umari, N. Vast, X. Wu, and S. Baroni, “Advanced capabilities for materials modelling with quantum ESPRESSO,” Journal of Physics: Condensed Matter 29, 465901 (2017).
9 P. E. Blöchl, Phys. Rev. B 50, 17953 (1994).
10 H. Meradji, S. Drablia, S. Ghemid, H. Belkhir, B. Bouhafs, and A. Tadjer, Phys. Status Solidi B 241, 2881 (2004).
11 L. Bing, L. R. Feng, and Y. X. Dong, Chin. Phys. B. 19, 076201 (2010).
12 J. F. Nye, Physical properties of crystals (Oxford science publications, 1985).
13 F. E. H. Hassan, H. Akbarzadeh, and M. Zoaeter, J. Phys.: Condens. Matter 16, 293 (2004).
14 H. Meradji, S. Drablia, S. Ghemid, H. Belkhir, B. Bouhafs, and A. Tadjer, Phys. Status Solidi B 241, 2881 (2004).
15 F. E. H. Hassan, H. Akbarzadeh, and M. Zoaeter, J. Phys.: Condens. Matter 16, 293 (2004).
16 J. F. Nye, Physical properties of crystals (Oxford science publications, 1985).
17 M. Palumbo and A. Dal Corso, J. Phys.: Condens. Matter 29, 395401 (2017).
18 M. Palumbo and A. Dal Corso, Phys. Status Solidi B 254, 1700101 (2017).
19 P. Giannozzi, S. Baroni, N. Bonini, M. Calandra, R. Car, C. Cavazzoni, D. Ceresoli, G. L. Chiarotti, M. Cococcioni, I. Dabo, A. Dal Corso, S. De Gironcoli, S. Fabris, G. Fratesi, U. G. Ralph Gebauer, C. Gougoussis, A. Kokalj, M. Lazzeri, L. Martin-Samos, N. Marzari, F. Mauri, R. Mazzarello, S. Paolini, A. Pasquarello, L. Paulatto, C. Sbraccia, S. Scandolo, G. Schlueter, A. P. Seitsonen, A. Smogunov, P. Umari, and R. M. Wentzcovitch, J. Phys.: Condens. Matter 21, 395501 (2009).
20 F. Giannozzi, O. Andreussi, T. Brumme, O. Bunau, M. B. Nardelli, M. Calandra, R. Car, C. Cavazzoni, D. Ceresoli, M. Cococcioni, N. Colonna, I. Carmineo, A. Dal Corso, S. De Gironcoli, P. Delugas, R. A. DiStasio, A. Ferretti, A. Floris, G. Fratesi, G. Fugallo, R. Gebauer, U. Gerstmann, F. Giustino, T. Gorni, J. Jia, M. Kamawura, H.-Y. Ko, A. Kokalj, E. Kucukbenli, M. Lazzeri, M. Marsili, N. Marzari, F. Mauri, N. L. Nguyen, H.-Y. Nguyen, A. O. de-la Roza, L. Paulatto, P. Poncè, D. Rocca, R. Sabatini, B. Santra, M. Schlip, A. P. Seitsonen, A. Smogunov, I. Timrov, T. Tomanhaus, P. Umari, N. Vast, X. Wu, and S. Baroni, “Advanced capabilities for materials modelling with quantum ESPRESSO,” Journal of Physics: Condensed Matter 29, 465901 (2017).
21 P. E. Blöchl, Phys. Rev. B 50, 17953 (1994).
22 P. Giannozzi, O. Andreussi, T. Brumme, O. Bunau, M. B. Nardelli, M. Calandra, R. Car, C. Cavazzoni, D. Ceresoli, M. Cococcioni, N. Colonna, I. C. Carmineo, A. Dal Corso, S. De Gironcoli, P. Delugas, R. A. DiStasio, A. Ferretti, A. Floris, G. Fratesi, G. Fugallo, R. Gebauer, U. Gerstmann, F. Giustino, T. Gorni, J. Jia, M. Kamawura, H.-Y. Ko, A. Kokalj, E. Kucukbenli, M. Lazzeri, M. Marsili, N. Marzari, F. Mauri, N. L. Nguyen, H.-Y. Nguyen, A. O. de-la Roza, L. Paulatto, P. Poncè, D. Rocca, R. Sabatini, B. Santra, M. Schlip, A. P. Seitsonen, A. Smogunov, I. Timrov, T. Tomanhaus, P. Umari, N. Vast, X. Wu, and S. Baroni, “Advanced capabilities for materials modelling with quantum ESPRESSO,” Journal of Physics: Condensed Matter 29, 465901 (2017).
23 http://dalcorso.github.io/thermo_pw/.
24 C. Kittel, Introduction to Solid State Physics (Wiley, New York, 1976).
25 D. A. Broido, L. Lindsay, and T. L. Reinecke, Phys. Rev. B 88, 214303 (2013).
26 F. Benkabou, C. Chikr.Z, H. Aourag, P. J. Becker, and M. Certier, Phys. Lett. A 252, 72 (1999).
27 H. Ma, C. Li, S. Tang, J. Yan, A. Alatas, L. Lindsay, B. C. Sales, and Z. Tian, Phys. Rev. B 94, 220303 (2016).
28 R. G. Greene, H. Luo, and A. L. Ruoff, Phys. Rev. Lett. 33, 2476 (1994).
29 G. G. M. Wemberley, D. A. Broido, L. Lindsay, and T. L. Reinecke, Phys. Rev. B 88, 214303 (2013).
30 S. Daoud, N. Bioud, and N. Lebga, Chinese J. Phys. 57, 165 (2019).