Ab-initio study of C15-type Laves phase superconductor LaRu$_2$

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Abstract: Structural, elastic, electronic, optical, thermodynamic, and superconducting properties of the Laves phase superconductor LaRu$_2$ with $T_c \sim 1.63$ K were investigated using the first-principles calculations for the first time. The corresponding evaluated structural parameters are in good agreement with the available theoretical values. The different elastic properties like as, elastic constants, bulk modulus $B$, shear modulus $G$, Young’s modulus $E$, and Poisson ratio $\nu$ were calculated using the Voigt–Reuss–Hill approximation. The ductility nature appears in both values of Cauchy pressure and Pugh’s ratio. The band structure and Cauchy pressure shows that the material behaves metallic nature. The calculated total density of state is 6.80 (electrons/eV) of LaRu$_2$. The optical properties such as reflectivity, absorption spectrum, refractive index, dielectric function, conductivity, and energy loss spectrum are also calculated. The photoconductivity reveals the metallic nature of LaRu$_2$ and absorption coefficient is good in the infrared region. The evaluated density and Debye temperature are 9.55 gm/cm$^3$ and 110.51 K, respectively. In addition, the study of thermodynamic properties like as minimum thermal conductivity, melting temperature, and Dulong–Petit limit are 0.26 (Wm$^{-1}$K$^{-1}$), 1,471.65 K, and 74.80 (J/mole K), respectively. Finally, the investigated electron-phonon coupling constant is 0.66 of LaRu$_2$ superconductor.

Subjects: Material Science; Physics; Condensed Matter Physics

Keywords: Laves phase; elastic properties; electronic properties; optical properties; thermodynamic properties; superconducting properties

1. Introduction
The Laves phase are the structure of AB$_2$, which is explained by Fritz Laves and divided the Laves phases in three types such as face centered cubic C15 (MgCu$_2$), hexagonal C14 (MgZn$_2$), and
double-hexagonal C36 (MgNi₂) (Okaniwa, Shindo, Yoshida, & Takasugi, 1999). Laves phase have some functional properties, those are excellent corrosion and creep resistance, magnetic, and electrical properties (Keitz & Sauthoff, 2002; Klein, Pickett, Papaconstantopoulos, & Boyer, 1983; Okaniwa et al., 1999; Thoma et al., 1997). C15-type Laves phase is better than any other two Laves phase because of cubic structure (Zhang et al., 2011). Due to simple structure, the study of different types of physical and superconducting properties are quite interesting and understand very clearly. The agreeable superconductivity is found in the Laves phase cubic MgCu₂ (C15)-type intermetallic compound with transition temperatures 0.07 K to above 10 K (Rapp, Invarsson, & Claeson, 1974). Rapp et al. (1974) studied the superconductivity in distinct Laves phase compounds in 1974, and reported the superconducting critical temperature of ZrW₂, HfW₂, and ZrMo₂, Lave phases are 0.12 K. Deligoz, Colakoglu, Ozisik, and Cifti (2013) investigate the detailed thermodynamic properties of Al₂Ca and Al₂ Mg Laves phases. Rahaman and Rahman (2016) investigated some physical properties of NbBe₂ Laves phase using theoretical means. Matthias and Corenzwit in 1957, and Matthias and Bozorth in 1958, investigated the superconductivity and ferromagnetism of Laves phase superconductor LaRu₂ and predicted the transition temperature is 1.63 K (Compton & Matthias, 1959). He also investigated LaRu₂ has a cubic structure with lattice parameter \( a = 7.702 \) Å and he reported YAl₂ compound and the hafnium compound such as HfRe₂ and HfOs₂.

In recent, the Laves phase LaRu₂ has no experimental and theoretical work about the physical and superconducting properties. Then we, therefore, decided to investigate the detailed physical properties of this compound theoretically. In this article, we have calculated different physical properties of LaRu₂ such as structural, elastic, electronic, optical, thermodynamic, and superconducting properties using the plane-wave pseudo-potential density functional theory method (DFT). The remaining parts of this paper are aligned as follows. The computational methods are discussed in Section 2, the investigated results and discussions are shows in Section 3 and finally, a summary of this present investigation is shown in Section 4.

2. Computational method

The study of the Laves phase LaRu₂ has performed with Cambridge sequential total energy package (CASTEP) code using the plane wave pseudo-potentials method based on density function theory (DFT) (Clark et al., 2005; Hohenberg & Kohn, 1964; Materials Studio CASTEP Manual_Accelrys, 2010; Perdew et al., 2008). The exchange-correlation energy function is defined by the generalized gradient approximation (GGA) of Perdew–Burke–Ernzerhof (PBE) (Perdew, Burke, & Ernzerhof, 1996). The interaction between ion core and valence electron is described using the ultrasoft pseudopotential (Fagan et al., 2001). The outermost electron configuration for La is 5d¹ 6s² and Ru is 4d⁷ 5s¹, respectively. The cut-off energy and the \( k \)-points are set to 350 eV and \( 7 \times 8 \times 8 \). The geometrical optimization of the Laves phase LaRu₂ structure was performed by the Broyden–Fletcher–Goldfarb–Shanno (BFGS) minimization method (Pfrommer, Côté, Louie, & Cohen, 1997). The crystal structure optimization, criteria of convergence was set to 1.0 × 10⁻⁵ eV/atom for energy, 0.03 eV/Å for force, 0.05 GPa for stress, and 0.001 Å for ionic displacement. The elastic stiffness constants of the Laves phase LaRu₂ were achieved by the stress—strain method (Nye, 1961). The elastic constants of LaRu₂ are calculated using the bulk modulus. For this reason, the criteria of convergence tolerance were set to 2.0 × 10⁻⁶ eV/atom for energy, 2.0 × 10⁻⁴ Å for maximum ionic displacement, 6.0 × 10⁻⁴ eV/Å for maximum ionic force, and 0.1 GPa for maximum stress component. In the present investigation, the maximum strain amplitude was set to be 0.003 of LaRu₂.

3. Results and discussion

3.1. Structural properties

The Laves phase LaRu₂ compound has a cubic lattice of MgCu₂-type structure with the space group Fd-3 m and number of space group is 227 (Compton & Matthias, 1959). The equilibrium lattice parameter has a value of 7.702 Å and the atomic positions of La and Ru atom in the unit cell are (0, 0, 0) and (0.625, 0.625, 0.625), respectively (Compton & Matthias, 1959; Rahaman & Rahman, 2016). The lattice constants and the atomic positions have been progress as a function of normal stress by
minimizing the total energy. The optimized three-dimensional structures are shown in Figure 1 and the two-dimensional conventional cell and primitive cell are also shown in Figure 2. The calculated values of the structural properties of LaRu₂ are presented in Table 1 along with the available experimental and other theoretical values. From Table 1, we see that our present theoretical results are very close to both experimental and other theoretical results. The calculated lattice constant of this present work is 7.786 Å which shows 1.07% deviation compared with the experimental value and slightly different than other theoretical values due to the different calculation methods. This indicates the reliability of our present DFT-based first-principles calculations.

![Figure 1. The three-dimensional crystal structures of LaRu₂ (a) conventional cubic cell and (b) primitive cell.](image1)

![Figure 2. The two-dimensional structure of cubic Laves phase LaRu₂ (a) conventional cell and (b) primitive cell.](image2)

| Properties | Expt. (Nye, 1961) | Present calculation | Other calculation | Deviation from expt. (%) |
|------------|------------------|---------------------|------------------|------------------------|
| \(a₀\) (Å) | 7.702            | 7.786               | 6.484\(^a\), 7.052\(^b\) | 1.07, 0.78\(^b\)       |
| \(V₀\) (Å\(^3\)) | –              | 472.00              | –                | –                      |
| \(B₀\) (GPa) | –               | 143.81              | –                | –                      |

\(^a\)Source: Rahaman and Rahman (2016).
\(^b\)Source: Liu et al. (2012).
3.2. Elastic properties

The resistance of a crystal to an applied stress can be determined from the elastic constant, which reveals the bonding characteristics near the equilibrium position (Wang & Zhou, 2004). The study of the elastic properties provides information about the chemical bonds and the cohesion of material (Wu, Wen, Tang, Peng, & Ding, 2010). Also, the detailed study of elastic constants provides information of the mechanical properties and dynamic information about the stability and stiffness of materials and various important materials parameters such as Debye temperature, chemical bonds, and the mechanical stability of materials (Wang & Zhou, 2004). The elastic constants were determined from a linear fit of the calculated stress–strain function according to Hook’s law (Nye, 1961). The LaRu$_2$ superconductor has three important elastic constants because of cubic structure these are $C_{11}$, $C_{12}$, and $C_{44}$. From the calculated value of $C_{ij}$, the crucial mechanical properties like as the bulk modulus $B$, shear modulus $G$, Young’s modulus $E$, and Poisson’s ratio $\nu$ of LaRu$_2$ are determined using the Voigt–Reuss–Hill (VRH) averaging scheme (Hill, 1952). The elastic constant data of this compound are recorded in Table 2. For cubic crystal, LaRu$_2$ fulfilled the Born stability criteria because of mechanically stable crystal (Born, 1940) and the criteria for cubic crystal are as follows,

$$C_{11} > 0, C_{44} > 0, C_{11} - C_{12} > 0 \text{ and } C_{11} + 2C_{12} > 0$$

From the data of Table 2 we see that the Born stability criteria for cubic crystal are satisfied.

| $C_{11}$ (GPa) | $C_{12}$ (GPa) | $C_{44}$ (GPa) | $C_{11} - C_{12}$ (GPa) | $B$ (GPa) | $G$ (GPa) | $E$ (GPa) | $B/G$ | $\nu$ | $A$ |
|----------------|----------------|----------------|-------------------------|--------|--------|--------|-------|-----|-----|
| LaRu$_2$       | 155.44         | 137.99         | 19.60                   | 118.39 | 143.80 | 14.16  | 10.15 | 0.45 | 2.24 |

Table 2. The calculated elastic constants $C_{ij}$ (GPa), Cauchy pressure ($C_{12} - C_{44}$), bulk modulus $B$ (GPa), shear modulus $G$ (GPa), Young’s modulus $E$ (GPa), $B/G$ values, Poisson’s ratio $\nu$, and anisotropy factor $A$ of LaRu$_2$.
The Zener anisotropy factor $A$ is determined using the following formula:

$$A = \frac{2C_{44}}{(C_{11} - C_{12})} \quad (8)$$

The calculated value of $C_{12} - C_{44}$, $B$, $G$, $E$, $B/G$, $\nu$, $A$ using the above equations are also shown in Table 2. We are not able to compare these values with experimental values because no experimental data are available yet.

The Cauchy pressure ($C_{12} - C_{44}$) reveals the angular character of atomic bonding in all compounds (Pettifor, 1992). Positive value of $C_{12} - C_{44}$ indicates the metallic nature and negative value shows the non-metallic (Liu et al., 2012). From Table 2, we see that the value of $C_{12} - C_{44}$ is positive and indicates the metallic nature of LaRu$_2$ Laves phase, which result is same as our present band structure nature. The negative value of Cauchy pressure of any compound behaves brittle and the positive indicates ductile nature (Pettifor, 1992). Since the Cauchy pressure is positive, our investigated compound behaves ductile nature. The ratio of $B/G$ is known as Pugh’s ratio, which also indicates the brittle or ductile nature and if the value of $B/G$ is less than 1.75 ($B/G < 1.75$) the material shows brittle manner otherwise ductile (Pugh, 1954). From our present calculation, the value of Pugh’s ratio is greater than 1.75 and behaves ductile nature. The both values of Cauchy pressure and Pugh’s ratio are same nature, which represent the reliability of our present investigation.

The shear modulus is the prominent parameter related with the stability of superconductor LaRu$_2$ because the value of bulk modulus $B$ is greater than shear modulus ($B > G$) (Liu, Liu, Feng, & Tian, 2011). The value of Poisson’s ratio $\nu$ provides crucial information about the bonding forces (Mayer et al., 2003). The values of Poisson’s ratio 0.25 and 0.5 shows the central forces in solids and these values are known as lower limit and upper limit of Poisson’s ratio, respectively (Fu, Li, Peng, Gao, & Cheng, 2008). From Table 2, we see that the calculated value of Poisson’s ratio $\nu$ is 0.45 of LaRu$_2$, which is larger than the lower limit value of 0.25 and which also represent that the interatomic forces of LaRu$_2$ are central forces. The value of anisotropy factor $A = 1$ for cubic crystal represent the material are completely isotropic material, otherwise smaller or larger value from $A = 1$ reveals the degree of elastic anisotropy (Karki et al., 1997). In our present investigation, the value of $A$ is 2.24, which indicates the degree of elastic anisotropy.

3.3. Electronic properties

The study of band structure, and the total and partial density of state give much crucial information about the physical phenomena of LaRu$_2$. The band structure of LaRu$_2$ in present calculation is shown in Figure 3 and dotted line shows the Fermi level. From this curve, we see that the valence band and conduction band overlap each other in the Fermi level which indicates the metallic nature of LaRu$_2$. The total and partial density of state of our present calculation is also shown in Figure 4. The values of total and partial density of state are shown in Table 3. The calculated value of total density of state is 6.80 (electrons/eV).

From Figure 4, we say that the main bonding peaks are obtained in the energy range between $-5$ and 5 eV. The contribution of La-5d and Ru-4d states is dominant and at the Fermi level Ru-4d orbital contributes largely than La-5d orbital. Coincidence between Ru-4d and La-5d orbital's implies that covalent bonds exist between those states (Rahman, Rahaman, & Sarker, 2016).

The investigation of Mulliken atomic population shows the covalent or ionic character of LaRu$_2$ superconductor (Mulliken, 1955). The investigated data are tabulated in Table 4. The zero value of bond population reveals the perfectly ionic bond and greater zero value indicates the increasing levels of covalency (Segall, Shah, Pickard, & Payne, 1996). Also lower than zero value indicates the ionic bond.
From Table 4, we see that the charge transfers from La to Ru atom, which indicates the ionic nature of La-Ru bonds (Rahaman & Rahman, 2016). The values of bond population of LaRu₂ are positive and greater than zero which also indicate the covalent character of this compound. The bond length of LaRu₂ are also determined and recorded in Table 4. Our calculated bond lengths are very close to the other theoretical values of same phase, which show the reliability of the present DFT-base calculation.
3.4. Optical properties

The dielectric function \( \varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega) \) is used to calculate the optical properties of LaRu\(_2\), which is frequency-dependent function and the study of the optical properties gives very crucial phenomena of different materials. Where \( \varepsilon_2(\omega) \) is the imaginary part achieved from the momentum matrix elements between the filled and the unfilled electronic states and which are determined using the following equation (Materials Studio CASTEP manual_Accelrys, 2010):

\[
\varepsilon_2(\omega) = \frac{2e^2}{\Omega \omega} \sum_{\mathbf{k}, \mathbf{k}'} |\psi_{\mathbf{k}}^e|^2 |\psi_{\mathbf{k}'}^c|^2 \delta(E_{\mathbf{k}}^c - E_{\mathbf{k}'}^c - \epsilon)
\]

where \( u \) is defined as the polarization of the incident electric field, \( \omega \) is defined as the frequency of light, \( e \) is denoted the charge of electron, \( \psi_{\mathbf{k}}^e \) is expressed as the conduction band wave function and \( \psi_{\mathbf{k}'}^c \) is the valence band wave function at \( K \), respectively. The Kramers–Kronig transform is used to express the real part. From Equations (49)–(54), Materials Studio CASTEP manual_Accelrys (2010) are used to determine all other optical constants. Figure 4 represents the optical functions of LaRu\(_2\) and which are investigated for photon energies up to 100 eV. The value of 0.5 eV Gaussian smearing is used for all calculations.

The reflectivity spectrum of LaRu\(_2\), is shown in Figure 5(a). From this figure, we see that the reflectivity start from the value of 0.78 in which zero energy appears. The value of the reflectivity drops in the visible region and the reflectivity is zero in the ultraviolet region.

Figure 5(b) shows the absorption coefficient of LaRu\(_2\) Laves phase. The absorption start from zero values and some highest peak appears in the infrared region and visible region. The highest peak value of absorption is \( 2.81 \times 10^5 \) where the photon energy is 5.98 eV. This value indicates that LaRu\(_2\) has good absorption coefficient in the infrared region.

Figure 5(c) shows the refractive index diagram of LaRu\(_2\). The static value of refractive index is 16.33 at zero energy, which decreases gradually in the visible region and becomes stable in the ultraviolet region.
The dielectric function shows in Figure 5(d). From this figure, we see that the maximum dielectric constant of LaRu$_2$ appears at zero photon energy level. In infrared region the values of dielectric function appears good but it is stable in visible and ultraviolet region, respectively.

Figure 5(e) represents the conductivity spectra of LaRu$_2$. In this figure, the photoconductivity starts with zero conductivity in which photon energy is also zero, which reveals the metallic nature of LaRu$_2$ superconductor. This result is similar with our present band structure result which is shown in Figure 3.

The energy loss function is a crucial optical phenomenon, which represents the energy loss of a fast electron traversing the material and huge energy loss appears at the plasma frequency (Hossain, Ali, & Islam, 2012). Figure 5(f) shows the energy loss spectrum of LaRu$_2$ as a function of photon energy. The static value of Loss function is 18.68 with photon energy 22.92 eV. The highest peak is related to the plasma resonance and in which involving frequency is called plasma frequency (Fox, 1972). Since the state peak is found in 22.92 eV which is equal to plasma frequency.

3.5. Thermodynamic properties

The study of thermodynamic properties gives very essential phenomena in solid. The Debye temperature is one of them. The Debye temperature can be calculated using the following equation (Aydin & Simsek, 2009).

$$\theta_D = \frac{h}{k_B} \left( \frac{3N}{4\pi V} \right)^{\frac{1}{3}} \times v_m$$

where $v_m$ is the average sound velocity and is calculated from the following equation,
where $v_t$ and $v_l$ are the transverse and longitudinal wave velocity, respectively, and which are also evaluated from the following equations,

$$v_m = \left[ \frac{1}{3} \left( \frac{2}{v_t^3} + \frac{1}{v_l^3} \right) \right]^{-\frac{1}{3}}$$  \hspace{1cm} (11)

The evaluated values of $\nu_m$, $\nu_t$, and $\nu_l$ from above equations are recorded in Table 5. Our calculated density and Debye temperature are 9.55 gm/cm$^3$ and 110.51 K, respectively.

Thermal conductivity, melting temperature, and Dulong–Petit limit also evaluate in present section. Thermal conductivity of a solid is defined as the heat transfer process from one part to other part of a material (Rahaman & Rahman, 2017b). The minimum thermal conductivity is denoted as $K_{min}$ which is associated with high-temperature applications of solid and when temperature increases thermal conductivity decreases to a certain limit. (Shen, Clarke, & Fuierer, 2008). The minimum thermal conductivity is calculated using the following formula (Clarke, 2003).

$$K_{min} = K_B v_m \left( \frac{M}{n_\rho N_A} \right)^{-2/3}$$  \hspace{1cm} (14)

where $K_B$ is the Boltzmann constant, $v_m$ is the average sound velocity, $M$ is the molecular mass, $n_\rho$ is the number of atoms per molecule, and $N_A$ is the Avogadro’s number.

For cubic metal, the value of the melting temperature can be calculated using the following formula which is discovered by Mehl, Klein, and Papaconstantopoulos (1994).

$$T_m = 553 + 5.91C_{11}$$  \hspace{1cm} (15)

The Dulong–Petit limit of solid can be determined using the following relation (Mao, Liu, Hou, Tan, & Zhou, 2016),

$\text{Dulong–Petit limit} = 3nN_A K_B$ \hspace{1cm} (16)

where $N_A$ and $K_B$ represents the Avogadro’s number and the Boltzmann constant, respectively.

Table 5. The evaluated density $\rho$ (in gm/cm$^3$), transverse ($\nu_t$), longitudinal ($\nu_l$), and average sound velocity $\nu_m$ (m/s) and Debye temperature $\theta_D$ (K) of laves phase LaRu$_2$

| Compound | $\rho$ (gm/cm$^3$) | $\nu_t$ (m/s) | $\nu_l$ (m/s) | $\nu_m$ (m/s) | $\theta_D$ (K) |
|----------|------------------|---------------|---------------|---------------|---------------|
| LaRu$_2$ | 9.55             | 1,217.67      | 4,127.29      | 1,387.96      | 110.51        |

Table 6. The calculated minimum thermal conductivity, $K_{min}$ (in Wm$^{-1}$ K$^{-1}$), melting temperature, $T_m$ (K) and the Dulong–Petit limit (J/mole K) of LaRu$_2$

| $K_{min}$ | $T_m$ | Dulong–Petit limit |
|-----------|-------|--------------------|
| 0.26      | 1,471.65 | 74.80              |
3.6. Electron-phonon coupling constant and superconductivity

The superconducting transition temperature is a crucial phenomenon of superconductor. The superconducting transition temperature of any compound can be calculated using the following McMillan formula (McMillan, 1968).

\[ T_c = \frac{\theta_D}{1.45} e^{-\frac{1.04 + 0.62 \mu^*}{1.45 T_c}} \]  

(17)

where \( T_c \) is the superconducting critical temperature, \( \theta_D \) is the Debye temperature, \( \lambda \) is the electron-phonon coupling constant, and \( \mu^* \) is the coulomb pseudo-potential.

For determining the value of \( T_c \) the electron-phonon coupling constant \( \lambda \) calculate accurately. From QUANTUM-EXPRESSO program the value of \( \lambda \) measured directly (Giannozzi et al., 2009). Also the value of \( \lambda \) can be calculated using Equation (20) of Rahaman and Rahman (2017a). But we have no experimental value of electronic specific-heat coefficient \( \gamma \). So, we are not able to calculate the value of \( \lambda \) accurately. The theoretical value of \( \lambda \) provides lower value (Savrasov & Savrasov, 1996). For this reason, also we are not able to calculate the value of \( T_c \) accurately under consideration.

In this present work, we only calculate the value of \( \lambda \) indirectly using the McMillan formula (McMillan, 1968).

\[ \lambda = \frac{1.04 + \mu^* \ln \left( \frac{\theta_D}{1.457} \right)}{(1 - 0.62 \mu^*) \ln \left( \frac{\theta_D}{1.457} \right) - 1.04} \]  

(18)

where \( \theta_D \) is the Debye temperature and \( \mu^* \)is the effective screened Coulomb repulsion constant.

The value of effective screened Coulomb repulsion constant for Laves phase compound lies between 0.10 and 0.16 (Rahaman & Rahman, 2016) and here, we consider the value of \( \mu^* \) is 0.15 for evaluating \( \lambda \). The calculated Debye temperature in our present study is 110.51 K and experimental value of \( T_c \) is 1.63 K. From these above values, the calculated electron-phonon coupling constant \( \lambda \), in this present work, is 0.66 for LaRu2, which is well agreed compared to \( \lambda = 0.46 \) in Rahaman and Rahman (2016) as a same phase material. So, our calculated value ensures the accuracy.

4. Conclusion

In summary, we investigated the structural, elastic, electronic, optical, thermodynamic, and superconducting properties of Laves phase LaRu2 using the first-principle calculation base on DFT. The evaluated equilibrium lattice parameters are in accordance with others theoretical values. We have also determined the independent elastic constants, Cauchy pressure, bulk modulus, shear modulus, Young’s modulus, Pugh’s ratio (B/G), Poisson’s ratio, and anisotropy factor using the Voigt–Reuss–Hill (VRH) approximation. The evaluated elastic constants of cubic superconductor LaRu2 satisfies the required stability criteria which indicate that the compound is mechanically stable under study. The both values of Cauchy pressure and Pugh’s ratio behave ductile nature. The Cauchy pressure also behaves metallic nature. Poisson’s ratio represent the interatomic forces of LaRu2, are central force and anisotropy factor indicates the degree of elastic anisotropy. The band structure of LaRu2 shows the metallic nature and our calculated total density of state is 6.80 (electrons/eV). It is observed that the Cauchy pressure and band structure both behaves metallic nature, which indicates the accuracy of our present investigation. In addition, the optical properties, e.g. reflectivity, absorption spectrum, refractive index, dielectric function, conductivity, and energy loss spectrum of LaRu2 have been investigated first time in our present study. The photoconductivity reveals the metallic nature of LaRu2. This result is also similar to our present band structure and Cauchy pressure, which also indicates reliability. The static value of Loss function is found in 22.92 eV which is equal to plasma frequency and LaRu2 has good absorption coefficient in the infrared region. Our calculated density and Debye temperature are 9.55 gm/cm³ and 110.51 K, respectively. Further the thermodynamic properties like as minimum thermal conductivity, melting temperature, Dulong–Petit limit have been study in our
present calculation. We also calculate the electron-phonon coupling constant which is 0.66. So, we predict that the superconductor LaRu$_2$ is a weakly coupled BCS superconductor.

The present work has a great implication for future theoretical investigation on the physical and superconducting properties of others Laves phase superconductors.

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