Abstract

The discovery of superconductivity in MgB$_2$ at 40 K has revived the attention of electron-phonon superconductors. We briefly outline the method of density functional theory for superconductors, recently proposed by the authors, describing without adjustable parameters the critical properties of real materials. We present the results obtained in elemental superconductors.

INTRODUCTION

The search of new superconducting materials with increasingly high critical temperature is a very active field of outmost importance. The recent discovery of phonon-mediated superconductivity at 39.5 K in MgB$_2$[1] has renewed the interest in the phonon-driven mechanism alive. While in fact the mechanism of superconductivity in cuprates is still under debate, there are many materials in which the electron-phonon interaction is certainly the mechanism responsible for superconductivity. MgB$_2$, in particular, has many important aspects which make it interesting from the point of view of applications. Disappointingly, many superconducting materials have so far been discovered by chance. In fact, predicting the superconducting properties of materials is a very important, but difficult challenge. The reason is the following: in the phonon mechanism of superconductivity, the interaction (denoted “e-ph” in the following) of electrons with quantized lattice waves (phonons) results into a net electron-electron attraction necessary to stabilize the superconducting state. This attraction, however, has to overcome the strong direct Coulomb repulsion (denoted “e-e”); this is only made possible by the difference of time scale in the electron and nuclear motion, a delicate mechanism that produce a large variety of critical temperatures, often due to little variations in the compound stoichiometry, pressure or other structural parameters.

On the theoretical side, most of nowadays calculations are based on the Eliashberg theory. While in the latter the phonon mediated attraction between is perfectly accounted for, the e-e effects are condensed in a single number, which is difficult to calculate from first principles and which, in most practical applications, is treated as an adjustable parameter, usually chosen as to reproduce the experimental critical temperature $T_c$. In this sense, Eliashberg theory, in spite of its tremendous success, can be considered a semi-phenomenological theory.

We have recently extended the density functional theory (DFT), a very successful standard approach in normal state electronic structure calculations, to deal with the superconducting state (SCDFT)[2-4]. Unlike in Eliashberg based calculations, within SCDFT there are no adjustable parameters, and the final critical temperature is the result of material specific quantities, all of which are computed ab-initio. SCDFT theory turns out to be able to treat superconductors with a wide range of couplings, as shown by several investigations.

In this paper we shall overview the properties of the most important new superconductors recently discovered. We start by sketching in the next section the necessary theoretical concepts beyond the modern calculations of the superconducting properties of materials. Then, we shall describe the properties of MgB$_2$, intercalated graphite CaC$_6$, and of alkali metals under pressure.

THEORETICAL METHODS

The modern calculations of electronic structure are based on Density Functional Theory (DFT)[5], introduced by Hohenberg and Kohn in 1965. DFT, especially in its Local Density Approximation (LDA), has enjoyed increasing popularity as a reliable and relatively inexpensive tool to describe real materials. In this approach, as applied to the normal state, the fundamental Hohenberg-Kohn (HK) theorem states that all observables are functionals of the electronic density alone. By approximating the functional dependence of the free-energy on the density, Kohn and Sham[5] were able to obtain a simple set of one-electron Schrödinger-like equations, containing an effective potential which is a functional of the density. The density, in turn, is obtained from the modulus square of the one-electron wavefunctions. The corresponding self-consistent solution of these coupled equations provides the electronic eigenenergies, which in metals are often successfully compared to the experimental excitation energies. From the point of view of superconductivity, the states around the Fermi surface are obviously the most relevant.

Before turning to the problem of superconductivity, it is instructive to reconsider how magnetic systems are usually treated within DFT. The HK theorem implies that also the magnetization, are functionals of the electronic density alone. This, however, assumes the knowledge of the magnetization as a functional of the density. To
approximate this functional is extremely hard and, in practice, one chooses a different approach. The task can be vastly simplified by treating the magnetization, i.e., the order parameter of the magnetic state, as an additional fundamental density in the density functional framework. An auxiliary field, here a magnetic field, is introduced, which couples to and breaks the corresponding (rotational) symmetry of the Hamiltonian. In other words, it drives the system into the ordered state. The resulting magnetization then leads to a finite value of the effective magnetic field. If the system wants to be magnetic, the order parameter will survive even if the auxiliary perturbation is switched off again. In this way, the ground-state magnetization density is determined by minimizing the total energy functional (free energy functional for finite temperature calculations) with respect to both the normal density and the magnetization density. Much simpler approximations to the exchange-correlation functional (now a functional of two densities) can lead to satisfactory results. This idea is the basis of the local spin density approximation and, likewise, of current density functional theory.

The same idea is also at the heart of density functional theory for superconductors[2-4], as formulated by Oliveira, Gross and Kohn. Here the order parameter is the so-called anomalous density, and the corresponding potential is the non-local pairing potential. It can be interpreted as an external pairing field, induced by an adjacent superconductor via the proximity effect. Again, this external field only acts to break the symmetry (here the gauge symmetry) of the system, and is set to zero at the end of the calculation. As in the case of magnetism, the order parameter will be sustained by the self-consistent effective pairing field, if the system wants to be superconducting. The formalism outlined so far captures, in principle, all electronic degrees of freedom. In order to describe phonon-mediated superconductors, also the electron-phonon interaction has to be taken into account. In the weak coupling limit, this phonon-mediated interaction can be added as an additional BCS-type interaction. However, in order to treat also strong electron-phonon coupling, the electronic and the nuclear degrees of freedom have to be treated on equal footing. This can be achieved by a multi-component DFT, based on both the electronic density and the nuclear density. The extension of this framework to a more general case is straightforward. Note that there is no external potential in the Hamiltonian. In addition to the normal and anomalous electronic densities, we also include the diagonal of the nuclear density matrix.

As usual, the Hohenberg-Kohn theorem guarantees a one-to-one mapping between the set of these three densities in thermal equilibrium and the set of their conjugate potentials. In standard DFT one normally defines a Kohn-Sham system, i.e., a non-interacting system chosen such that it has the same ground-state density as the interacting one. In our formalism, the Kohn-Sham system consists of non-interacting and superconducting electrons, and interacting nuclei. The problem of minimizing the Kohn-Sham grand canonical potential can be transformed into a set of three differential equations that have to be solved self-consistently: One equation for the nuclei, which resembles the familiar nuclear Born-Oppenheimer equation, and two coupled equations which describe the electronic degrees of freedom and have the algebraic structure of the Bogoliubov-de Gennes equations. With a few physically sound approximations, we finally arrive at the formulation of a gap equation, formally looking like that of BCS theory, but with interaction parameters completely ab-initio and derived from normal state DFT calculations.

To show the capability of our method, we show in Fig. 1 and Fig. 2 the critical temperatures and superconducting gaps for several, elemental materials[4]: we clearly see that the agreement is very good.
MgB$_2$

MgB$_2$, with its $T_c=39.5$ K, is very likely the most remarkable electron-phonon superconductor known to date. Besides the high $T_c$ value, it has rather peculiar properties, such as the presence of two superconducting gaps at the Fermi level. The possibility of two-band superconductivity has long been known to favor a high critical temperature. MgB$_2$, however, is the best realization of such concept, with a large enhancement of $T_c$ by multiband effects. We first outline its electronic structure (Fig. 3), and then describe the application of density functional theory for the superconducting state to the case of MgB$_2$[6,7].

The Fermi surface (FS) of MgB$_2$ has several sheets with different orbital character. In particular, two tubular structures with $\sigma$ character are very strongly coupled to the $E_{2g}$ phonon mode, corresponding to a B-B bond-stretching in the boron planes. MgB$_2$ also has three-dimensional bands, that give rise to a complicated Fermi surface. Without holes in the bands, the compound would not be superconducting, like AlB$_2$. The $\pi$ bands are coupled much less efficiently to phonons, but are nevertheless crucial to superconductivity. A remarkable feature of this compound is the presence of two gaps on the $\sigma$ and $\pi$ bands, as clearly demonstrated by several different experiments.

In our density-functional calculations we used the four, band resolved, Eliashberg functions by Golubov et al.[8]. Our procedure keeps the fundamental distinction between $\sigma$ and $\pi$ gaps, analogously to the Eliashberg calculations reported to date.

In Fig. 4(a), the superconducting gaps are plotted versus temperature, together with a few recent experimental results. The agreement is striking: the values of $T_c$ (34.1 K) and of $\Delta_\sigma$ and $\Delta_\pi$ at $T=0$ K are very close to the experimental data. Moreover, the temperature behavior of both gaps, along with their strongly non-BCS behavior, are very well reproduced. Obviously, unlike calculations performed using Eliashberg theory, we do not reproduce exactly the experimental critical temperature, as our calculations are not fitted to match any experimental quantity.

We also calculated the Kohn-Sham entropy as a function of temperature and, from its temperature derivative, the specific heat. In order to compare our results with experiments, we plot in Fig. 4(b) the reduced specific heat versus temperature, normalized to $T_c$ (using the corresponding experimental and calculated $T_c$ values). Both the shape of the curve as well as the discontinuity at $T_c$ are almost perfectly reproduced. We recall that the low temperature shoulder comes from the presence of the smaller gap and that our is slightly different from the experimental ratio.

The predictive power of our method, it is only one part of our investigation. Another important aspect is to gain further insight into the peculiar superconductivity of MgB$_2$. To this end, we performed a calculation using an average functional form for the Coulomb interaction, not distinguishing between $\sigma$ and $\pi$ bands. This functional corresponds to a semiclassical $t$-reatment valid in the limit of slowly varying densities, and actually leads to a good agreement with the full matrix element calculation for s-p metals, and works reasonably also in d metals as Nb. We obtain $T_c$ = 52 K, with the gaps being 9.8 meV and 1.9
meV, respectively. This test shows that the repulsion among \( \sigma \) states, stronger than within \( \pi \) and between \( \sigma \) and \( \pi \) is crucial in determining the experimental \( T_c \). If we, on the other hand, average the \( \sigma \) and \( \pi \) electron-phonon interactions, we obtain \( T_c = 20 \) K, which clearly shows the importance of multiband effects in enhancing the critical temperature of this material.

**INTERCALATED GRAPHITE CaC\(_6\)**

MgB\(_2\) has triggered the interest on materials sharing structural similarities, such as graphite. Graphite intercalated compounds (GICs) were first found to be superconductors in 1965. Doping with Li, Na and K however, produced superconductivity only at low temperatures around 1 K. During the past year, GICs have enjoyed renewed attention after the discovery of superconductivity in CaC\(_6\) and YbC\(_6\) at 11.5 and 6.5 K respectively[9].

From the theoretical point of view, the most important question is related to the pairing mechanism active in these compounds. Ab initio calculations of the electronic and dynamical properties of CaC\(_6\) have pointed out that electron-phonon coupling is sufficient to yield the observed \( T_c \)[10].

The phonons mostly contributing to superconductivity belong to an optical branch involving Ca displacements and, to a lower extent, to two C-related branches at a much higher frequency. However, despite these detailed investigations, some aspects have remained unsolved in particular, the experimental specific heat behavior was first interpreted as an indication of isotropic one-gap BCS superconductivity, but later this interpretation was questioned; experimental results on the isotopic effect, a clear indication of the e-ph mechanism, report a large Ca isotope coefficient 0.5, while ab-initio calculations based on the McMillan equation report a much lower value 0.25. These problems were used to discuss the possibility of anisotropic superconductivity[11]. In fact, the electronic structure of CaC\(_6\) around the Fermi level \( E_F \) as shown in the upper panel of Fig. 5, is quite rich. Together with nearly two dimensional C bands (blue in Fig. 5), there is a three-dimensional band with a free-electron interlayer behavior (yellow). In CaC\(_6\) this band gains a further strong contribution from Ca 4s and 3d orbitals. This band is coupled to the Ca optical in-plane phonon branch; these low-frequency modes provide a strong contribution to the e-ph constant, as can be seen in the electron-phonon coupling function in the lower panel of Fig. 5. On the other hand stiff C modes are also strongly coupled with electrons providing both to a second important contribution to the coupling, and to high energy modes that increase the energy with which the superconducting coupling is effective around the Fermi energy.

We report here the results of ab-initio calculations of anisotropic superconductivity in CaC\(_6\). We use our results to interpret the experimental temperature dependence of the specific heat in CaC\(_6\), and discuss tunneling experiments.

![Fig. 5: Upper Panel: Band structure of CaC\(_6\) in a small energy window around the Fermi Energy (chosen as the zero of the scale). Colors, going from light green to yellow, indicate the charge projection over the atomic orbitals of C and Ca atoms. Lower Panel: Phononic dispersions of CaC\(_6\); green, blue and bordeaux dots correspond respectively to in plane C, out of plane C and Ca modes. The electron-phonon coupling function is reported on the left.](image)

![Fig. 6: Color Fermi surfaces of CaC\(_6\), with a color coding indicating (a) the larger contribution to the charge projection; (b) superconducting gap; (c) electron-phonon coupling summed over the three major groups of phonon modes; the number indicates the factor by which one should multiply the value read in the scale.](image)
In our calculations the full anisotropy is maintained, which results in a band- and k-dependent superconducting gap over the FS’s. In CaC₆, the σ bands are completely filled, and at the Fermi level only the C π bands are present, forming two-dimensional, wrapped cylindrical FS sheets running along the direction perpendicular to the graphene layers. However, we also find a part of the FS coming from the interlayer bands, mixed with Ca s and dₓ²−ᵧ² states; the latter orbitals, empty in atomic Ca, are partially occupied in the solid. These states form an almost spherical FS, intersecting the C FS. Because of the k-point-dependent mixing, the nature of electron states changes in the different FS sheets but also within each sheet. Clearly, this situation suggests the possibility of a strongly k-dependent superconducting gap.

In Fig. 6a we show the dominant orbital character over the Fermi surface. We see that, while C states are dominant and homogeneous on the tubular FS structures with a minor contribution from dₓ²−ᵧ² and dₓ²+y² Ca states, Ca orbitals contribute anisotropically on the internal, spherical FS: the dₓ² components dominate on the portions oriented along the directions perpendicular to the graphene planes, whereas on the remaining parts of the FS a mixture of s and interlayer states dominates. The tubular and spherical FS’s mix on the intersection regions, but the mixing is small.

Our calculations lead to a electron-phonon coupling constant λ = 0.85, in good agreement with previous calculations[10]. Solving the gap equation for the superconducting gap as a function of T, we calculate the critical temperature. We obtain Tc,calc = 9.4 K, in good agreement with the experimental value Tc,exp = 11.5 K. We emphasize in this context that our calculations have no adjustable parameter, and that the superconducting properties have an intrinsically exponential dependence on the couplings, which makes an accurate calculation of Tc a hard task.

Figure 6b shows, under two different perspectives, the T = 0 K superconducting gap, on the different parts of the FS. We clearly see a correlation between the orbital character of states and the gap, which is larger for the Ca-dominated FS. Furthermore, we notice the presence of some anisotropy on the individual FS sheets; in particular, the region close to the intersection between tubular and spherical parts shows the largest variations.

This structure of the superconducting gap is mainly due to the different electron-phonon couplings on the FS sheets. Figure 6c shows the coupling summed over modes belonging to three main groups of peaks in the phononic density of states, i.e., the group of soft Ca modes centered at about 15 meV; that of out-of-plane C modes at 60 meV; and that of C in-plane modes at 170 meV (see Fig. 5). The first and to a lesser extent second groups give a large contribution to the global coupling with the interlayer band spherical FS; while the Ca modes give a roughly homogeneous coupling, the C out-of-plane modes interact mainly with the s region of this part of the Fermi surface. The C in-plane modes give a contribution to the global coupling which is smaller and, as expected, couple strictly with C states. The energy dependent gap distribution emphasizes more clearly this anisotropy. To each isoenergy surface corresponds a large spread of gaps: the largest and the smallest values differs roughly by a factor of 2, smaller than the difference between the gaps in MgB2 but far from negligible. Unlike in MgB2, we have a continuum of gap values; their average value, 1.63 meV, compares well with experiments giving 1.79 and 1.6 eV by penetration depth and scanning tunneling microscope STM measurements, respectively.

In Fig. 7a we plot the temperature dependence of the difference between the superconducting and normal specific heats of CaC₆, compared with experiment[12]. To avoid the amplification of differences between experimental and theoretical Tc and Sommerfeld constant γ, we normalize T and C/T, respectively, to Tc and C/T both experimental and theoretical. Our calculations (full black curve) compare rather well with experiment, basically in the whole temperature range. The discontinuity at Tc is quite close to the BCS value 1.43, as expected in the presence of medium coupling strength. Specific heat data were originally used to argue for an isotropic superconducting order parameter, and later questioned by Mazin et al.[13] who found that the experimental specific heat cannot be reconciled with the isotropic model. To investigate this point further, we performed a calculation of the specific heat using isotropically averaged interactions. We can see that the corresponding results show a clear discrepancy from experiment, much larger than that of the anisotropic calculation, with a general shape quite similar to the one
found in the calculations by Mazin et al. In particular, in the low-temperature region the isotropic results are too low compared with experiments. To investigate this point further, we plot in Fig. 7a similar data for Nb. It turns out that, when properly renormalized, the same general trend is common to these isotropic calculations, with some obvious differences due to the strength of the coupling jump at $T_c$.

Scanning tunneling microscopy experiments have been recently performed\[14\] on polycrystalline CaC6 films oriented along the c axis. According to the authors, the tunneling current should come mainly from the Ca-related three-dimensional spherical FS, but this analysis could be modified by several experimental effects. They could obtain a good fit of experiments by smearing a BCS single-gap curve with a 0.2 meV broadening. Figure 7b shows the experimental data, together with our results, obtained by calculating the superconducting density of states DOS, normalized to the normal-state DOS and filtered with a thermal broadening similar to the experimental one. We use both the anisotropic gap results and its average over isoenergy surfaces. The agreement is pretty good, apart from the two bumps at $\pm 5$ meV, which depend on the computational details e.g., FS sampling and are equal in the anisotropic and isotropic calculations. We conclude that the experimental results can be equally well reproduced using an anisotropic gap, or by a larger smearing of a BCS isotropic curve, originating from experimental reasons. Clearly, we do not have two distinct gaps.

**ALKALI METALS AND AI UNDER HIGH PRESSURE**

The effect of high pressure on phonon-mediated superconductors has been the subject of many investigations. These studies revealed a strong material dependence: applied pressure suppresses superconductivity in some materials and favors it in others. Even in simple metals, the physics underlying pressure effects on the superconducting properties can be very complicated (see Ref. [15] and references therein). For example, Li, K and Al behave in many circumstances like nearly free-electron gases, but they exhibit very different behaviors under pressure, still only partially understood within the Eliashberg theory. At ambient pressure, Al is a superconductor with $T_c \approx 1.18$ K. Pressure rapidly reduces $T_c$, bringing it down to 0.075 K at 6.2 GPa. Lithium, on the other hand, is a rather complex material: Below 77 K and at zero pressure, it shows a martensitic transition to energetically competing closed packed structures; from 7.5 to 70 GPa, it undergoes several structural transitions suggesting the presence of strong electron-phonon interactions. No sign of a transition to a superconducting state above 4 K was found up to $\approx 20$ GPa, while, at higher pressures, Li becomes a superconductor. In the range 20 – 38.3 GPa, where Li crystallizes in an fcc structure, experiments found that $T_c$ increases rapidly with pressure, reaching values around 12 –17 K (the highest $T_c$ observed so far in any elemental superconductor). K undergoes several phase transitions and is stable in the fcc phase between 11.6 and 23 GPa, but no experimental evidence of superconductivity exists. Precedent theoretical studies based on the Eliashberg theory have shown a satisfactory agreement with experiments for Al, whereas in the case of Li, much too high $T_c$ (45 –75 K) were obtained clearly overestimating the measured critical temperature. For K, $T_c = 9$ K was obtained at 13.5 GPa.

Using the SCDFD we explored the superconducting properties of Li, K, and Al under pressure[15,16]. This study provides a detailed description of the subtlety of superconductivity in Li, where the incipient phase transitions produce a phonon softening and a very strong electron-phonon coupling, thus enhancing $T_c$ up to values unusually large for simple elemental metals. We predict K to be superconducting, with a $T_c$ up to $\approx 2$ K in the experimental stability range of the fcc structure and up to 11 K in the range of stable calculated phonon frequencies.

![Fig.8: Comparison between calculated and experimental critical temperatures for fcc Al (upper panel), K (middle panel), and Li (lower panel). Different symbols with the same color refer to the same experimental report with different setups. Vertical dashed lines indicate the experimental structural transition pressures for Li and K.](image)

The LDA underestimates the equilibrium volume of Li and Al, as it can be observed by calculating the equation of state using Murnaghan’s formula. To compensate for this systematic error, we apply a positive pressure shift of about 3.5 and 2 GPa for Al and Li, respectively. This is the amount required to match the experimental equation of state. These shifts will always be included in the values given in the following. No shift is needed for K.
In Fig. 8, we compare the calculated pressure dependence of $T_c$ for Al, K, and Li with available experimental results. For Al, SCDFT calculations match exactly the experimental zero pressure $T_c = 1.18$ K and reproduce the rapid decrease of the transition temperature. In the same figure, we report the estimation of $T_c$ by means of McMillan’s formula.

In the case of Li (lower panel in Fig. 8), despite the poor agreement among the four sets of experimental data, the most recent experiments agree in: (i) Li is not superconducting at ambient pressure; (ii) $T_c$ is lower than 4 K up to 20 GPa; and (iii) $T_c$ then increases with pressure, reaching 14 K at about 30 GPa. The only exception to this behavior is a very early report. At even higher pressures, experiments show a quite complex behavior (see below).

In Li, on the other hand, the phonon frequencies exhibit a quite different behavior. In Fig. 9, we present the phonon dispersion of the lowest branch along the X-K line of the Brillouin zone. For pressures up to 8 GPa, there is an increase of the phonon frequencies, as in the case of Al.

However, as the pressure is raised further, the phonons near the K point start to soften. The softenings continue up to 33 GPa, when this frequency becomes imaginary. A closer inspection of Fig. 9 reveals that, already at around 30 GPa, a phonon mode close to the X point develops an imaginary frequency. We believe that this marks the transition to the hR1 (rhombohedral symmetry) phase, but further analysis would be required to fully validate this assumption. In addition, the Eliashberg spectral function shows a high-frequency peak whose height decreases as a function of pressure. These factors contribute to the decrease of $T_c$ (see the inset in Fig. 8) and, consequently, of the critical temperature $T_c$.

Within this scenario, our calculated SCDFT results are in excellent quantitative agreement with the most recent experiments up to about 30 GPa. We find that Li is not superconducting up to 8 GPa and that $T_c$ shows two different trends with pressure, a first region (8 – 20 GPa), in which $T_c$ increases at a rate of region (20 – 30 GPa) at K shows a behavior quite similar to Li: Beyond a pressure threshold (20 GPa), $T_c$ rises rapidly. In the range where phonons were found to be stable, it reaches 11 K at 29 GPa; the experimentally observed instability of the fcc phase, however, limits this value to 2 K at 23 GPa.

The differences between Al and Li can be understood by looking at the e-ph coupling as a function of pressure. In Al, the phonon frequencies increase as the pressure rises (this corresponds to the normal stiffening of phonons with increased pressure). In addition, the Eliashberg spectral function $\alpha^2 F$ (which gives the frequency-resolved contribution to the electron-phonon coupling) shows a high frequency peak whose height decreases as a function of pressure. These factors contribute to the decrease of $\lambda$ (see the inset in Fig. 8) and, consequently, of the critical temperature $T_c$.

In Fig. 10, we present the phonon dispersion of the lowest branch along the X-K line of the Brillouin zone. For pressures up to 8 GPa, there is an increase of the phonon frequencies, as in the case of Al.

On the top right: a FS cut on a (110) plane, including both the L and the $\Gamma$ k-points, highlights the FS nesting. The arrows represent the nesting vectors.

**Fig. 10:** On the left: 3D view of the Fermi surface of Li, at 28.6 GPa, with a color scale indicating the value of $\Delta$. The red color indicates high values of $\Delta$.

**Fig. 9:** Upper panel: Phonon dispersion of Li, at different pressures, for the lower frequency mode. Lower panel: e-ph coupling $\lambda_{\text{el},\text{ph}}$ and phonon linewidth $\gamma_{\text{el},\text{ph}}$. 

The observed phonon softening as a function of pressure is a direct consequence of the presence of FS nestings. To demonstrate this idea, we plot in Fig. 10 a cut of the FS parallel to the (110) plane which includes the L and the $\Gamma$ point. We clearly recognize nesting vectors (indicated by arrows) connecting fairly flat and parallel lines. The effects of nesting are remarkably enhanced by the strong e-ph matrix elements. The observed phonon softening as a function of pressure is a direct consequence of the presence of the FS nesting. In turn, the progressive FS nesting with the increase of pressure is a consequence of the FS topological transition from a spherical free-electron like to a distorted anisotropic shape (see Fig. 3). This topological transition is a manifestation of an “s-p” transition of the electronic states near $E_F$. In particular, we can see in Fig. 3(a) that the k-resolved $\Delta$ is maximum on
the rings of the FS around the L-point, arising from mostly p-like and strongly covalently bonded states. An analogous “s-d” transition occurs in K.

CONCLUSIONS

In conclusion, we showed how modern developments in solid state theory, with the help of the availability of large computing facilities, can lead to a detailed understanding of superconductivity in newly discovered electron-phonon superconductors. We examined the cases of MgB$_2$, CaC$_6$, and simple metals under high pressure; each of these systems introduces new features which make it unique and interesting in its own.

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