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The influence of spin orbit interaction on phonons and superconductivity in the noncentrosymmetric superconductors $LaPt_3Si$ and $LaPtSi_3$

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ABSTRACT

We have performed *ab initio* study of structural, electronic, vibrational and electron-phonon interaction properties of $LaPt_3$ Si and $LaPtSi_3$ by employing the density functional theory, a linear-response formalism, and the plane-wave pseudopotential method. The electronic structure, phonon dispersion relations and the Eliashberg spectral function for these materials have been examined with and without the inclusion of spin-orbit interaction (SOI). Our electron-phonon interaction results reveal that the influence of spin-orbit interaction on phonons and superconductivity in these noncentrosymmetric superconductors is very small. Thus, we can conclude that a mixing of the spin-singlet and the spin-triplet components in these superconductors is weak and the spin-singlet Cooper pairs dominate. By integrating the Eliashberg spectral function $\alpha^2F(\omega)$, the average electron-phonon coupling parameter λ is obtained to be 0.470 for $LaPt_3$ Si and 0.488 for $LaPtSi_3$, indicating these to be weak-coupling BCS superconductors. Using an acceptable value of $\mu^* = 0.13$ for the effective Coulomb repulsion parameter, the superconducting critical temperature T_c is calculated to be 0.67 K for $LaPt_3$ Si and 1.39 K for $LaPtSi_3$, in good accordance with experimental values of 0.65 K and 1.52 K, respectively.

Noncentrosymmetric (NCS) superconductors have been known for decades but have become an outstanding research topic recently following the discovery of superconductivity in $CePt_3$ Si [1]. The superconducting order parameters in NCS superconductors cannot be categorized in terms of parity, and the coexistence of both spin-singlet and spin-triplet states is permitted [2–6]. Two types of NCS superconductors have been noted: strongly correlated systems such as $CePt_3$ Si [1] and UIr [7], and weakly correlated systems such as Li_2 Pt_3 B and Y_2 C_3 [8,9]. The superconducting properties of heavy-fermion NCS superconductors are strongly affected by electron correlation effects, and the weakly correlated NCS superconductors provide a fertile ground for studying mixing of the singlet-triplet pairing derived from the break down of inversion symmetry and a strong Rashba-type asymmetric spin-orbit-coupling (ASOC) interaction. Despite the anticipation of mixed parity pairing in NCS superconductors, single-gap BCS-like superconductivity is clearly found in many NCS superconductors. For instance, $LaPt_3$ Si (with superconducting transition temperature $T_c = 0.65$ K), which is isostructural with $CePt_3$ Si, displays no sign of magnetic order or strong electronic correlation. Thus, $LaPt_3$ Si is expected to be an ideal system for studying the effect of the lack of inversion symmetry on the superconducting state [1,10–14]. In addition, similar to $LaPt_3$ Si, NCS superconductors such as $BaPtSi_3$ [15], $LaRhSi_3$ [16], $CaPtSi_3$ [17,18], $CaIrSi_3$ [17,18], $LaPtSi_3$ [19] and $LaPdSi_3$ [19] also do not exhibit strong electronic correlations, and exhibit superconductivity with the BCS characteristics at ambient pressure. Recently, Krannich and co-workers [20] have measured the dispersion of transverse acoustic and low energy optical phonon branches for $CePt_3$ Si along the [110] direction using inelastic neutron scattering. In these branches they have found deviations from their *ab initio* lattice dynamical calculations, which overall gives good explanation of the phonon dispersion in $CePt_3$ Si. Thus, they emphasize that the lattice dynamics of $CePt_3$ Si is conventional and that the observed deviations between their experimental and theoretical calculations are not linked to effects of

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ASOC. These authors have also mentioned that a strong Rashba-type ASOC plays less a role in noncentrosymmetric superconductors than widely believed [20].

The discovery of superconductivity in NCS materials has motivated theoretical physicists to study their structural, electronic, vibrational and superconducting properties. Bauer and co-workers [15] have studied electronic, phononic and superconducting properties of $BaPtSi_3$ by using the density functional theory (DFT) within the local density approximation (LDA). This theoretical work [15] has mentioned that the non-inversion symmetry plays only a minor role for the superconducting properties of $BaPtSi_3$ due to rather small spin-orbit splitting at the Fermi energy level. The electronic structures of $CaPtSi_3$ and $CaIrSi_3$ have been calculated by means of the full-potential linearised augmented plane wave (FLAPW) [21]. This theoretical work [21] reveals that the electronic structures of these superconductors display similarities to the corresponding structure of $BaPtSi_3$ [15]. Terashima and co-workers [22] have performed angle-resolved de Hass-van Alphen (dHvA) measurements and FLAPW band-structure calculations for $LaRhSi_3$. They have indicated that the dHvA frequency branches observed in this superconductor can quantitatively be described by the calculated Fermi surface, which is composed of three pairs of inversion-asymmetry-split sheets. The electronic properties of $LaPdSi_3$ have been investigated by using the full-potential local-orbital method (FPLO) within the density functional theory [23]. This theoretical work reveals that the influence of spin-orbit coupling in this NCS superconductor, particularly in small energy range around the Fermi level, is rather low. Recently, the electronic structure of $LaPt_3$ Si has been calculated by using the DFT within the LDA [20]. Very recently, Uzunok and co-workers [24] have carried out an *ab initio* study of the electronic, vibrational and electron-phonon interaction properties of $CaIrSi_3$ by employing the DFT, a linear response formalism, and the plane-wave pseudopotential method. This theoretical work reveals that the influence of spin-orbit interaction (SOI) on the average electron-phonon coupling parameter is very small. Thus, Uzunok and co-workers [24] conclude that a mixing of the spin-singlet and the spin-triplet components in the superconducting condensate is weak and the spin-singlet Cooper pairs dominate.

In spite of some theoretical progress in examining the electronic properties of $LaPt_3$ Si, no experimental or theoretical works have been performed to investigate the electronic properties of $LaPtSi_3$. Furthermore, the electron-phonon interaction properties of these materials have not yet been investigated. It is important to examine the spectral distribution function of the electron-phonon interaction as a number of important physical properties of solids are governed by it, such as the electrical and thermal resistivities, superconductivity, softening of phonon modes, renormalization of the low-temperature electronic component of the heat capacity, and a number of other physical phenomena. For this reason, this work is aimed at making *ab initio* calculations of the structural and electronic properties of $LaPt_3$ Si and $LaPtSi_3$ by using a generalized gradient approximation (GGA) of the DFT with and without the inclusion of spin-orbit interaction (SOI) [25]. We have further performed *ab initio* linear response calculations [25] of phonon dispersion relations and electron-phonon matrix elements in these NCS materials. A detailed comparison of the SOI and non-SOI electronic structures and the electron-phonon matrix elements is made. The phonon density of states and the electron-phonon matrix elements are used to determine the Eliashberg spectral function [26,27], from which the average electron-phonon coupling parameter can be determined. Using the average electron-phonon coupling parameter and the logarithmic average of phonon frequency, we finally compute the superconducting transition temperature.

1. Theory

All calculations have been made using the density functional theory with and without SOI. We have used the plane wave-pseudo-potential method as implemented in the QUANTUM-ESPRESSO simulation package. The atomic pseudopotentials generated using the projected-augmented wave [25] (PAW) are used to simulate interactions between valence electrons and ion cores, and the electron wave function is expanded in plane waves up to an energy cutoff of 60 eV for all calculations. The electron exchange−correlation energy is evaluated using the GGA of the Perdew− Burke− Ernzerhof (PBE) formalism [28]. Self-consistency in solutions to the Kohn-Sham equations [29] is achieved by considering special $\boldsymbol{k}$ points within the irreducible Brillouin zone (IBZ). The energy calculations in the simple tetragonal IBZ have been made with a $(8 \times 8 \times 8)$ $\boldsymbol{k}$-point mesh using the Monkhorst-Pack scheme [30] while a $(24 \times 24 \times 24)$ Monkhorst-Pack $\boldsymbol{k}$-point grid has been utilized to describe the electronic properties of both materials.

Phonon calculations for both materials have been performed within the framework of the self-consistent density-functional perturbation theory [25] with and without SOI. Within this approach, second-order derivatives of the total energy are computed to determine the dynamical matrix. A static linear response of the valence electrons is considered in terms of the variation of the external potential corresponding to periodic displacements of the atoms in the unit cell. The screening of the electronic system in response to the displacement of the atoms has been taken into account in a self-consistent manner. We have used a $(8 \times 8 \times 8)$ grid for sampling the irreducible segment of the Brillouin zone (BZ) in our phonon calculations for both materials. We find that the phonon frequencies for both studied materials are accurate to within 0.05 THz for the present choice of the kinetic energy cutoff and the special $\boldsymbol{k}$ points. In order to achieve phonon dispersion curves and density of states, we have computed 18 dynamical matrices for $LaPt_3$ Si and 13 dynamical matrices for $LaPtSi_3$ on a $4 \times 4 \times 4$ grid in $\mathbf{q}$ space. Finally, these dynamical matrices have been Fourier transformed to procure the full phonon spectrum and density of states. The technique for the calculation of the electron-phonon interaction has been explained in detail in our previous study [32]. Fermi-surface sampling for the evaluation of the electron-phonon matrix elements has been made using $24 \times 24 \times 24$ $\boldsymbol{k}$-mesh with a Gaussian width 0.02 Ry. The phonon density of states and the Eliashberg function have been also worked out using this $\boldsymbol{k}$-mesh.

2. Results

2.1. Structural and electronic properties

$LaPt_3$ Si crystallizes in a simple tetragonal $CePt_3$ B-type crystal structure lacking inversion symmetry, with space group *P4mm*, and one formula unit per primitive unit cell. The five atoms inside a primitive unit cell can be grouped as four nonequivalent crystallographic sites: La, Pt1, Pt2, and Si according to the symmetry. The atomic positions are: La (1b) (1/2, 1/2, z_{La}), Pt1 (2c) (1/2, 0, z_{Pt1}), (0, 1/2, z_{Pt1}), Pt2 (1a) (0,0,0) and Si (1a) (0, 0, z_{Si}). As a consequence, this simple tetragonal structure is formed by two lattice parameters (a and c) and three internal parameters (z_{La}, z_{Pt1} and z_{Si}). The calculations have been performed to find total energy results, which are then fitted into Murnaghan equation of state to calculate bulk modulus (B). The calculated equilibrium lattice parameters (a and c), the equilibrium volume (V), the internal parameters (z_{La}, z_{Pt1} and z_{Si}), the Pt1−Si bond length (d_{Pt1-Si}), the Pt2−Si bond length (d_{Pt2-Si}) and the bulk modulus (B) are given in Table 1, together with