Electron-phonon superconductivity in $A\text{Pt}_3\text{P} (A=\text{Sr}, \text{Ca}, \text{La})$ compounds: From weak to strong coupling

Alaska Subedi, Luciano Ortenzi, and Lilja Boeri

Max Planck Institute for Solid State Research, Heisenbergstr. 1, D-70569 Stuttgart, Germany

We study the newly-discovered Pt phosphides $A\text{Pt}_3\text{P} (A=\text{Sr}, \text{Ca}, \text{La})$ [T. Takayama, et al., Phys. Rev. Lett. 108, 237001] using first-principles calculations and Migdal-Eliashberg theory. Given the remarkable agreement with the experiment, we exclude the charge-density wave scenario proposed by previous first-principles calculations, and give conclusive answers concerning the superconducting state in these materials. The pairing increases from La to Ca and Sr due to changes in the electron-phonon matrix elements and low frequency phonons. Although we find that all three compounds are well described by conventional $s$-wave superconductivity and spin orbit coupling of Pt plays a marginal role, we show that it could be possible to tune the structure from centrosymmetric to non centrosymmetric opening new perspectives towards the understanding of unconventional superconductivity.

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I. INTRODUCTION

In the last ten years, several important discoveries have sensibly advanced our understanding of superconductivity: a record $T_c$ of 39 K in the BCS superconductor MgB$_2$, exotic superconductivity with $T_c$ of up to 56 K in the iron-based superconductors, as well as superconductivity in boron-doped diamond, aromatic compounds, and so on. At the same time, ideas percolating from other fields of condensed matter have brought in new twists into this old and fascinating phenomenon. For example, the recent interest in spin-orbit coupling (SOC) has revived the discussion on superconductivity in non-centrosymmetric crystals (NCSC), boosted by the discovery of the heavy fermion CePt$_3$Si ($T_c$=0.75 K) in 2004. In crystals without inversion symmetry, a strong antisymmetric SOC that lifts the spin degeneracy can be conducive to exotic pairing symmetry. Because of the large SOC of Pt ($Z=78$), this makes Pt-based compounds promising candidates for exotic superconductivity, as discussed for SrPtAs.

Recently, Takayama et al. discovered a new family of ternary platinum phosphide superconductors with chemical formula $A\text{Pt}_3\text{P} (A=\text{Sr}, \text{Ca}, \text{La})$ and $T_c$'s of 8.4 K, 6.6 K and 1.5 K, respectively. Besides the relatively high $T_c$, these compounds exhibit a very interesting crystal structure, which is a centrosymmetric variant of the CePt$_3$Si one. The authors have suggested that this discovery would have a very strong impact in the field of superconductivity if one could synthesize both centrosymmetric and non-centrosymmetric variants of superconductors consisting of the electronically equivalent elements. This would in fact allow to study the effect of inversion symmetry on superconductivity in a controlled way. The nature of the superconducting pairing in the $A\text{Pt}_3\text{P}$ compounds has been debated through experiments and ab initio calculations. In the original discovery paper, it was proposed that, at least in SrPt$_3$P, the superconductivity is of strong-coupling $s$-wave type with clear signatures of low-lying phonons and large BCS ratios suggestive of multiband behavior. Ref. has instead proposed that $T_c$ is enhanced by the proximity to a dynamical charge-density wave (CDW) instability, and that a strong SOC could eventually lead to exotic superconductivity in LaPt$_3$P. Ref. found no indication of CDW instability, and supported a conventional electron-phonon (EP) scenario.

In this paper, we employ first principles calculations and Migdal-Eliashberg theory to study superconductivity in the $A\text{Pt}_3\text{P}$ phosphides. We find that SOC plays a marginal role in all three compounds and show that the available experimental data are quantitatively reproduced by conventional EP theory, based on well-converged electronic and phonon spectra. This rules out exotic pairing and CDW instabilities. In fact, the $A\text{Pt}_3\text{P}$ series is a textbook example for EP superconductivity: LaPt$_3$P, where $T_c$ is only 1.5 K, is a typical low-$T_c$ superconductor in which all phonon branches are moderately coupled to the electrons at $E_F$. Lowering the electronic filling from trivalent La to divalent Sr and Ca brings about an intense EP coupling that is concentrated in low-lying phonon branches with substantial Pt in-plane breathing character. In SrPt$_3$P, these branches are flat and have low frequencies, and this entirely explains the large value of its BCS ratios with no need for multiband effects.

II. METHODS

Our calculations employ density functional perturbation theory (GGA) as implemented in the Quantum-ESPRESSO package. We use ultrasoft pseudopotentials and basis set cutoffs of 40 Ry and 400 Ry for wave function and charge density, respectively. We use an $8 \times 8 \times 8$ grid for zone integration in the self-consistent calculations, while a denser $16 \times 16 \times 16$ grid is used in the electron-phonon

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coupling calculations. The dynamical matrices are calculated on an 8 \times 8 grid, and phonon dispersions and DOS are then obtained by Fourier interpolation. The results of the structural relaxation were tested with the all-electron code Wien2k, which employs the full potential linear augmented plane wave method.\[2,20\]

### III. STRUCTURE

Fig. 1(a) shows the crystal structure of the APt$_3$P phosphides (space group P4/nmm). In these tetragonal antiperovskites, the ionic radii of Pt and P ions are similar, and the P ions off-center from the octahedral basal plane formed by the Pt(1) ions as the P ion is too big to fit into the center of the Pt(1) square. The apical Pt(2) ion that is further from the P ion also moves closer to the basal plane to ensure closer packing of the constituent ions. The distortions of the XPt$_6$ octahedra occurs in both the phosphides (X=P) and in the non-centrosymmetric rare-earth silicides CePt$_3$Si and LaPt$_3$Si (X=Si), with space group P4mm. What distinguishes the two structures is the in-plane arrangement of the octahedra. In the silicides, the distortions have a polar arrangement, i.e. they all point in the same direction, and the resulting structure has a inversion symmetry. The corresponding unit cell that contains one formula unit (f.u.) is shown with dashed lines in Fig. 1(c). With full lines we show the $\sqrt{2} \times \sqrt{2}$ cell of the phosphides, where the distortions alternate in a checkerboard fashion and restore the inversion symmetry (antipolar structure). Therefore, the unit cell comprises two f.u., and $A$, Pt(1), Pt(2) and P occupy 2a, 4e, 2c and 2e Wyckoff positions respectively. We relaxed the structures fully within GGA such that the force on each atom is less than $10^{-5}$ Ry/Bohr. The relaxed parameters are given in Table I.

The crystal structure of APt$_3$P, with space group P4/nmm, and that of REPt$_3$Si (RE=La, Ce), with space group P4/mmm, can be seen as variants of the same antiperovskite structure, which differ only for the in-plane polar arrangement of the distorted XPt$_6$ octahedra. For A=La both the non-centrosymmetric (P4/nmm) silicide and the centrosymmetric (P4/mmm) phosphide compound exist, and are superconducting with low $T_c$’s $\lesssim 2K$, while for A=Ca, Sr to our knowledge only the phosphides have been synthesized.

We have studied the relative stability of the two structures for APt$_3$ silicides and phosphides, using total energy calculations. The structures were fully relaxed in GGA at zero pressure. For the existing compounds, the relaxed parameters are within $\sim$2% of the experimental values.

In Fig. 2 we plot the difference in total energies between the antipolar and polar structures ($E_{AP} - E_P$). The difference is negative for phosphides (full symbols), and positive for silicides (empty symbols), with approximately an order of magnitude difference between the two cases. The small energy differences found in the phosphides (a few tens meV), and in particular for CaPt$_3$P, indicates that it might be indeed possible to synthesize these compounds also in the polar variant, realizing the proposal of Takayama et al. to study the lack of inversion symmetry in electronically-equivalent compounds.\[11\]

### TABLE I: Fully relaxed structural parameters (GGA) for the APt$_3$P compounds in the experimental P4/nmm structure.

|       | a(\AA) | c(\AA) | $z_{P12}$ | $z_P$ |
|-------|--------|--------|-----------|-------|
| SrPt$_3$P | 5.898  | 5.470  | 0.1362    | 0.7227|
| CaPt$_3$P | 5.758  | 5.494  | 0.1357    | 0.7303|
| LaPt$_3$P | 5.838  | 5.553  | 0.1418    | 0.7719|

FIG. 1: (Color online) (a) Crystal structure of APt$_3$P, space group P4/nmm. The $\sqrt{2} \times \sqrt{2}$ in-plane arrangement of the distorted XPt$_6$ octahedra (b) distinguishes the APt$_3$P compounds from the non-centrosymmetric CePt$_3$Si superconductor (space group P4mm); the corresponding unit cells are shown as full and dashed lines in panel (c).

FIG. 2: Total energy difference between the antipolar and polar structure for phosphides (full symbols) and selenides (empty symbols), in the fully relaxed GGA structure at zero pressure.
IV. ELECTRONIC STRUCTURE

In the following, we stick to the $\text{APt}_3\text{P}$ compounds in the $P4/nmm$ structure, employing fully relaxed lattice constants and internal parameters. Our electronic structures are in very good agreement with previous calculations.\cite{12,13} A zoom-in of the bands for energies $\pm 1$ eV around the Fermi level ($E_F$), with (red, dashed) and without (black, solid) SOC, is shown in Fig. 3. Only in LaPt$_3$P does the SOC lead to a visible lifting of some band degeneracies. But even in this case, the bands remain spin degenerate, in contrast to what is claimed by Ref.\cite{13}. Since the SOC plays only a marginal role on the electronic states near $E_F$, we neglect it in the following.

Fig. 4 shows the “fat” bands without the SOC of the three $\text{APt}_3\text{P}$ compounds, highlighting the orbital characters which give the highest contribution to the electronic states at the Fermi surface. The axes are oriented along the shortest in-plane Pt-Pt distance. The Fermi surface of the $A^{2+}$ compounds comprises a large, low dispersive sheet, formed by the band with prominent Pt(1) $d_{x^2-y^2}$ character which crosses $E_F$ along the $\Gamma - X - M$ line; two other bands, with more Pt(2), P and interstitial character, form two more dispersive pockets, \textit{i.e.} a large, flat, structure centered around the $\Gamma$ point, and a small cigar-shaped hole pocket around the $Z$ point. These bands

FIG. 3: (Color online) Electronic structure of $\text{APt}_3\text{P}$ with (red, dashed line) and without (black, solid line) spin orbit coupling (SOC); the zero of the energy is the Fermi level.

FIG. 4: “Fat bands” of $\text{APt}_3\text{P}$, decorated with partial orbital characters. $xy(1)$ and $yz(1)$ are in-plane Pt (Pt(1)) partial characters; $yz(2)$ refers to Pt apical atoms (Pt(2)); Int is interstitial.
cross $E_F$ along the $Z - R - A$ line. This unequal distribution of orbital characters on the Fermi surface suggests that the superconducting gap may be anisotropic. LaPt$_3$P, with one more electron per f.u. has its Fermi level shifted up by $\sim 0.5$ eV, and the band with low dispersion along $M - \Gamma$ is completely full. The Fermi surface is composed of highly dispersive sheets, with strongly mixed orbital contributions of Pt(2), P and Pt(1) characters.

V. PHONON DISPERSIONS AND ELECTRON-PHONON COUPLING

The three compounds have very similar phonon dispersions, shown in the left panels of Fig. 5. The thirty phonon branches extend up to $\sim 450$ cm$^{-1}$, with two upper branches of mostly out-of-plane P character, four intermediate branches at $\sim 300$ cm$^{-1}$ that show mostly in-plane vibration of P, and a lower manifold of the twenty-four strongly intertwined branches, with mixed $A$, Pt(1) and Pt(2) character.

There is a substantial difference in the three Eliashberg functions $\alpha^2 F(\omega)$, plotted in the rightmost panels of Fig. 5 and defined as:

$$\alpha^2 F(\omega) = \frac{1}{N(0)} \sum_{\kappa, q, n, m} \delta(\epsilon^m_{\kappa q})\delta(\epsilon^m_{\kappa q}) g_{\kappa q}^{n \kappa q} |2 \delta(\omega - \omega^{\nu}_q)|,$$

where $\omega^{\nu}_q$ are phonon frequencies, $\epsilon^n_{\kappa}$ electronic energies, and $g_{\kappa q}^{n \kappa q}$ EP matrix elements. The $\alpha^2 F(\omega)$ yield information not only on the intensity of the total EP coupling (EPC) $\lambda$, but also on the nature of the bonding and character of the superconducting state. In general, an $\alpha^2 F(\omega)$ roughly proportional to the PDOS is characteristic of metals with a weak to moderate total coupling and low $T^*_c < 5$ K. The best EP superconductors, such as MgB$_2$ and A15’s, are instead characterized by $\alpha^2 F(\omega)$ which display sharp peaks only at specific parts of the phonon spectrum, reflecting a strong coupling between specific electron and phonon states. This requires (partly) covalent bonding. It is not uncommon that within the same family of materials the electron count changes the EP coupling regime from weak to strong, depending on the nature of the electronic states at $E_F$ selected by the two $\delta$ functions in Eq. 1.

Fig. 5 shows that while the coupling is uniform in LaPt$_3$P, in the two $A^{2+}$ compounds it is strongly enhanced at low frequencies. Furthermore, it is almost entirely concentrated in the low-lying phonon branches with substantial Pt(1) in-plane breathing character, which at the $\Gamma$ point has $B_{2u}$ symmetry — $\omega_2^*$ in the following 33,34. These modes are very low in energy and almost dispersionless in SrPt$_3$P ($\omega \sim 50$ cm$^{-1}$) and slightly harder in Ca, where they have a sizable dispersion that extends up to $\sim 100$ cm$^{-1}$. One can trace their evolution in the two compounds by following the largest $\lambda^{\nu}_q$ symbols that decorate the phonon dispersions, or looking at the partial Pt(1) phonon DOS plotted in the middle panel of Fig. 5. In-plane Pt breathing modes couple more strongly to the Pt(1) in-plane electronic states, and less to other partial characters. This causes some anisotropy in the $k$ space distribution of the EPC and, as a consequence, in the $q$-dependence of the $\lambda^{\nu}_q$ in the $A^{2+}$Pt$_3$P, and explains the much lower coupling in LaPt$_3$P.

The total EPC constant $\lambda = \sum_{\kappa q} \lambda^{\nu}_q = 2 \int_0^\infty \alpha^2 F(\omega) d\omega$ is quite low in LaPt$_3$P ($\lambda = 0.57$) but sizable both in CaPt$_3$P ($\lambda = 0.85$) and SrPt$_3$P ($\lambda = 1.33$). Due to the $1/\omega$ factor, the EPC is strongly enhanced in SrPt$_3$P with respect to CaPt$_3$P because a considerable part of the breathing branches is shifted to low frequen-
cies. A similar softening of the breathing branch is discussed by Chen et al., who find a dynamical instability of the breathing branch, which we cannot reproduce. For some q points where the differences in $\omega_{q}^{\text{br}}$ are large, the partial EPC constants $\lambda_{q}^{\text{br}} = \text{const} \times I_{q}^{\text{br}}/\omega_{q}^{\text{br}}$ differ by as much as a factor three despite a very small difference ($\sim 10\%$) in the matrix elements ($I_{q}^{\text{br}}$), as shown in Table II. These results demonstrate that the lowering of the frequencies in Sr with respect to Ca is not due to increased EP coupling. Rather, this is almost entirely a structural effect, since we find that $\omega_{q}^{\text{br}}$ is increased (reduced) by reducing (increasing) the in-plane lattice constant, which in CaPt3P is $\sim 0.14$ A smaller than in SrPt3P. To confirm the strong sensitivity of the Pt(1) breathing branch to the in-plane lattice constant, we have calculated the Γ-point phonon frequencies of SrPt3P as a function of pressure using the theoretical structures that are optimized within the GGA. The frequency of the $B_{2u}$ mode as a function of pressure is plotted in Fig. 6 together with the corresponding value of the in-plane lattice constant $a$. For pressures of $\pm 4$ GPa, we estimate a linear dependence $\omega_{q}^{\text{br}}(P) = +5\text{cm}^{-1}/\text{GPa}$. This translates in an almost linear dependence in terms of the in-plane lattice constant: $\omega_{q}^{\text{br}}(a) \sim -20\text{cm}^{-1}/\text{A}$. From the calculated pressure derivative of the zone-center frequency of SrPt3P, we estimate that this would correspond to a 30 cm$^{-1}$ hardening of the phonon frequency, in remarkable agreement with the values calculated for CaPt3P.

The sensitivity of $\lambda_{q}^{\text{br}}$ to the value of the in-plane lattice constant explains why the regime for superconductivity is weak coupling in Ca and strong coupling in Sr, despite the very close critical temperatures. In fact, the shift of spectral weight in $\alpha^{2}F(\omega)$ to lower energies causes a strong enhancement in $\lambda$, but it also induces a decrease in $\omega_{n}$ as $\omega_{n} = \text{exp} \left(\frac{\mu}{T} \int_{0}^{\infty} d\omega/\omega^{2}F(\omega) \ln \omega\right)$—see Table III. These two factors compensate in the Allen-Dynes expression for $T_{c}$:

$$T_{c} = \frac{\omega_{n}}{1.20} \exp \left(\frac{-1.04(1 + \lambda)}{\lambda - \mu^{*} - 0.62\lambda\mu^{*}}\right),$$

but not in the BCS ratios $(2\Delta/T_{c}, \Delta C/T_{c}, \text{etc.})$, which to a very good approximation depend only on the quantity $T_{c}/\omega_{n}$.

VI. MIGDAL-ELIASHBERG THEORY

In Refs. 13 Marsiglio and Carbottae have shown that the BCS ratios of all known superconductors fall on a universal curve when plotted as a function of $T_{c}/\omega_{n}$. We have obtained the values of the superconducting and thermodynamical quantities from the full solution of the single-band Migdal-Eliashberg equations to locate the A$P_{3}P$ compounds on the Marsiglio-Carbottae plots. As shown in Fig. 7 and from the data summarized in Table III, LaPt3P and CaPt3P, with $T_{c}/\omega_{n}$=0.013 and 0.058, respectively, lie together with elemental metals, while SrPt3P ($T_{c}/\omega_{n}$ = 0.110) is placed at the lower end of a broad class of the low-phonon, strong-coupling superconductors, together with the A15 and Chevrel compounds.

In order to calculate the critical temperatures, gap values and specific heat data presented in Fig. 7 and Table III we solved the Migdal-Eliashberg equations in the single-band case:

$$\phi(\omega_{n}) = \pi T \sum_{m=\pm M} \left[\lambda(\omega_{n} - \omega_{m}) - \mu^{*}\right] \frac{\phi(\omega_{m})}{\sqrt{\omega_{m}^{2}Z^{2}(\omega_{m}) + \phi^{2}(\omega_{m})}}$$

$$Z(\omega_{n})\omega_{n} = \omega_{n} + \pi T \sum_{m=\pm M} \lambda(\omega_{n} - \omega_{m}) \frac{Z(\omega_{m})\omega_{m}}{\sqrt{\omega_{m}^{2}Z^{2}(\omega_{m}) + \phi^{2}(\omega_{m})}}$$

$$\lambda(\omega_{n} - \omega_{m}) = 2 \int_{0}^{\infty} \frac{\Omega^{2}F(\Omega)d\Omega}{\omega_{n} - \omega_{m}^{2} + \Omega^{2}},$$

where $\phi(\omega_{n}) = \Delta(\omega_{n})Z(\omega_{n})$, $\Delta(\omega_{n})$ is the superconducting gap, $Z(\omega_{n})$ is the mass enhancement factor and $M$ is the number of Matsubara frequencies $\omega_{n}$ used in the calculations. We used the Eliashberg functions in Fig. 7 and

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**TABLE II:** Some calculated results for A$P_{3}P$: Electronic density of states at the Fermi level $N(0)$ in states/eV/spin/unit cell; $\omega_{n}$ in $K$; Frequency $\omega_{q}^{\text{br}}$ in cm$^{-1}$; e-ph coupling $\lambda_{q}^{\text{br}}$, and e-ph coupling strength $I_{q}^{\text{br}}$ in cm$^{-1}$ for the in-plane Pt(1) breathing mode at $\Gamma$.

| $P$ (GPa) | $\omega_{n}$ (cm$^{-1}$) | $\omega_{q}^{\text{br}}$ (cm$^{-1}$) | $\lambda_{q}^{\text{br}}$ | $I_{q}^{\text{br}}$ (cm$^{-1}$) |
|-----------|--------------------------|-----------------------------------|--------------------------|-----------------------------|
| 1.94      | 1.47                     | 67.5                              | 0.85                     | 3.95                        |
| 2.36      | 1.47                     | 67.5                              | 0.85                     | 3.95                        |
| 2.37      | 1.47                     | 67.5                              | 0.85                     | 3.95                        |
| 1.94      | 1.47                     | 67.5                              | 0.85                     | 3.95                        |

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**FIG. 6:** SrPt3P: Calculated frequency of the $B_{2u}$ mode of SrPt3P (top) and in-plane lattice constant (bottom) as a function of pressure.
the densities of states in Table I. The value of \( \mu^* \) was chosen to reproduce the experimental \( T_c \)—we obtained \( \mu^* = 0.1 \pm 10\% \) for all three compounds—and kept fixed in the calculations of the specific heat jump and superconducting gap. The specific heat jump was obtained by numerically calculating the difference \( \Delta F(T) \) between the normal state (N) free energy and the superconducting one (S):

\[
\Delta F(T) = -\pi T \sum_{m=-M}^{m=M} \left\{ |\omega_n| |Z_N(\omega_n) - 1| \right. \\
- \frac{2\omega_n^2[|Z_N(\omega_n)| - 1] + 2\phi^2(\omega_n)}{|\omega_n| + \sqrt{\omega_n^2Z_N^2(\omega_n) + \phi^2(\omega_n)}} \\
+ \frac{\omega_n^2Z_S(\omega_n)(Z_S(\omega_n - 1)) + \phi^2(\omega_n)}{\sqrt{\omega_n^2Z_S^2(\omega_n) + \phi^2(\omega_n)}} \right\}
\]

and fitting the obtained curve with a 12th order polynomial. The specific heat was then obtained from the second derivative of the polynomial expansion.

Fig. 8 shows a comparison of the specific heat data with experiments from Ref. 11. In the inset, we compare calculations (solid lines) and experiments (symbols) for the normal total state specific heat of SrPt3P. The lattice specific heat is fitted with: \( c(T) = bT^3 + dT^5 \), \( b = 1.29(1.26) \) mJ/mol K^4, \( d = 8.9(13.0) \) mJ/mol K^6 for theoretical (experimental) data, respectively. This remarkable agreement suggests that our calculated phonon spectra, with a sharp peak at \( \omega \sim 50 \) cm\(^{-1}\), are very close to the actual ones. This allows us to rule out the dynamical instabilities calculated in Ref. 13.

In the main panel of Fig. 8 the superconducting state data for SrPt3P are shown as a blue curve. The single-band Migdal Eliashberg calculations, which yield \( \Delta 0 \sim 4.06 \), reproduce almost exactly the experimental curve. As for the low-\( T_c \) compounds, we again obtain critical temperatures in very good agreement with experiments, with \( \mu^* = 0.1 \), which is a strong indication in favor of conventional superconductivity. CaPt3P (red curves in Fig. 8) displays a mass enhancement in the normal state that is 2.5 times larger than the calculated one, which we attribute to the presence of additional superconducting phases in the sample. All other quantities are in line with our calculations. In fact, using the calculated value of \( \gamma_N = 10.5 \) mJ mol\(^{-1}\) K\(^{-2}\), we obtain also a reasonable fit to the specific heat jump, as shown in Fig. 8. For LaPt3P (green curves in Fig. 8) we obtain a fairly good agreement for the normal state quantities, while the superconducting state data are probably too noisy for a meaningful comparison.

Fig. 7 clearly shows that the values we obtain for all three APr3P compounds are fully in line with other EP superconductors. The very high BCS ratio \( 2\Delta/T_c = 5.0 \) reported from Takayama et al.\(^{11}\) for SrPt3P lies instead out of the general trend. In Fig. 7 \( 2\Delta/T_c = 5.0 \) corresponds to \( T_c/\omega_{\text{in}} \sim 0.18 \), which, given the calculated \( \omega_{\text{in}} \), leads to a \( T_c \sim 14 \) and \( \lambda \sim 3 \), clearly inconsistent with the experiment. In Ref. 11 the value \( 2\Delta/T_c = 5.0 \) is one of the strongest arguments for multiband superconductivity. We believe that this is an artifact of the simplified \( \alpha \) model used by the authors to fit the experimental specific heat. In fact, as we have shown above, a single gap Migdal Eliashberg model perfectly fits the electronic specific heat for SrPt3P, with a lower \( 2\Delta/T_c = 4.06 \). Therefore, also the possible anisotropy in the gap suggested by the uneven distribution of orbital characters on the Fermi surface is either negligible, or washed out by impurities in real samples. At the same time, the good agreement of the calculated lattice specific heat, allows us to rule out the dynamical instability of the low-lying
phonon branches in SrPt$_3$P and the CDW scenario based thereon. The same single-band analysis, applied to the lower $T_c$ compounds, yields critical temperatures in very good agreement with experiments, which is a strong indication in favor of conventional superconductivity.

TABLE III: Superconducting properties of APt$_3$P, from first-principles calculations and Migdal-Eliashberg theory; $\gamma_N$ is the electronic normal-state specific heat, in mJ mol$^{-1}$ K$^{-2}$, $\Delta(0)$ is the value of the superconducting gap, $\Delta C$ is the specific heat jump at $T_c$. Experimental data from Ref.[11] are in parentheses. The Coulomb pseudopotential $\mu^*$ was fixed to reproduce the experimental $T_c$.

|     | $\gamma_N$ | $T_c$ | $2\Delta(0)/T_c$ | $\Delta C/T_c$ | $T_c/\omega_{ph}$ | $\mu^*$ |
|-----|------------|------|------------------|----------------|------------------|--------|
| Sr  | 12.9 (12.7)| 8.5  | 0.46             | 29.0 (28 )     | 0.110            | 0.11   |
| Ca  | 10.3 (17.4)| 6.34 | 3.66             | 16.8 (11 )     | 0.058            | 0.09   |
| La  | 7.18 (6.7) | 1.56 | 3.53             | 10.5 (2 )      | 0.013            | 0.11   |

VII. CONCLUSIONS

In conclusion, the first-principles calculations and Migdal-Eliashberg analysis presented in this work allow us to make some conclusive statements about the nature of superconductivity in the recently-discovered APt$_3$P compounds (A=Sr, Ca, La). Superconductivity in APt$_3$P (A=Sr, Ca, La) compounds is of conventional $EP$ nature and the SOC plays a negligible role, thus ruling out the proposals of exotic superconductivity of Refs.[12,13]. The electronic filling brings about an $EP$ coupling which is moderate in La, and much stronger in Ca and Sr, where Pt(1) breathing phonons couple to in-plane electronic states. The frequency and dispersion of the breathing phonons can be tuned acting on the in-plane lattice constant, leading to weak and strong-coupling values of the BCS ratios in Ca and Sr, despite the very close critical temperatures.

Furthermore, our total energy calculations suggest that the APt$_3$P compounds could also be synthesized in the related, non-centrosymmetric CePt$_3$Si structure, through appropriate synthesis conditions or partial replacement of P with Si. This would realize the original proposal of Takayama et al.[11] and open the way to the exciting possibility of studying the effect of the lack of inversion symmetry on superconductivity in a controlled way.

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