Letter

Electronic structure studies on single crystalline Nd$_2$PdSi$_3$, an exotic Nd-based intermetallic: evidence for Nd 4f hybridization

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Abstract

In the series R$_2$PdSi$_3$, Nd$_2$PdSi$_3$ is an anomalous compound in the sense that it exhibits ferromagnetic order unlike other members in this family. The magnetic ordering temperature is also unusually high compared to the expected value for a Nd-based system, assuming 4f localization. Here, we have studied the electronic structure of single crystalline Nd$_2$PdSi$_3$ employing high resolution photoemission spectroscopy and ab initio band structure calculations. Theoretical results obtained for the effective on-site Coulomb energy of 6 eV corroborate well with the experimental valence band spectra. While there is significant Pd 4d–Nd 4f hybridization, the states near the Fermi level are found to be dominated by hybridized Nd 4f–Si 3p states, which is possibly responsible for the ferromagnetism in Nd compound. Nd 3d core level spectrum exhibits multiple features manifesting strong final state effects due to electron correlation, charge transfer and collective excitations. These results serve as one of the rare demonstrations of hybridization of Nd 4f states with the conduction electrons possibly responsible for the exoticity of this compound.

Keywords: strongly correlated system, photoemission spectroscopy, hybridization, density of states

(Some figures may appear in colour only in the online journal)

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Intermetallic compounds containing rare-earths or actinides with partially filled $f$ shells allow for the realization of complex magnetic ground states, which can be driven by the presence of competing magnetic interactions [1, 2]. The intersite magnetic interaction among the local $f$-electrons has been known to be mainly governed by indirect exchange interaction, viz, Rudermann–Kittel–Kasuya–Yosida (RKKY) interaction in such metallic compounds. Following intense research during 1970s, it was recognized that partial delocalization of $4f$ electrons in Ce-based materials leads to anomalous magnetism in its intermetallic alloys due to finite $4f$-hybridization with conduction electrons (Kondo effect); exoticity in their electronic properties emerges due to the competition between the RKKY and Kondo interactions [1]. In fact, the $4f$-hybridization induced effects can extend to other rare-earths, such as Pr, Nd etc as was actually demonstrated through photoemission spectral features [3–5]. This conclusion from such exact state techniques found further evidence from subsequent studies of hybridization-related ground state properties like heavy-fermion superconductivity or magnetic anomalies in some Pr and Nd based systems, the most famous ones being skutterudites [6]. However, the fact remains that such examples for Nd are less abundant. A notable example in the field of multifermiology having relevance to magnetoelectric coupling is NdCrTiO$_5$, where magnetic ordering temperature is substantially enhanced [7, 8] with respect to isostructural Gd analogues due to $4f$-hybridization. A recent density functional theoretical calculations, supported by inelastic x-ray scattering experiment on Nd(0001) thin film, reveal strong $4f$ electron correlation and its influence on lattice dynamics [9], which stresses unexplored avenues of Nd $4f$ hybridization [10]. Judged by such reports, investigations of more Nd systems should present interesting situations.

In this respect, the material class, $R_2MSi_3$ ($R =$ rare-earth, $M =$ transition metal) is of great interest, where the $R$ sublattice is sandwiched by the $MSi$ sublattice and the hybridization between $4f$ and valence electrons leads to varied novel properties among Ce-based systems [11]. These materials form in A1B$_2$-type structure; $M$ and Si atoms are placed in ‘$ab$’ basal plane in an ordered manner making a hexagonal sublattice as shown in the inset of figure 1(a) and contribute in the conduction band formation. These planes are separated by hexagonal $R$ sublattice along ‘$c$’-axis [12, 13]. Use of Pd at the $M$ sites instead of $3d$ transition metals has led to the discovery of plethora of exotic phenomena; such as, Ce$_2$PdSi$_3$ is a Kondo lattice [14], Gd, Dy and Tb show large negative magnetoresistance [15], Gd$_2$PdSi$_3$ exhibits strong magneto-caloric effect and unexpected electrical resistivity minimum [16], which led to emergence of interesting theoretical studies [17]. Quasi-one dimensional magnetism is observed in Tb$_2$PdSi$_3$ [18]. It is intriguing to note that evidence of ‘topological Hall effect’ was reported [16] as early as 1999 in Gd$_2$PdSi$_3$, a centrosymmetric material as emphasized recently [19] although this terminology was coined in late 2000. A recent study [20] attributed these anomalies to magnetic skyrmions.

The behavior of Nd$_2$PdSi$_3$ is different from the other members in this series as it exhibits an unusual ferromagnetic order [21–23] while most other members exhibit antiferromagnetic order. Moreover, the magnetic ordering occurs at a significantly higher temperature ($T_C \sim 16$ K) than the expected value according to de Gennes scaling [23]. Such complex magnetism is of great relevance in view of the observation of magnetic skyrmion in Gd$_2$PdSi$_3$, as remarked in ‘editor’s suggestion’ for reference [24]. The electronic properties of this compound and some of its solid solutions (substituting nonmagnetic ion at various sites) have been studied extensively using magnetization, heat capacity and resistivity measurements. The results indicate existence of a competition between ferromagnetic and antiferromagnetic interactions at low temperatures. It was proposed [23] that strong Nd $4f$ hybridization with the conduction electrons plays an important role behind its unusual behavior. Thus, there is an urgent need to find a direct evidence from electronic structure studies. Here, we report our results of the study of electronic structure of Nd$_2$PdSi$_3$ using high resolution photoemission spectroscopy. The experimental results provide evidence for strong Nd $4f$-hybridization.

The single crystal of Nd$_2$PdSi$_3$ was grown and characterized as reported elsewhere [22]. Photoemission measurements were carried out using a Scienta electron analyzer, R4000 WAL and monochromatic laboratory sources of Al K$_\alpha$ ($h\nu = 1486.6$ eV), He $\pi$ ($h\nu = 40.8$ eV) and He $\uparrow$ ($h\nu = 21.2$ eV) photon energies. Energy resolution for ultraviolet photoemission measurements were fixed to 2 meV and for x-ray photoemission, it was 350 meV. The experiments were carried out in transmission mode with wide angle lens configuration to get $k$-integrated data. The temperature down to 10 K was achieved by an open cycle He cryostat from advanced research systems, USA. The single crystal was cleaved at a base pressure of $3 \times 10^{-11}$ torr just before the measurements.

Figure 1. Calculated partial density of states of (a) Nd $4f$ and (b) Pd $4d$ and Si $3p$ states for $U = 6$ eV (upper panel) and $U = 0$ eV (lower panel). Nd $4f$ contributions are rescaled and shown in (a) to emphasize weak intensity features. A view of the crystal structure along c-direction is shown in the inset. Si and Pd are represented by blue and orange balls, respectively. Nd is represented by big purple balls.
The band structure calculations were carried out using full potential linearized augmented plane wave method within the local density approximation (LDA) as adapted in WIEN2k software [25]. The convergence was achieved using 1000 k-points within the first Brillouin zone; the energy and charge convergence was achieved to be less than 0.2 meV/f.u. and $10^{-3}$ electronic charge. The effect of spin–orbit interaction and on-site Coulomb energy, $U$ was introduced in the calculation following LDA + U method, [26] where the ‘effective’ $U$ is defined as $U_{\text{eff}} = U - J$, setting the exchange term, $J = 0$. The space group used in our calculations is $P6_3/mmc$ and lattice parameters were taken from the reference [23].

Band structure calculation converges to a metallic ground state as also found experimentally. The valence band is found to be primarily constituted by Nd 4f, Pd 4d and Si 3p states; partial density of states (PDOS) calculated for $U = 0$ and $U = 6$ eV are shown in figure 1. The calculated results exhibit significant modification for the consideration of $U$. For example, Nd 4f PDOS is essentially concentrated as a narrow band at the Fermi level in $U = 0$ case—weak intensities are observed at higher binding energies after we rescaled the intensities by a factor of 200. Si 3p PDOS exhibit two broad bands in the energy range (0–2.5 eV) and (2.5–6 eV). On the other hand, Pd 4d states primarily contribute between 2.5–6 eV energy regime. From the distribution of various PDOS, it is evident that Nd 4f states hybridize with the Si 3p states and Nd 4f–Pd 4d hybridization appears to be weak. Pd 4d–Si 3p hybridization leads to bonding features between 2.5–6 eV binding energies with the dominance of Pd 4d contributions and the antibonding bands appear between 0–2.5 eV having large Si 3p contributions.

With the inclusion of $U$ among Nd 4f electrons, the electronic structure exhibits significant change. We have varied $U$ to get a good description of the experimental results and observe that $U = 6$ eV provides a representation similar to the experimental results. This value of $U$ is consistent with the estimate found for elemental Nd considering a small enhancement due to positive valancy of Nd in this system [9]. The calculated moment for Nd is 3.2 $\mu_B$, which is consistent with the earlier experimental findings [22]. The results show that the sharp Nd 4f band of the $U = 0$ case splits into 4 distinct features. The features centered at about 4.5 eV, 1 eV and $-1.5$ eV in the LDA + $U$ data are absent in the LDA results and match well with the experiment. While the features at 4.5 eV and $-1.5$ eV roughly in line with the consideration of $U = 6$ eV, the origin of the 1 eV feature is not clear. We believe that the origin of this feature is linked to the complex interplay of the crystal field splitting and on-site Coulomb interactions. Further studies are required to understand the origin of this feature. Consequent to the appearance of correlation induced features, the feature at the Fermi level becomes less intense in LDA + $U$ data relative to the LDA results. Although the scenario involving Pd 4d and Si 3p remains similar to the $U = 0$ case, the shift of Nd 4f PDOS to the proximity of Si 3p and Pd 4d bands leads to enhanced Pd 4d–Nd 4f hybridization.

In figure 2, we show the experimental valence band spectra collected at 10 K using monochromatic laboratory sources, He I, He II and Al Kα after normalizing by the intensity of the intense peak around 4 eV binding energy. There are several features in the experimental spectra in the energy range shown down to 6 eV below the Fermi level. To identify the features, we have calculated the spectral functions from LDA + $U$ results for $U = 6$ eV. Each of the PDOS are multiplied by the atomic photoemission cross section for Al Kα spectroscopy [27]. These results are then broadened by a Gaussian representing the energy resolution and a Lorentzian representing various lifetime broadenings. The simulated total spectrum and the constituent components are shown in the figure by line exhibiting good representation of the experimental Al Kα data. It is evident that the intense feature at 4 eV binding energy is primarily contributed by Pd 4d states and the feature at 4.5 eV is contributed by Nd 4f states; here, rare-earth 4f signal appears at binding energy higher than that of Pd 4d (reference [28]).

The photoexcitation cross sections of Pd 4d and Si 3p show similar trend of change in the photon energies used in our study. The relative photoemission cross section of Nd 4f with respect to Pd 4d at He I energy increases by about 3.5 times at He II energy and by about 15 times at Al Kα energy. Therefore, the He I spectrum mainly represents the Pd 4d and Si 3p characters in the valence band, whereas He II and Al Kα yield enhanced information of Nd 4f state along with other contributions; Al Kα data has the highest Nd 4f contribution compared to that in the other spectra. Thus, significantly smaller intensity at 4.5 eV in the UV spectra compared to the Al Kα spectrum can be attributed to the change in relative photoemission cross section [27]. This provides an experimental evidence of the Nd 4f contribution at this energy.

The features at 0.3 eV and 1 eV are distinct in the Al Kα data, while the intensities in the UV spectra is somewhat flat in this energy range. This indicates Nd 4f contribution at
Figure 3. (a) Pd 4d, (b) Si 3p and (c) Nd 3d core level spectra collected at 10 K. In (a), the extended energy region in Pd 3d spectrum is rescaled in intensity to reveal loss features indicated by arrows. In (c), the arrows show the location of distinct features. High binding energy part is shown in enlarged intensity scale to emphasize the peak positions. The inset shows the Nd 3d_{5/2} intense signal in an expanded energy scale.

Figure 4. (a) Simulation of the Nd 3d core level spectrum; experimental data (open circles) and simulated spectrum (red line) are superimposed over each other exhibiting good representation. (b) The constituent peaks are shown in an expanded intensity scale. Arrows with the numbers represent the energy position of the features corresponding to Nd 3d_{5/2} signal and the dashed vertical lines indicate features corresponding to Nd 3d_{3/2} signal.

these energies, which is in good agreement with the calculated results for $U = 6$ eV. Si 3p states primarily contribute at 1.8 eV along with significant intensities in the 3–5 eV binding energy range. All these results indicate that the group of features below 3 eV binding energy are the bonding peaks and the ones between 0–3 eV are antibonding peaks arising due to hybridization between Nd 4f, Pd 4d and Si 3p states. It is to note here that in the case of Ce$_2$PdSi$_3$, Ce 4f states are closer to the Fermi level along with significant 5d contributions leading to a large 4f–5d hybridization in this system [28]. Since the Nd 4f states in Nd$_2$PdSi$_3$ appear at higher binding energy, the Si 3p contribution at the Fermi level becomes relatively larger which might be the driving force for unusual magnetic ground state in this material.

Some selected core level spectra collected at 10 K are shown in figure 3. Pd 3d core level spectrum shown in figure 3(a) exhibits two sharp features at about 337 eV and 342.3 eV corresponding to spin–orbit split 3d_{5/2} and 3d_{3/2} excitations, respectively; the intensity ratio is 3:2 as expected from the multiplicity of the features and the spin–orbit splitting is 5.3 eV. Higher binding energy regime exhibits a hump with significant intensity. For clarity, we show the spectrum with rescaled intensity exhibiting signature of two peaks (see arrows) separated by the energy of Pd 3d spin–orbit splitting. This suggests their origin to be associated to plasmon-type collective excitations. The photoemission signal from Si 2p core level spectra shown in figure 3(b) exhibits two spin–orbit split features at 99 eV and 99.5 eV representing 2p_{3/2} and 2p_{1/2} excitations, respectively; spin–orbit splitting is close to 0.5 eV. We could not probe the loss feature at the higher binding energy regime in this case due to the overlap of photoemission signals from Nd 4d core level.

In figure 3(c), we show the Nd 3d core level spectrum, which reveals two sharp and intense peaks at 982 eV and 1004.7 eV corresponding to the spin–orbit split features 3d_{5/2} and 3d_{3/2} excitations, respectively. In addition, there are several features; distinct signature of the features are clearly visible in the experimental data as denoted by ‘arrows’ in the figure. Presence of such multiple features indicate that strong orbital dependent Coulomb interactions are important in this system and charge transfer from the ligand levels to Nd is possible that allows screening of the photoemission core hole.

In order to delineate the signature of these features, we have simulated Nd 3d core level spectrum using a set of asymmetric functions having Doniach–Sunjić lineshape [29]. The results are shown in figure 4 exhibiting good representation of the experimental spectra. Such a lineshape indicates metallic ground state that allows low energy excitations across the Fermi level and hence, asymmetry in the peak. The constituent peaks are represented by solid lines. It is evident that there are at least five features (marked by numerics in figure 4(b)) associated to the excitation of each of the spin–orbit split features.

In photoemission, the incident photon beam excites electrons from its ground state (initial state); the excited state is called the final state. The final state Hamiltonian contains all
the interaction parameters present in the ground state and in addition, the core hole potential created by the excitation process. If the electrons are non-interacting, the final states will be identical to the initial states and one observes a feature corresponding to each excitations. For \( U \neq 0 \), the eigenstates of the final state Hamiltonian will be different from those for the initial state Hamiltonian and there will be finite overlap of multiple final states with the ground state wave function leading to multiple features; this is known as final state effects [30–33]. Assuming a configuration interaction model, the electronic configuration of the final states are as follows. Electronic configuration of Nd (atomic number 60) is \([\text{Xe}]4f^3(5d^16s^2)\). Usually, Nd is found in \((3^+ \) valence state similar to other rare earth based materials. Therefore, the ground state will be dominated by the electronic configuration, \( |4f^3\rangle \). Due to creation of Nd 3d core hole, the final states will be comprised of \(|4f^3 \rangle\) states and the charge transferred states, \(|4f^3L_1 \rangle\), \(|4f^3L_2 \rangle\), etc. Here, \( L \) is a hole in the ligand band, (Pd4dSi3p).

From various core level calculations [30–33], it is well established that the lowest binding energy feature corresponds to the most stabilized final state, where the stabilization comes from the screening of the core hole with the conduction electrons. Thus, the feature ‘1’ in the figure can be associated to the final state, \(|4f^3L_1 \rangle\) for 3d\(_{3/2}\) excitations. All other cases for 3d\(_{5/2}\) excitations appear at higher binding energies; they are labelled as 2, 3, 4 and 5 with vertical arrows in figure 4. Evidently, hybridization of Nd 4f with the valence electrons (mostly Si 3p) is significant leading to charge transfer induced final state features. The features ‘4’ and ‘5’ appear about 16 eV and 32 eV away from the main peak. In Ce-based systems, similar features are observed and are often attributed to Kondo physics [34]. However, we observe loss features in Pd 3d core level spectrum shown in figure 3(a) at similar energy separations, which is also consistent with the observation of plasmon excitations in other \(R_2\)PdSi\(_3\) systems [28]. These observations suggest that the features ‘4’ and ‘5’ are indeed loss features due to the plasmon excitations along with the photoexcitation of core electrons.

In summary, we studied the electronic structure of Nd-PdSi\(_3\) using high resolution photoemission spectroscopy and \textit{ab initio} band structure calculations. The comparison of the experimental valence band spectra with the calculated results provide an estimate of the on-site Coulomb energy of Nd 4f electrons close to 6 eV. The electronic states close to the Fermi level is constituted by hybridized Nd 4f and Si 3p states unlike in Ce case having significant 5d contributions, which is possibly the origin of anomalous magnetism of Nd compound. The core level spectra exhibit multiple features indicating strong final state effects. These results provide an evidence of strong Nd 4f–Si 3p hybridization despite the fact that Nd 4f has stronger atomic character than Ce-based systems, which could be the key for the apparent anomaly for the exotic magnetism of this system.

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