

# Insights into the unconventional superconductivity in $\text{HfV}_2\text{Ga}_4$ and $\text{ScV}_2\text{Ga}_4$ from first-principles electronic-structure calculations

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The  $\text{HfV}_2\text{Ga}_4$  compound was recently reported to exhibit unusual bulk superconducting properties, with the possibility of multiband behavior. To gain insight into its properties, we performed *ab initio* electronic-structure calculations based on the density functional theory (DFT). Our results show that the density of states at the Fermi energy is mainly composed by V-*d* states. The McMillan formula predicts a superconducting critical temperature ( $T_c$ ) of approximately 3.9 K, in excellent agreement with the experimental value at 4.1 K, indicating that superconductivity in this new compound may be explained by the electron-phonon mechanism. Calculated valence charge density maps clearly show directional bonding between Hf and V atoms with 1D highly populated V chains and some ionic character between Hf-Ga and V-Ga bonds. Finally, we have shown that there are electrons occupying two distinct bands at the Fermi level, with different characters, which supports experimental indications of possible multiband superconductivity. Based on the results, we propose the study of a related compound,  $\text{ScV}_2\text{Ga}_4$ , showing that it has similar electronic properties, but probably with a higher  $T_c$  than  $\text{HfV}_2\text{Ga}_4$ .

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## I. INTRODUCTION

Although superconductivity has attracted the attention of the scientific community for a long time, the understanding of the phenomenon, which started with the model proposed by Bardeen, Cooper, and Schrieffer (BCS) [1] is still very challenging. The BCS theory, although useful for a large class of superconducting materials, fails to correctly explain other experimentally observed superconducting elements or compounds [2] and a plethora of different behaviors demands new approaches.

First-principles electronic-structure calculations, within the framework of the density functional theory (DFT), has proven to be an important tool to study superconducting materials. Although strongly correlated systems are beyond the scope of the Kohn-Sham scheme of the DFT, many successful attempts have been made to deal with the description of superconducting materials. In particular, some specific properties of the normal state, e.g., electronic band dispersions and electronic density of states, are very useful to elucidate aspects of the superconducting mechanism and to predict relevant parameters, such as the critical temperature  $T_c$  and the electron-phonon coupling constant  $\lambda$ . In the last few years, an increasing number of studies appeared using this methodology, either as support for experimental discoveries [3–5] or fully theoretical investigations [6–9].

Superconductivity was recently experimentally reported, by some of the present authors, for the  $\text{HfV}_2\text{Ga}_4$  compound, with a critical temperature ( $T_c$ ) of 4.1 K [10]. The investigators observed some deviations from the more conventional BCS theory signatures, such as an unusual inflection near  $T_c$  in lower

and upper critical field as a function of reduced temperature, and a second jump in the specific heat vs temperature curve. The authors speculated that the experimental results could be either due to sample inhomogeneity or to the presence of more than one superconducting gap at the Fermi surface, resulting in a two-band superconductivity [11].

These recent experimental results for the bulk  $\text{HfV}_2\text{Ga}_4$  point to a new promising class of materials to study unconventional superconducting behavior. Motivated by these results, here we perform *ab initio* electronic-structure calculations for  $\text{HfV}_2\text{Ga}_4$ . We focus our attention on the analysis of the possible mechanisms behind the superconducting properties. The theoretical study was extended to a new (possibly) bulk superconducting compound with the same prototype structure,  $\text{ScV}_2\text{Ga}_4$ , as a way to manipulate the electronic structure aiming at enhancing the superconducting transition temperature.

## II. COMPUTATIONAL METHODS

The *ab initio* electronic-structure calculations were performed in the framework of the Kohn-Sham scheme [12] within density functional theory (DFT) using the full potential-linearized augmented plane wave plus local orbitals (FP-LAPW+lo) method [13], as implemented in the WIEN2K computational code [14]. The exchange and correlation (XC) functional was described by the generalized gradient approximation (GGA) in the Perdew-Burke-Ernzerhof (PBE) formulation [15], taking relativistic corrections and spin-orbit coupling (SOC) effects into account. We used muffin-tin spheres with radius  $R_{\text{MT}} = 2.0 a_0$  (Bohr's radius) for all atoms, with  $R_{\text{MT}} K_{\text{max}} = 9.0$ , where  $K_{\text{max}}$  is related to the basis set size [14]. Self-consistent-field (SCF) calculations were carried out with a  $32 \times 32 \times 32$  Monkhorst-Pack [16] shifted *k*-point mesh discretization in the first Brillouin zone. All lattice parameters

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and internal degrees of freedom were relaxed in order to guarantee a ground state convergence to about  $10^{-5}$  Ry in the total energy,  $10^{-4}$  e for electron density, and 0.5 mRy/ $a_0$  for forces acting on the nuclei. The Birch-Murnaghan equation of state [17] was used to fit the total energy as a function of the unit cell volume (keeping  $c/a$  constant) at several  $c$  values in order to obtain the ground state lattice constants and bulk modulus.

Finally, six different lattice distortions, with 15 intensities for each one (a total of 90 different structures), were used to provide data for the determination of the elastic properties with the ElaStic code [18], using QUANTUM ESPRESSO [19] for DFT calculations of deformed structures. The QUANTUM ESPRESSO calculations were performed using PBE SG15 optimized norm-conserving vanderbilt (ONCV) pseudopotentials [20], with a cutoff energy of 220 Ry and 1728  $k$  points in the first Brillouin zone. Anderson's simplified method [21] was then employed for the calculation of the Debye temperature.

### III. RESULTS AND DISCUSSION

#### A. HfV<sub>2</sub>Ga<sub>4</sub> electronic-structure calculations

HfV<sub>2</sub>Ga<sub>4</sub> crystallizes in the YbMo<sub>2</sub>Al<sub>4</sub> prototype (space group  $I4/mmm$ , Pearson symbol  $tI14$ ), a body-centered tetragonal structure composed by a cagelike structure, where Hf sites, at  $2a$  (0, 0, 0) Wyckoff positions, are surrounded by V and Ga sites at  $4d$  (0, 1/2, 1/4) and  $8h$  (0.303, 0.303, 0), respectively [22], as schematically shown in Fig. 1.

The calculated optimized lattice parameters are in excellent agreement with the experimental data reported in the literature [23], as seen in Table I. There is a slight difference of at most 1% with respect to the experimental values, which is commonly related to the inherent imprecision of the approximations required by the computational method [24–26]. The calculated

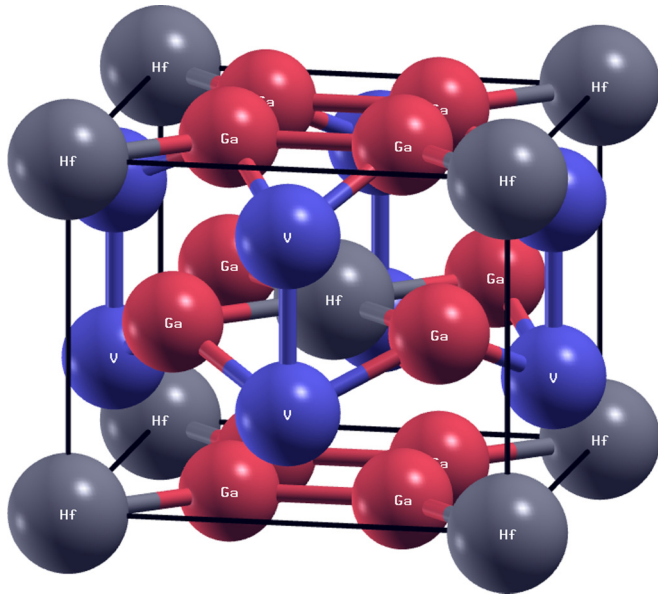


FIG. 1. HfV<sub>2</sub>Ga<sub>4</sub> body-centered tetragonal unit cell (conventional setting). Hf (gray), V (blue), and Ga (red) sites are at the  $2a$  (0, 0, 0),  $4d$  (0, 1/2, 1/4), and  $8h$  (0.303, 0.303, 0) Wyckoff positions, respectively.

TABLE I. Calculated lattice parameters and optimized  $8h$  (Ga) atomic position for the HfV<sub>2</sub>Ga<sub>4</sub> tetragonal compound, compared to experimental values [23].

	Calc.	Expt.
$a, b$ (Å)	6.459	6.45
$c$ (Å)	5.197	5.20
$8h$ (Ga)	(0.303, 0.303, 0)	(0.303, 0.303, 0)

bulk modulus is 134.75 GPa, with a Poisson ratio of 0.24, resulting in 416.3 K for the Debye temperature ( $\Theta_D$ ). Our *ab initio* calculations for  $\Theta_D$  reproduce with great accuracy the 418.97 K value obtained through experimental measurements [10].

The total density of states (DOS), as well as the site and orbital projected density of states (PDOS), are shown in Figs. 2(a)–2(d). Both occupied and unoccupied states involve considerable hybridization, as seen in Fig. 2(a). In the lowest energy region Ga orbitals are dominant, with some contribution from V; in the region around the Fermi level (from  $-2.5$  eV to 3 eV), V states are prevailing, mainly due to V- $d$  character (notice the different PDOS scales on Figs. 2(b)–2(d), with some Hf- $d$  and Ga- $p$  contributions; in the higher (above 3 eV), unoccupied energy region, Hf and V states contribute equally. Almost half of the total DOS at the Fermi level is due to V, although these states are extended along the whole studied energy region.

The calculated total DOS at the Fermi level is  $N(E_F) = 2.29$  states/eV. This quantity is related to the linear coefficient of the electronic specific heat  $\gamma$ , known as Sommerfeld coefficient, given by

$$\gamma = \frac{\pi^2}{3} k_B^2 N(E_F), \quad (1)$$

where  $k_B$  is the Boltzmann constant. The calculated  $N(E_F)$  leads to a value of  $5.41$  mJ mol<sup>-1</sup> K<sup>-2</sup> for the theoretical  $\gamma_{\text{calc}}$ . From the value of the Sommerfeld coefficient  $\gamma_{\text{calc}}$  resulting from the *ab initio* calculations and the experimentally measured value ( $\gamma_{\text{exp}} = 8.263$  mJ mol<sup>-1</sup> K<sup>-2</sup>) [10], we can estimate reasonably well the electron-phonon coupling constant  $\lambda$  using the well-known approximation [27,28]

$$\lambda = \frac{\gamma_{\text{exp}}}{\gamma_{\text{calc}}} - 1, \quad (2)$$

which stems from the fact that the calculations give static (0 K) results. Following Eq. (2), we arrive at  $\lambda = 0.53$ . This value can be used to calculate the superconducting transition temperature  $T_c$  using the empirical McMillan formula [29],

$$T_c = \frac{\Theta_D}{1.45} \exp \left[ -\frac{1.04(1 + \lambda)}{\lambda - \mu^*(1 + 0.62\lambda)} \right], \quad (3)$$

where  $\mu^*$  is the Coulomb pseudopotential, which measures the strength of the electron-electron Coulomb repulsion [30]. A typical value of  $\mu^*$  is 0.12, as used in many previous works [27,28,31]. For the HfV<sub>2</sub>Ga<sub>4</sub> compound, using the calculated  $\Theta_D$  and the above values for  $\lambda$  and  $\mu^*$ , we arrive at an estimated critical temperature  $T_c = 3.9$  K, in excellent agreement with the experimental (4.1 K) value. This indicates

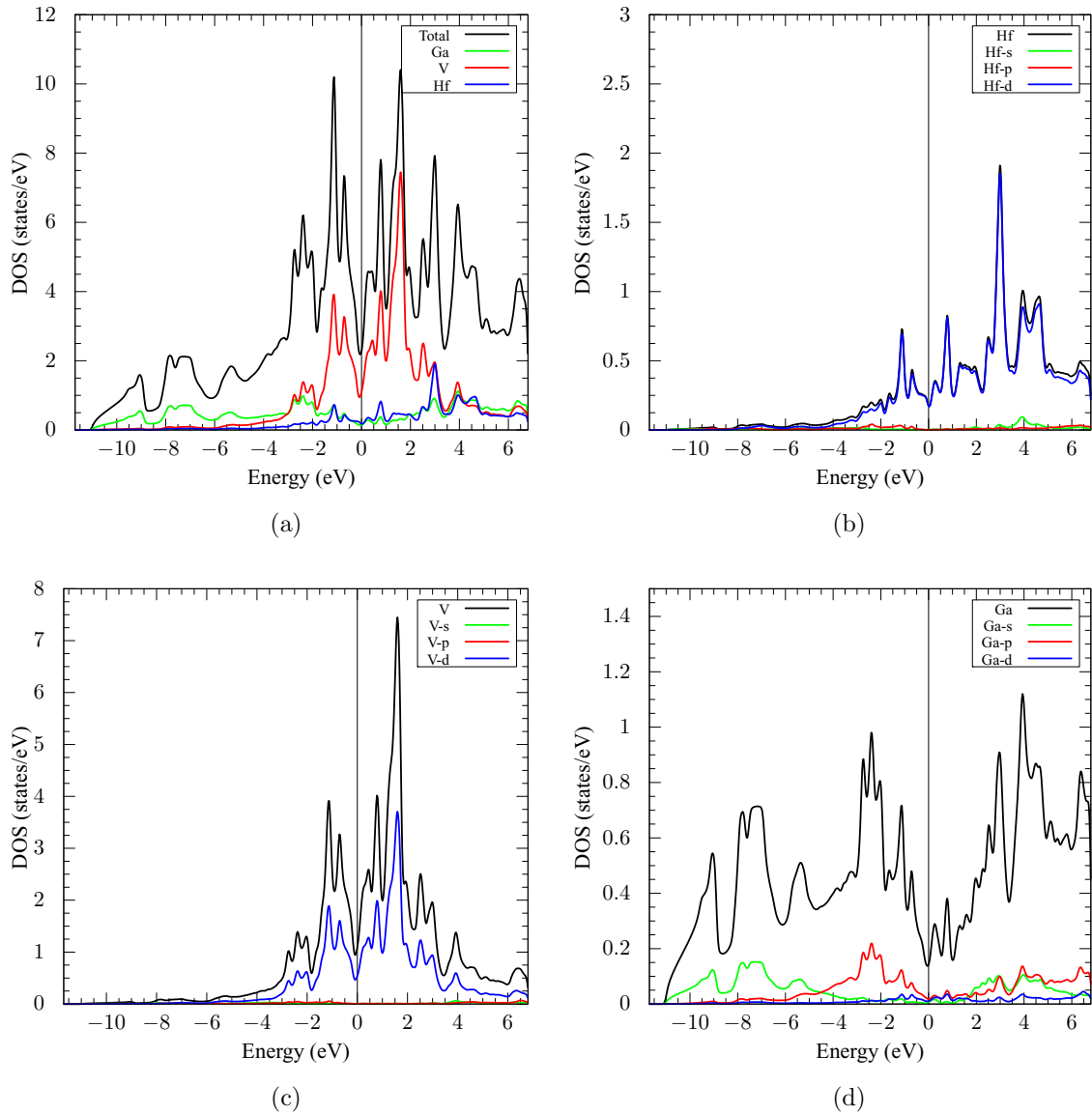


FIG. 2. (a) Total and site projected density of states for HfV<sub>2</sub>Ga<sub>4</sub>. The orbital-projected (*s*, *p*, and *d*) contributions at each site are also shown: (b) Hf, (c) V, and (d) Ga. The Fermi level is set at 0 eV in all figures.

that the electron-phonon interaction may be the mechanism behind superconductivity in HfV<sub>2</sub>Ga<sub>4</sub>. The V states dominate the  $N(E_F)$  and therefore have the major contribution for the pairing. It is important to stress the fact that our approach to the calculation of  $T_c$ , despite being widely and successfully employed in the literature, has several drastic approximations. A perturbative approach to DFT [32] is a more precise formalism to describe the electron-phonon coupling constant  $\lambda$ . The Coulomb pseudopotential  $\mu^*$  can be obtained using the GW quasiparticle correction to DFT [33], as employed in superconducting gap calculations [9]. Such methodologies are computationally very expensive and are justified when a higher degree of precision is required.

The nature of the atomic bonding can be further elucidated with the help of valence electron density plots such as those shown in Figure 3, in which the electron density is plotted, with an appropriate logarithmic scale in a (001) plane, passing through the center of Hf and Ga nuclei within a unit cell

[Fig. 3(a)], and a (100) plane, passing through the center of Hf and V nuclei [Fig. 3(b)]. It should be noted that, in Fig. 3(a), the nonlabelled high-density regions are V nuclei not centered on the (100) plane. The plots clearly show a directional shared bond between Hf and V atoms, evidenced by the density contours in the (100) and (001) planes. This reveals that Hf atoms, which are “locked” in the center of a cagelike structure, are not simply passive electron donors: They stabilize the charge transfer to the V atoms (as also observed in Fig. 2) that, in turn, commands the electronic properties.

Furthermore, it is interesting to note that the charge density gives rise to a kind of electron sharing channel in the lattice, composed by directional, strongly-bonded, highly populated V chains in the (100) and (010) crystallographic planes. The same characteristic has previously been found in other compounds with the same crystal structure [34,35]. The Hf nuclei are weakly bonded with the two V atoms within adjacent unit cells in these 1D chains. As a consequence of these



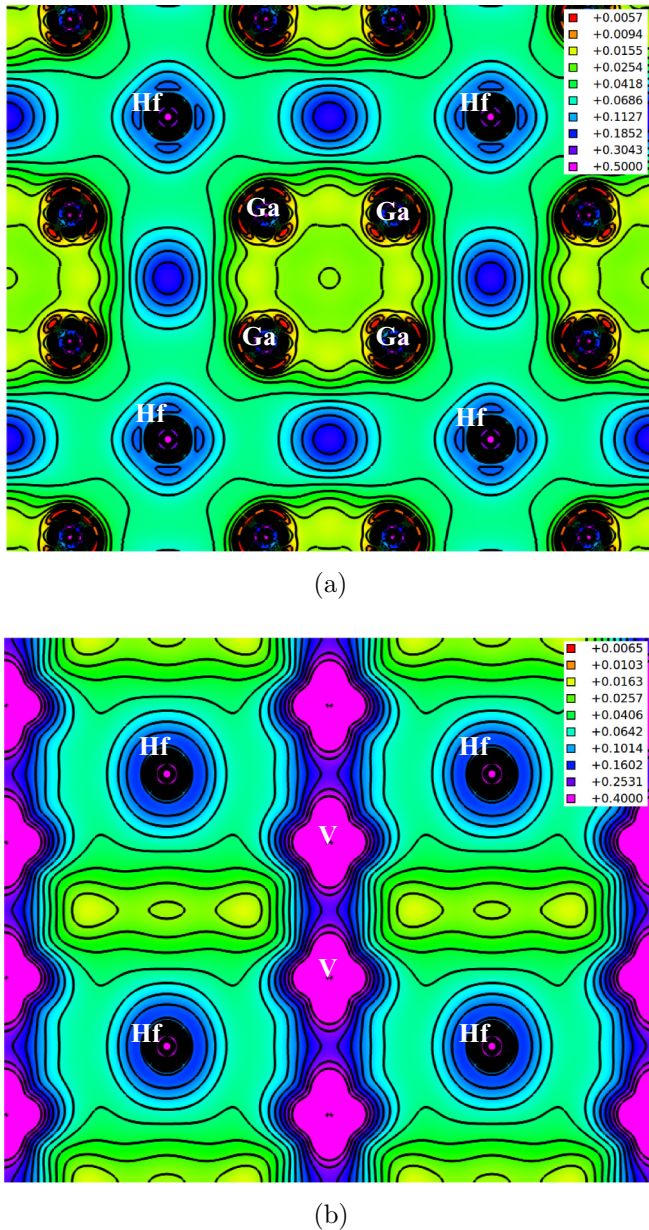


FIG. 3. Valence electron density plot in (001) plane (a) and (100) plane (b) for  $\text{HfV}_2\text{Ga}_4$ . Along a contour the electron density is constant.

V chains that concentrate most of the electronic states that will give rise to Cooper pairs, this electronic configuration may lead to a high anisotropy that could be identified via transport measurements. Finally, despite the small difference in electronegativity between the atomic species, Hf-Ga and V-Ga bonds exhibit some ionic character. In Fig. 3(a) we can clearly observe isolated clusters containing four Ga atoms within a unit cell, forming weak bonds with adjacent Hf atoms.

Figure 4 shows the resulting band character plots along high symmetry points in the first Brillouin zone, not including [Fig. 4(a)] and including [Fig. 4(b)] spin-orbit coupling (SOC) effects in the calculations. In the band character plots, stronger colors mean stronger character due to the respective orbital projection. Indeed, the cage-like symmetry of the lattice gives

rise to complex dispersive metallic bands in the vicinity of the Fermi level. There are two bands crossing the Fermi energy, with very different Hf and V characters. The existence of two bands is better seen in the Fermi surface plot shown in Figs. 5(a) and 5(b), in which the contributions of the two bands are shown separately for clarity. The fact that there are electrons occupying two distinct bands in disconnected sheets of the Fermi surface (corresponding to the two bands crossing the Fermi level) supports the experimental evidence of a possible two-gap superconductivity [10]. These results open a promising scenario for a possible multiband behavior, so a superconducting gap calculation [32,36] would be a very interesting test for that hypothesis.

In the band character plots for  $\text{HfV}_2\text{Ga}_4$  shown in Fig. 4, we can see that a hole pocket develops around the M point, with a maximum at  $\approx 0.4$  eV, originated mainly from the Hf- $d$  states containing some mixing with the V- $d$  states. In Fig. 5(a), it corresponds to a small region around M, in the midpoint of the edge between two hexagons. The electron band crossing P just below  $E_F$  is made up mostly of V- $d$  states, and this corresponds to the pockets shown in Fig. 5(b). Notice that, near the Fermi level, the band plot unveils dispersive cones with zero gap at M and also along the M- $\Gamma$  direction, as well as one such feature at P. However, when SOC effects are considered, these features are gapped. Indeed, SOC leads to a visible lifting of some band degeneracies, mainly at M and M- $\Gamma$ , and less-pronounced at P (just a few meV). Moreover, although these compounds are metallic, SOC broken degeneracy creates a continuous pseudogap around the Fermi energy, although the gap almost closes at P [not visible in the scale of Fig. 4(b)]. This kind of signature also occurs in a few nontrivial topological materials like  $\text{Bi}_{14}\text{Rh}_3\text{In}_9$ ,  $\text{PbTaSe}_2$ , and  $\text{Cu}_x\text{ZrTe}_{2-y}$  [5,37,38]. Therefore, more detailed experimental and theoretical studies about the possibility of nontrivial topological effects in  $\text{HfV}_2\text{Ga}_4$  could be an interesting subject for future investigations.

### B. Theoretical predictions for $\text{ScV}_2\text{Ga}_4$

Several compounds that crystallize in the same body-centered tetragonal prototype  $\text{YbMo}_2\text{Al}_4$ , such as  $\text{RTi}_2\text{Ga}_4$  ( $R = \text{Ho, Er, Dy}$ ) and  $\text{RV}_2\text{Ga}_4$  ( $R = \text{Sc, Zr, Hf}$ ), have been reported in the literature. These compounds are poorly investigated, most efforts having been focused exclusively on magnetic properties in rare-earth compounds [39,40].

The results reported above for  $\text{HfV}_2\text{Ga}_4$  led us to consider an effective way to manipulate the electronic structure of such compounds, aiming at enhancing superconducting properties. In Fig. 2 we can observe that the Fermi level is situated down a deep valley in the total DOS. As a consequence, the density of states at  $E_F$  is extremely sensitive. So, considering a rigid band model, it is reasonable to assume that an element with a different valence configuration in the  $2a$  site of  $\text{HfV}_2\text{Ga}_4$  could shift the Fermi level to higher states. Based on what has been presented, we also have carried out first-principles electronic-structure calculations for  $\text{ScV}_2\text{Ga}_4$ , to test this hypothesis.

Table II shows the relaxed calculated lattice parameters, together with experimental reported values for  $\text{ScV}_2\text{Ga}_4$ . Following the same methodology applied in the previous section, we reached  $\Theta_D = 447.8$  K for  $\text{ScV}_2\text{Ga}_4$ . Unfortunately, in this case, there are no experimental data for comparison.

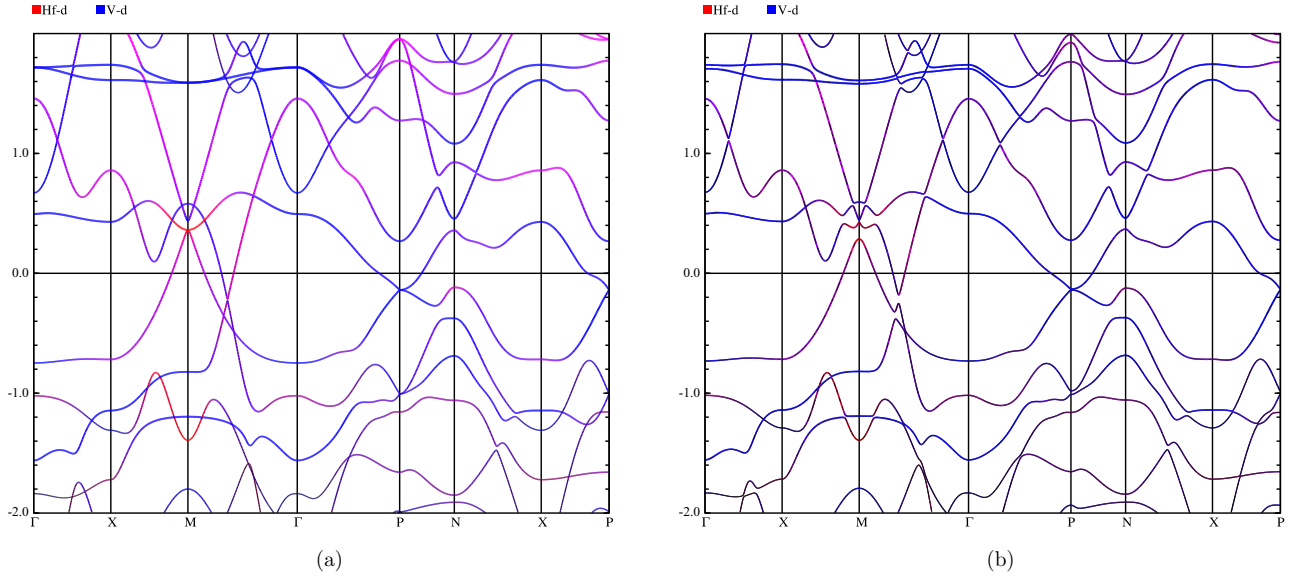


FIG. 4. Band character plots along high symmetry points in the first Brillouin zone of  $\text{HfV}_2\text{Ga}_4$ , without (a) and with (b) SOC effects. Colors give a picture about the band character, with color intensity indicating qualitatively the strength of the contribution of a given state. Only the Hf- $d$  (red) and V- $d$  (blue) states are represented (the Fermi level is set at 0 eV).

The nature of atomic bonding is the same showed for the  $\text{HfV}_2\text{Ga}_4$  in Fig. 3, with high populated 1D covalent V chains and Sc atoms acting to stabilize the transfer of charge to the V atoms. Therefore, the DOS overall appearance for  $\text{HfV}_2\text{Ga}_4$  is qualitatively identical to  $\text{ScV}_2\text{Ga}_4$ , as can be verified in Fig. 6(a). Hence, the contribution of each orbital in the density of states for  $\text{ScV}_2\text{Ga}_4$  is also very similar to  $\text{HfV}_2\text{Ga}_4$ , with a higher contribution due to Sc- $d$  states in the unoccupied bands. The calculated value of  $N(E_F)$  is 3.62 states/eV, that leads to  $\gamma_{\text{calc}} = 8.53 \text{ mJ mol}^{-1} \text{ K}^{-2}$  using Eq. (1). Confirming our hypothesis, the presence of Sc atoms instead of Hf in the  $2a$  sites causes the Fermi level to shift to a higher DOS value, an increase of about 60%, escaping from the bottom of the well.

In Figs. 6(b) and 6(c) we show the calculated band structure without and with SOC effects, respectively. It may be seen that the band structure is related to that presented for  $\text{HfV}_2\text{Ga}_4$  (Fig. 4), with similar features in the vicinity of the Fermi energy. Fermi bands in  $\text{ScV}_2\text{Ga}_4$  are well described as coming from hybridization between mainly V- $d$  and some Sc- $d$  states. However, SOC in  $\text{ScV}_2\text{Ga}_4$  plays only a marginal role,

making nontrivial topological effects unlikely. Nevertheless, the important point here resides on the fact that, similar to  $\text{HfV}_2\text{Ga}_4$ , there are two bands crossing the Fermi level, as seen in the Fermi surface plots shown in Figs. 6(d) and 6(e), opening again the possibility for a multiband scenario. Notice that the Fermi surface for  $\text{ScV}_2\text{Ga}_4$  is quite different from  $\text{HfV}_2\text{Ga}_4$ , as expected from the dissimilar valence configuration of the caged element (Hf or Sc) in the structure.

The large contribution of V- $d$  state electrons and the higher DOS value at the Fermi level, attached to the fact that there are electrons originated from two distinct bands in the Fermi surface, strongly suggest that  $\text{ScV}_2\text{Ga}_4$  could be a new example of two-band electron-phonon superconducting material with a considerable higher critical temperature than the one reported for the  $\text{HfV}_2\text{Ga}_4$  compound.

#### IV. CONCLUSIONS

In this paper we presented *ab initio* calculations for the bulk superconductor  $\text{HfV}_2\text{Ga}_4$ . The McMillan formula predicts a  $T_c$  of 3.9 K, in excellent agreement with experimental reported values (4.1 K), indicating that superconductivity can be readily explained in an electron-phonon framework. From the signature of the DOS in the vicinity of the Fermi energy, we have proposed to improve the superconducting critical temperature by investigating the  $\text{ScV}_2\text{Ga}_4$  compound.

TABLE II. Calculated lattice parameters and optimized  $8h$  (Ga) atomic position for the  $\text{ScV}_2\text{Ga}_4$ , compared to experimental values [23].

	Calc.	Expt.
$a, b$ (Å)	6.497	6.432
$c$ (Å)	5.200	5.216
$8h$ (Ga)	(0.3004, 0.3004, 0)	(0.303, 0.303, 0)

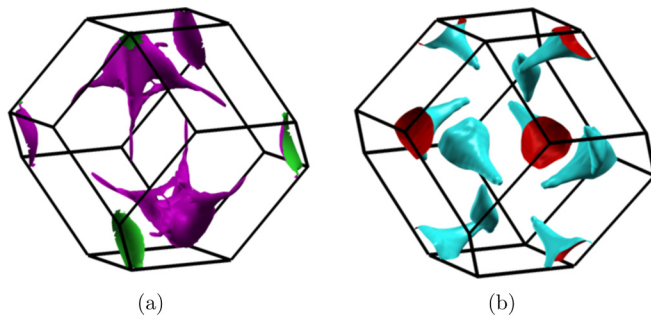


FIG. 5. Fermi surface plots for the compound  $\text{HfV}_2\text{Ga}_4$ . The two bands crossing the Fermi level have a predominant (a) Hf- $d$  and (b) V- $d$  character, as seen on the band plots in Fig. 4.

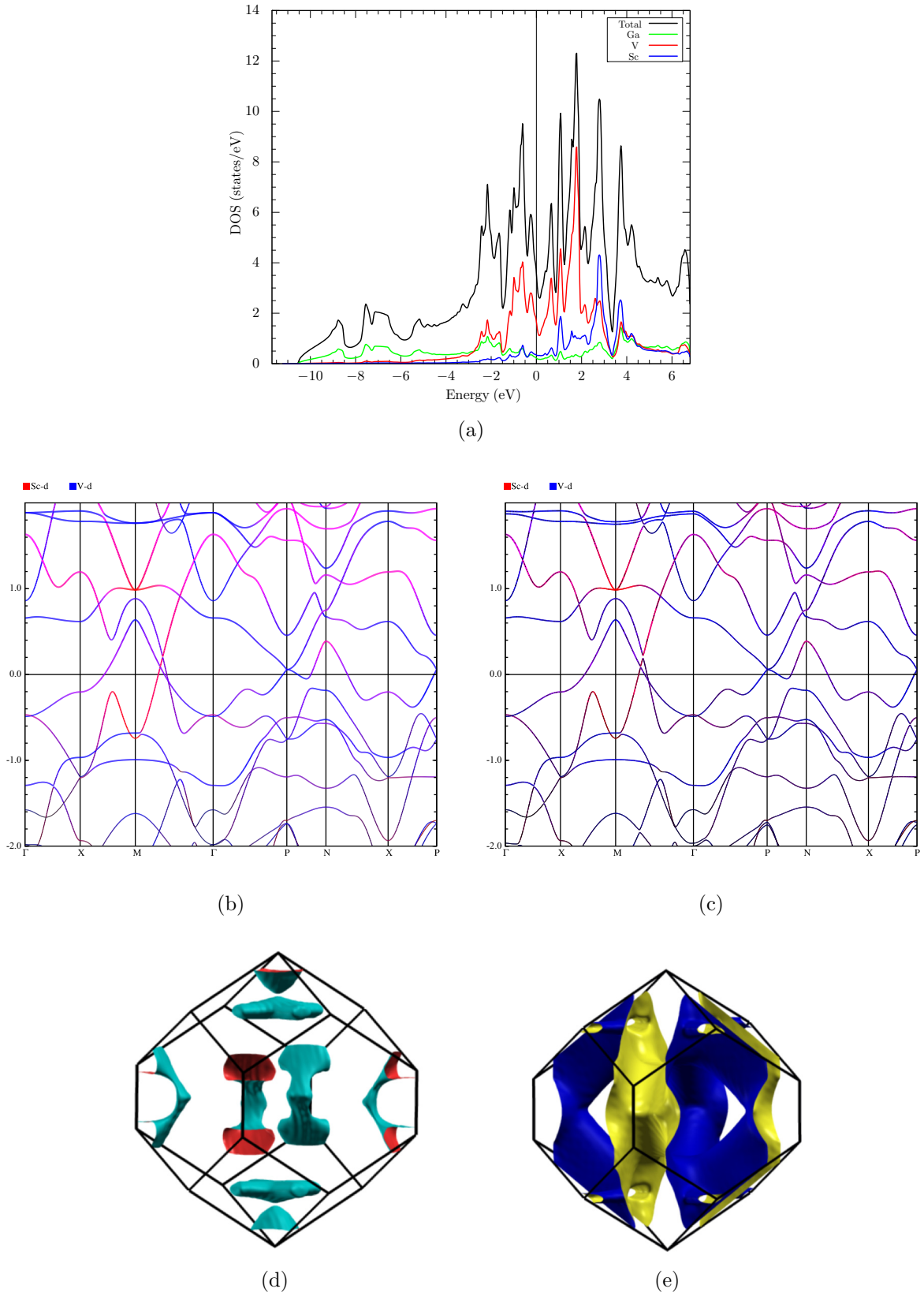


FIG. 6. Total and projected density of states for  $\text{ScV}_2\text{Ga}_4$  (a); band character plots along high symmetry points in the first Brillouin zone (b) without (b) and (c) with SOC effects; Fermi surface plots for the two bands crossing the Fermi level (d) and (e).



Theoretically, we have shown that the presence of Sc instead of Hf in the crystal structure causes the Fermi level to shift to a higher DOS value. The band structure around the Fermi level, which comes mainly from V-*d* states, and the DOS overall appearance, are qualitatively very similar for both compounds. Valence electron density plots unveil Hf(Sc)-V shared bonding and 1D highly populated V chains, while Hf(Sc)-Ga and V-Ga bonds have a partially ionic character. It was found that there are electrons derived from two distinct bands in disconnected sheets of the Fermi surface for both compounds, in agreement with the experimental evidence [10] of a possible two-gap superconductivity for HfV<sub>2</sub>Ga<sub>4</sub>. Finally,

we argue that ScV<sub>2</sub>Ga<sub>4</sub> is presumably a new candidate for two-band electron-phonon superconductivity with a higher  $T_c$  than HfV<sub>2</sub>Ga<sub>4</sub>, a result that should be confirmed experimentally.

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