

Silencing electron correlations in the open Ni 3d shell system NiTe₂

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The van der Waals transition metal dichalcogenide NiTe₂ is investigated through soft x-ray photoelectron and absorption spectroscopy combined with density functional plus dynamical mean-field theory. We derive an electronic configuration of d^9 for the Ni ions with some admixture of d^8 and d^{10} , yielding an average 3d occupation of about 8.9. Despite the d shell being open with non-negligible hole concentrations, calculations reveal the absence of local moments, thereby explaining the Pauli paramagnetic behavior as observed in magnetic susceptibility measurements. This behavior is unusual, particularly given that many Ni-based compounds exhibit strong electron correlations. We ascribe the silencing of correlation effects in this material to the fact that without the Ni–Te hybridization, the Ni would have the nonmagnetic full d^{10} configuration, and that the Ni bands that get partially unfilled due to hybridization are extremely broad, making the holes “bandlike” or “highly delocalized”. The large Hubbard U interaction does not become operative in this material.

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I. INTRODUCTION

Transition metal (TM) compounds constitute a class of materials that exhibit emergent properties arising from the interaction of different electronic degrees of freedom [1,2]. These include metal-insulator transitions, high-temperature superconductivity, and colossal magnetoresistance [3–5]. A particularly important subclass comprises compounds with 3d TMs, where the atomlike nature of the 3d orbitals makes the on-site Coulomb interaction significant, rendering one-electron approximations inadequate [6]. Nickel-based materials serve hereby as prototypical systems in which strong electron correlations play a dominant role in determining the electronic and magnetic properties. In NiO, for example, correlations lead to a Mott insulating state [7–9] or, more precisely, following the Zaanen-Sawatzky-Allen classification [10], a charge-transfer insulating state. In rare-earth (R) nickelates, such as $R\text{NiO}_2$ [11] and $R_{n+1}\text{Ni}_n\text{O}_{3n+1}$ [12], high-temperature superconductivity was observed. Apart from

oxides, correlation effects of nickel are also reported to be present with other chalcogens, such as the Mott insulator NiS_2 [13] and the correlated metal NiSe_2 [14]. Remarkably, even in elemental nickel, with itinerant d electrons, correlations manifest in its ferromagnetism that goes beyond the simple Stoner mean-field theory [15–18]. These examples underscore the ubiquity of electron correlations across diverse electronic phases in nickel compounds.

Recently, TM dichalcogenides (TMDCs) have garnered interest as a family of two-dimensional van der Waals materials. Their layered structure and highly tunable properties—which depend on the choice of TMs and chalcogens (S, Se, and Te)—offer a broad range of potential applications [19–21]. Nickel ditelluride (NiTe_2) is one of the TMDCs reported to be a semimetal with a nontrivial topological feature [22]. Its 1T-type crystal structure is displayed in Fig. 1. Superconductivity was observed in a Te-deficient sample under hydrostatic pressure reaching $T_c = 7.5$ K at 52.8 GPa [25] and, recently, intrinsic superconductivity was detected in a stoichiometric sample below $T_c = 261$ mK [26]. Angle-resolved photoelectron spectroscopy studies reveal a series of inverted band gaps that give rise to topological surface states and a type-II Dirac point close to the Fermi level [27–30]. The Te plays hereby the dominant role by forming dispersive bands that cross the Fermi level and help generate the topological surface states.

The role and character of Ni in NiTe_2 , however, have received less attention and have only been discussed briefly. It has been reported that the position of the Dirac node in NiTe_2 is different from the Pd and Pt counterparts [28]. Electron

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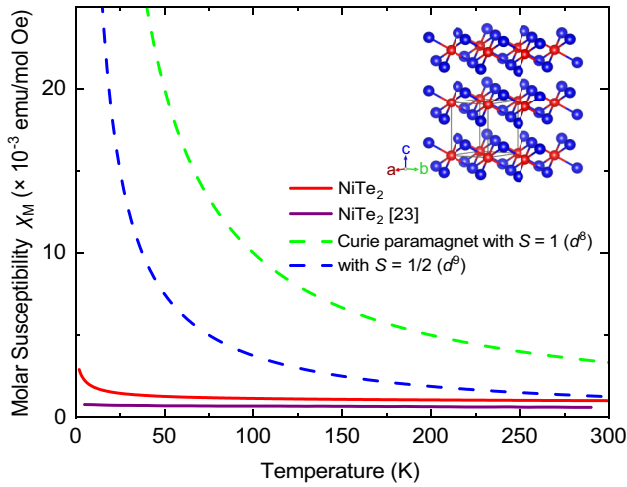


FIG. 1. Magnetic susceptibility of our NiTe_2 sample and that of Ref. [23] together with the calculated Curie paramagnetic behavior for an $S = 1$ (d^8) and an $S = 1/2$ (d^9) system. The inset shows the 1T- NiTe_2 van der Waals crystal structure and its unit cell (red: Ni; blue: Te), visualized by VESTA [24].

correlation effects have been mentioned only for the surface states based on DFT+ U analysis [30]. The Ni valence is often even not considered or assumed to be +2 (d^8) [31]. Only very recently, an x-ray spectroscopy study combined with cluster-model calculations examined the Ni electronic configuration, assigning an average Ni 3d occupation close to 9 and classifying NiTe_2 as a negative charge-transfer compound starting from a d^8 ansatz [32].

Magnetic susceptibility measurements on NiTe_2 single crystals have reported a temperature-independent Pauli paramagnetic behavior up to 300 K [23,26,33], indicating the absence of local moments. This is surprising if one considers an open d shell for this Ni compound [31,32]. In Fig. 1, we contrast the expected Curie behavior for a d^9 and a d^8 ion against the measured temperature dependence of the magnetic susceptibility [23]. It is immediately evident that the NiTe_2 behavior is not reflected by either of the Curie-Weiss curves. The susceptibility is considerably smaller, and there is generally no indication of magnetic ordering. The underlying origin of the absence of local moment behavior remains, however, unclear. One may speculate whether a Kondo screening mechanism can be present, as in the case of the $\text{CaCu}_3\text{Ru}_4\text{O}_{12}$ [34] where the magnetic moments of the Cu- d^9 ions are screened by the metallic Ru-O bands with an estimated Kondo temperature of around 1000 K.

To investigate Ni electronic behavior and the origin of its absence of local moment behavior, we present a soft x-ray photoelectron spectroscopy (PES) and x-ray absorption spectroscopy (XAS) study on NiTe_2 combined with density functional theory (DFT) plus dynamical mean-field theory (DMFT) calculations. A theoretical framework beyond cluster models is hereby required, as the hybridization with the extended metallic Te bands may play an essential role. Here, we will adopt the approach in which we constrain the DMFT calculations by tuning the model parameters, including specifically the double-counting correction, to reproduce accurately

the measured spectra [34–37]. The DFT + DMFT results are then used to quantify the Ni valence state and its charge fluctuations, and to further explore the Ni spin dynamics and the temperature dependence of the magnetic properties over a temperature range extending well beyond previous measurements. We examine why this material behaves so differently from other nickel-based compounds.

II. METHODS

PES, resonant PES (ResPES), and $\text{Ni-L}_{2,3}$ XAS were performed at the NSRRC-MPI TPS45A submicron soft x-ray spectroscopy beamline at the Taiwan Photon Source. PES were carried out at the normal emission geometry using an MB Scientific A-1 photoelectron analyzer and linear horizontal polarized light with the electrical field vector in the plane of the storage ring. For XAS, a 30° grazing incidence angle relative to the sample surface was used in total electron yield mode. All measurements were performed at $T = 40$ K. The overall energy resolution of the PES for $h\nu = 1200$ and 620 eV is approximately 135 and 125 meV, respectively, determined by fitting the Fermi edge of platinum. During $\text{Ni-L}_{2,3}$ XAS, NiO was measured simultaneously as a reference for the energy scale, which allows for the comparison of the relative absorption edge position with other compounds. Clean sample surfaces were prepared by *in situ* cleaving the NiTe_2 single crystal under ultrahigh-vacuum conditions with pressures below 1×10^{-10} mbar.

Reference Te 3d PES data for Bi_2Te_3 [38] and elemental Te were taken at room temperature using a monochromatic Al $K\alpha$ x-ray source, $h\nu = 1486.6$ eV, and a Scienta R3000 electron energy analyzer. The overall energy resolution was approximately 350 meV, and a polycrystalline Ag sample was used for calibration.

Appendix A describes in detail the sample preparation and characterization. Figure 1 shows the magnetic susceptibility of our NiTe_2 sample as a function of temperature, revealing similar Pauli paramagnetic behavior as reported in the literature [23].

We perform DFT + DMFT calculations [39,40] using the same implementation as described in Refs. [34,41,42]. Starting from a standard DFT calculation within the local density approximation (LDA) for the exchange-correlation functional, carried out using the WIEN2K package [43], we derive a tight-binding Hamiltonian spanning the Ni 3d and Te 5p states [44,45]. The tight-binding model is augmented by local electron-electron interaction within the Ni 3d shell, which is parametrized by the Hubbard interaction U and the Hund's coupling J . We employ $U = 5.0$ eV and $J = 1.0$ eV, consulting with previous studies on Ni chalcogenides [46]. The interacting lattice problem is solved within the DMFT approximation. The continuous-time quantum Monte Carlo (CT-QMC) method [47–50] is adopted to compute the local self-energy $\Sigma(i\omega_n)$ of the Ni electrons by solving the Anderson impurity model (AIM) on the Matsubara axis. Once convergence is achieved in the DMFT self-consistent cycle, the self-energy $\Sigma(\omega)$ on the real-frequency axis is obtained via analytic continuation [51], from which the one-particle spectral functions as well as the hybridization densities on the real-frequency axis are computed. In addition, the local

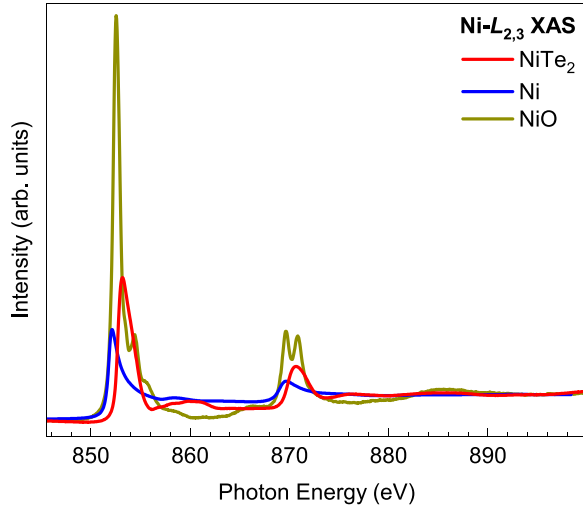


FIG. 2. Ni- $L_{2,3}$ XAS spectra of NiTe₂, Ni metal, and NiO. The spectra were normalized to the continuum at 895 eV and higher energies.

spin correlation function $\chi_{\text{spin}}(\tau)$ is computed from the AIM using the CT-QMC [52], and the temperature-dependent local spin susceptibility is obtained as $\chi_{\text{loc}}(T) = \int_0^\beta d\tau \chi_{\text{spin}}(\tau)$, where τ is the imaginary time and $\beta = 1/k_B T$ is the inverse temperature. To analyze the core-level spectra based on the DFT + DMFT valence electronic structure, we employ the AIM with the DMFT hybridization densities $V(\omega)$, which is extended to include the Ni 2*p* core orbitals and their Coulomb interaction with the Ni 3*d* valence electrons. This step follows the same numerical procedure as described in Refs. [41,42]. Unless otherwise stated, all calculations are performed at 300 K.

III. RESULTS: HIGH-ENERGY EXCITATIONS

Figure 2 shows the Ni- $L_{2,3}$ XAS spectrum of NiTe₂ in comparison with those of nickel metal and NiO. All spectra are normalized to the continuum at 895 eV and higher energies. The spectra are dominated by the Ni 2*p* core-hole spin-orbit coupling that splits the spectrum roughly in two parts, namely, the L_3 ($h\nu = 851\text{--}865$ eV) and L_2 ($h\nu = 868\text{--}882$ eV) regions. The NiTe₂ spectrum consists of two intense, asymmetric white lines, accompanied by weak, broad structures peaked at about 6 eV higher energies. The Ni- $L_{2,3}$ edges predominantly probe dipole-allowed 2*p* $\rightarrow$ 3*d* transitions. Notably, the weak, broad features at higher energies are likely associated with excitations into the unoccupied 4*s* states [53].

The white line intensity provides information about the number of available holes in the Ni 3*d* shell. The more holes, the higher intensity the white line will have. The comparison with the NiO and nickel metal suggests that the *d* occupation $\langle n_d \rangle$ of NiTe₂ falls between that of NiO ($\langle n_d \rangle \sim 8.2\text{--}8.4$) [8,54] and nickel metal ($\langle n_d \rangle \sim 9\text{--}9.2$) [55–60]. This is our first indication that the Ni 3*d* shell is open and that the hole concentration is substantial, albeit smaller than 2 per Ni ion.

Figure 3 shows the Ni 2*p* core-level PES spectrum of NiTe₂ together with that of nickel metal and NiCl₂. The latter

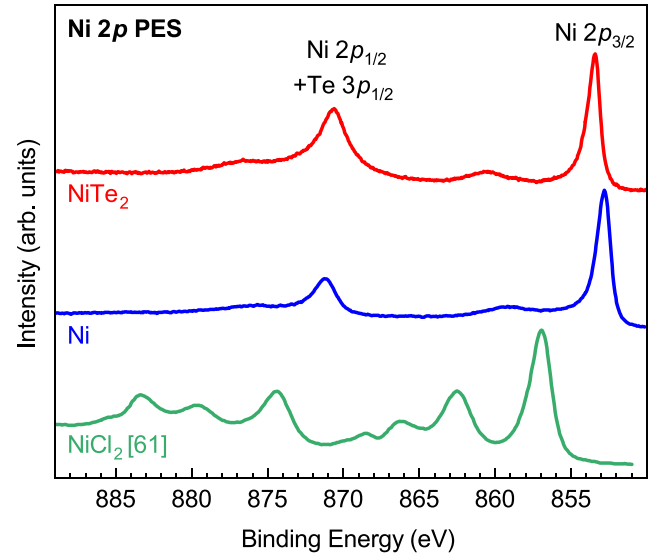


FIG. 3. Ni 2*p* core-level PES of NiTe₂, Ni metal, and NiCl₂. The NiTe₂ and Ni metal spectra were taken at $h\nu = 1200$ eV. The NiCl₂ spectrum is reproduced from Ref. [61] where $h\nu = 1486.6$ eV x-rays were used.

is reproduced from Ref. [61]. The spectra are split by the Ni 2*p* spin-orbit interaction into the 2*p*_{3/2} and 2*p*_{1/2} regions. We note that in NiTe₂ the Ni 2*p*_{1/2} peak overlaps with the Te 3*p*_{1/2} peak, complicating a comparison between the materials on the basis of the Ni 2*p*_{1/2}. Focusing on the 2*p*_{3/2} regions, the spectral line shape of the NiTe₂ is quite similar to that of nickel metal. It consists of a slightly asymmetric main peak accompanied by a satellite at about 6–7 eV higher binding energies. In contrast, the line shape of NiCl₂ is quite different. There the main peak is accompanied by multiple strong satellites.

These observations suggest that both the main peak and the satellite in NiTe₂ are similar in character to those in nickel metal and very different from those in NiCl₂. Based on several studies employing three-configuration Anderson impurity model calculations and cluster model calculations, the Ni 3*d* electronic configurations have been quantified as 14%–21% $d^8 + 48\%\text{--}65\%$ $d^9 + 17\%\text{--}38\%$ d^{10} for nickel metal [55–60] and as 71% $d^8 + 23\%$ $d^9 + 6\%$ d^{10} for NiCl₂ [54,62,63]. We thus can infer that the average *d* count in NiTe₂ is likely to be closer to 9 rather than 8.

We also have performed valence-band resonant photoelectron spectroscopy at the Ni- L_3 edge in order to identify the electronic configurations contributing to the electronic structure of especially d^8 , d^9 , and d^{10} systems [58,60,64,65]. Figure 4 displays the valence-band spectrum of NiTe₂ taken with the photon energy tuned to the Ni- L_3 absorption white line (on-resonant) and with the photon energy set at 5 eV below the white line (off-resonant). At resonance, two processes with the same final state are present: (1) the direct PES, $d^n + h\nu \rightarrow d^{n-1} + e_k$, and (2) the resonant process in which the photoabsorption is followed by an Auger decay, $d^n + h\nu \rightarrow \underline{c}d^{n+1} \rightarrow d^{n-1} + e_k$. Here, $\underline{c}$ denotes a core hole in the Ni 2*p* shell and e_k the emitted photoelectron. In principle, the two processes are coherent and can lead to interference

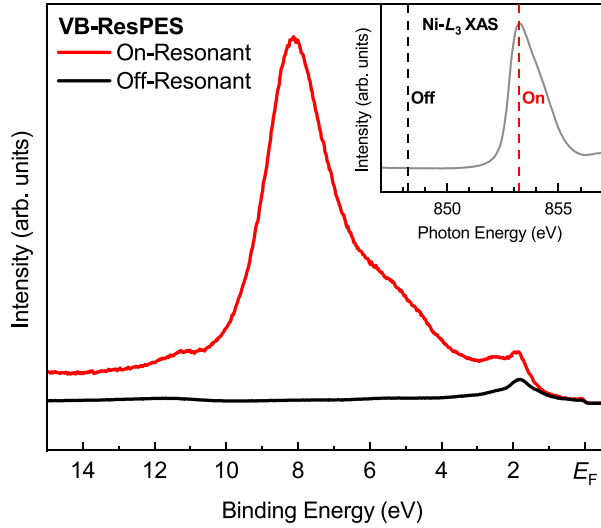


FIG. 4. Valence-band PES spectra of NiTe_2 taken with the photon energy tuned to the Ni-L_3 absorption white line (on-resonant) and with the photon energy set at 5 eV below the white line (off-resonant). These ResPES spectra are normalized to the incident photon flux.

effects. Yet, at the L_3 edge, the resonant process dominates and provides direct information about the configurations involved in the ground state (d^n), intermediate state ($\underline{c}d^{n+1}$), and final state (d^{n-1}) [64].

The resonant enhancement as shown in Fig. 4 has the typical line shape as observed earlier for CuO [64] and nickel metal [58,60]. The main peak at 8 eV binding energy is characteristic for the so-called atomiclike ^1G state in the d^8 final state spectrum, and the high-energy feature at 11 eV binding energy can be assigned to the ^1S state [66], the d^8 multiplet state with the highest energy. Consequently, the XAS white line must be of mainly $\underline{c}d^{10}$ character and the ground state must contain appreciable d^9 configuration.

Having established using high-energy excitations that the $\text{Ni } 3d$ shell is filled with about nine electrons, we can look at the Te valency to check the charge balance. Using PES, we collect the Te $3d$ core-level spectrum and compare its energy position with that of Bi_2Te_3 and elemental Te. The data are displayed in Fig. 5. We find a $\text{Te } 3d_{5/2}$ peak position of 572.56 eV for NiTe_2 , which falls in between the 572.05 eV position of Bi_2Te_3 [38] as a Te^{2-} system and the 572.94 eV of elemental Te as a Te^0 reference. Assuming a linear relationship between the chemical shift of $\text{Te } 3d_{5/2}$ and its valence state [31], we may estimate the Te valence to be about -0.6 in NiTe_2 . This is not inconsistent with the short (3.44, 3.46, 3.86 Å all <4 Å) inter- and intralayer adjacent Te-Te distances [67]. Using charge neutrality arguments, the Te results suggest a Ni valence of about $+1.2$ (i.e., a d count of 8.8), which is consistent with the above findings from the Ni XAS, PES, and ResPES spectra.

IV. RESULTS: VALENCE BAND AND DMFT

We now focus on the electronic structure of the valence band of NiTe_2 in more detail. The spectra were collected at

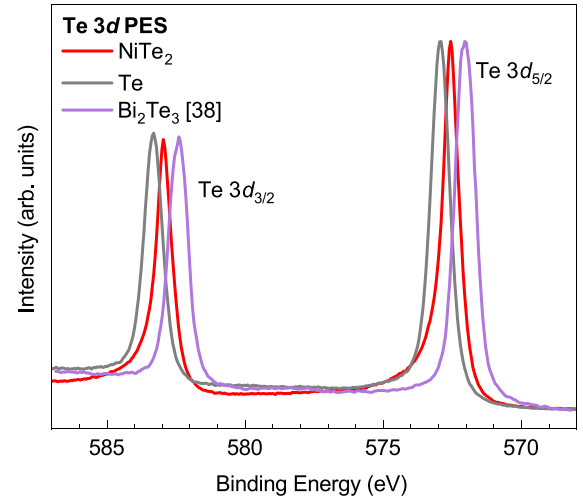


FIG. 5. $\text{Te } 3d$ core-level PES of NiTe_2 , Bi_2Te_3 from Ref. [38], and elemental Te.

$h\nu = 620$ and 1200 eV and are shown in Fig. 6. A clear Fermi cutoff is observed, reflecting the metallic nature of NiTe_2 , along with the $\text{Te } 5s$ states at a binding energy of about 12 eV. To disentangle the $\text{Ni } 3d$ contribution to the valence band, we utilize the photon-energy dependence of the photoionization cross sections, σ . Based on the calculated subshell photoionization cross sections obtained from Ref. [68], the $\text{Ni } 3d$ spectral intensity is expected to change more significantly than those of $\text{Te } 5s$ and $\text{Te } 5p$ ($\sigma_{620\text{ eV}}/\sigma_{1200\text{ eV}} \sim 3.15, 3.11$, and 8.89 for $\text{Te } 5s$, $\text{Te } 5p$, and $\text{Ni } 3d$, respectively). By normalizing the spectra to the $\text{Te } 5s$ peak at around 12 eV binding energy, we observe that the sharp 2 eV peak changes significantly, enabling us to identify this peak as of predominantly $\text{Ni } 3d$ character. In return, we can also infer that the $\text{Te } 5p$ states are spread out over the entire valence-band region, i.e., from 6.5 eV binding energy and upward crossing

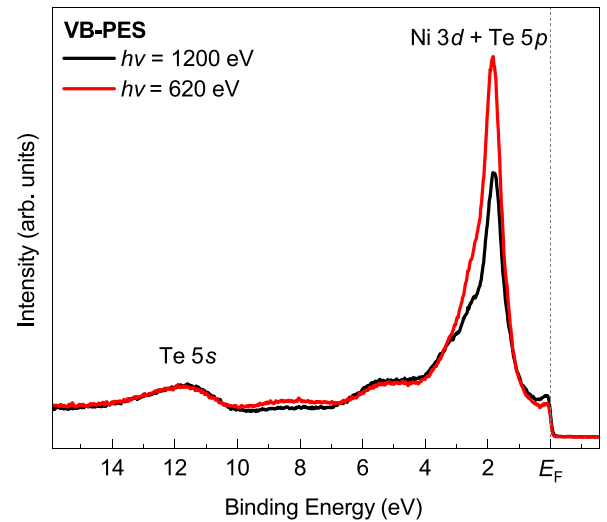


FIG. 6. Valence-band PES spectra of NiTe_2 taken with 620 eV (red line) and 1200 eV (black line) photon energy. The spectra were normalized to the $\text{Te } 5s$ peak.

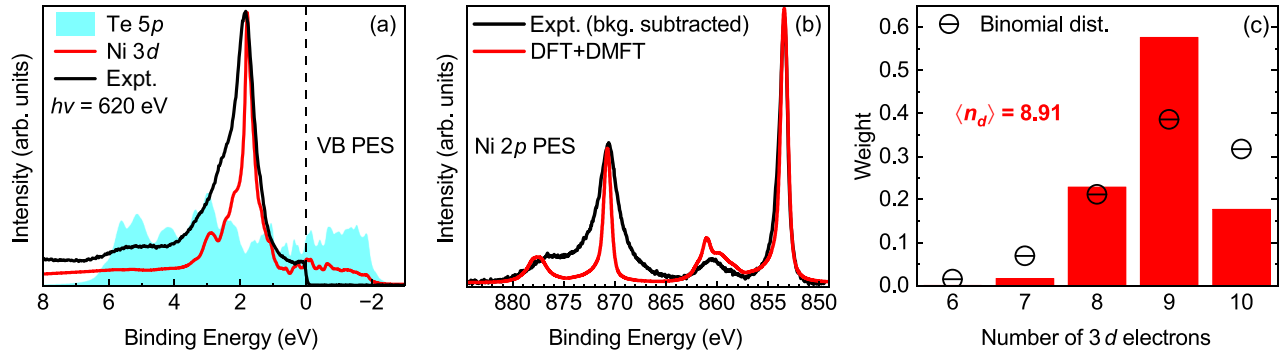


FIG. 7. DFT + DMFT calculations with $\mu_{dc} = 37.7$ eV, $U = 5$ eV, and $J = 1$ eV. (a) Ni 3d and Te 5p spectral functions together with the valence-band PES spectrum ($h\nu = 620$ eV). (b) Ni 2p spectral function and Ni 2p core-level PES spectrum. (c) Ni 3d configuration histogram, average 3d shell occupation, and corresponding binomial configuration distribution.

the Fermi level, as we will confirm later from the theoretical calculations.

To investigate the contribution of the Ni 3d states to the electronic structure of NiTe₂ and especially to the presence or absence of electron correlation effects, we performed DFT + DMFT calculations. As mentioned in the introduction section, a double-counting correction μ_{dc} must be introduced to subtract the electron-electron interaction effects that were already included in the DFT step [40,69,70]. However, a universal expression for μ_{dc} is not available. Rather than adopting standard schemes, we determine μ_{dc} by reproducing the experimental valence-band spectrum [34–37]. This approach is justified by the fact that μ_{dc} effectively renormalizes the relative energy position of the correlated 3d levels with respect to other, noncorrelated orbitals, namely, the Te 5p states in the present compound. Photon-energy-dependent PES measurements enable an experimental identification of the dominant peaks associated with the constituent orbitals, thereby guiding the optimization of μ_{dc} .

As shown in Fig. 7(a), we are able to obtain the Ni 3d and Te 5p spectral functions with the correct line shape and energy positions for both subshells. The optimal value for μ_{dc} is about 37.7 eV, while the parameters describing the Ni 3d Coulomb and exchange interactions were set at $U = 5$ eV and $J = 1$ eV. In order to verify the consistency of our results, we also have performed calculations for the Ni 2p spectral weight. Figure 7(b) shows that also the Ni 2p core-level PES spectrum can be accurately reproduced.

A search over a wide parameter range of μ_{dc} values is summarized in Appendix B (Fig. 10). In the valence-band spectrum, we find a systematic shift of the Ni 3d peak with respect to the Te bands as a function of μ_{dc} . In the Ni 2p PES, both the position and the intensity of the satellite features are also sensitive to the μ_{dc} value. As μ_{dc} controls the position of the Ni 3d levels, it influences the Ni 3d occupation. A deeper Ni 3d level, i.e., a larger value of μ_{dc} , favors a higher Ni 3d occupation. The plots in Appendix B allow us to unambiguously determine a reasonable range of μ_{dc} around 37.7 eV.

V. VALENCE STATE AND MAGNETIC BEHAVIOR

In the following, we analyze the DFT + DMFT results of NiTe₂ with the optimized $\mu_{dc} = 37.7$ eV. It yields an average

occupation of $\langle n_d \rangle = 8.91$ and a configuration distribution of $<2\%$ d^7 , 23% d^8 , 58% d^9 , and 18% d^{10} [see Fig. 7(c)]. The predominant d^9 configuration with comparable admixture of d^8 and d^{10} supports our spectroscopic assignments above and the similarities we noticed to nickel metal. The cluster model mentioned earlier [32] found Ni configuration weights of 19.5% d^8 , 57.4% d^9 , and 23.1% d^{10} . These values are close to our DMFT results, but have been derived in a model that does not take into account the extended metallic character of the Te bands. This cluster model produces inevitably a local moment for the Ni.

Along with the configuration histogram from our DMFT calculations, we also plot the binomial distribution $P(d^n)$, which is given by

$$P(d^n) = \binom{10}{n} \times \left(1 - \frac{\langle n_d \rangle}{10}\right)^{10-n} \times \left(\frac{\langle n_d \rangle}{10}\right)^n.$$

This represents the noncorrelated itinerant limit [35,71]. As the width of the histogram reflects the magnitude of charge fluctuations, deviations from this binomial distribution serve as a measure of the degree of electron correlation within the d shell [35,36]. We observe that the substantial admixture of the three main configurations results in a relatively broad distribution, with a moderate narrowing as compared to the hypothetical itinerant limit, as the Hubbard U interaction is not small.

Our finding that the Ni d^9 configuration is dominant and that the local Coulomb interaction is sizable may lead to the expectation that $S = 1/2$ local moments can be formed. This then would not be compatible with the experimentally observed Pauli paramagnetic behavior shown in Fig. 1. To address this, we examine in Fig. 8 the temperature-dependent local spin susceptibility $\chi_{loc}(T)$, and the local spin-spin correlation function $\chi_{spin}(\tau)$, obtained from the DFT + DMFT calculations. We present the data for the optimal model with $\mu_{dc} = 37.7$ eV, as well as the results for other μ_{dc} values in the range $\mu_{dc} = 33.7$ –40.7 eV.

The spin-spin correlation function $\chi_{spin}(\tau)$ at $\tau = 0$ encodes the instantaneous Ni 3d spin moment. Yet, $\chi_{spin}(\tau)$ exhibits a rapid decay on a short timescale and does not develop into a long-lived local moment, as shown in Fig. 8(a). This behavior persists from 300 up to 3000 K, the maximum temperature covered in the calculations. As a consequence,

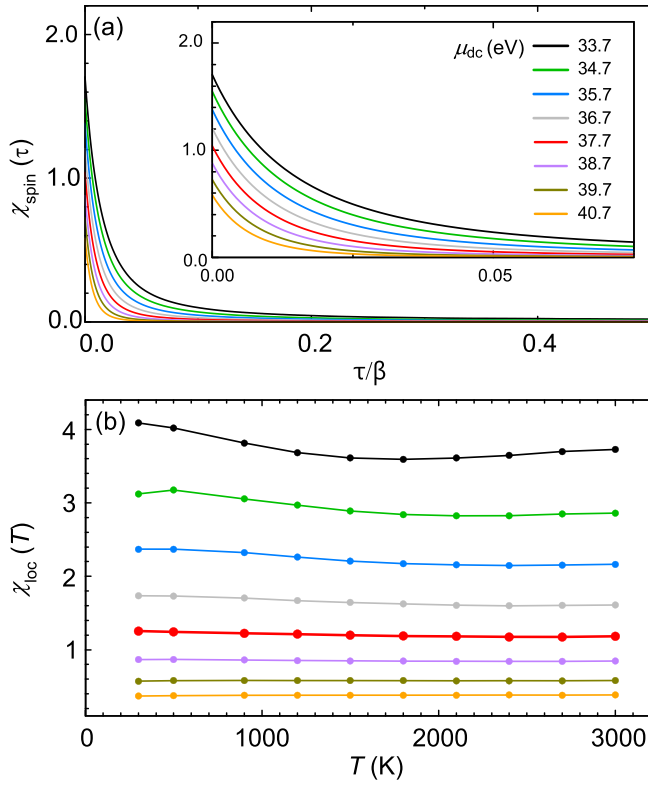


FIG. 8. (a) Spin-spin correlation function, $\chi_{\text{spin}}(\tau)$, for different μ_{dc} . (b) Temperature dependence of the local spin susceptibility, $\chi_{\text{loc}}(T)$, from $T = 300$ to 3000 K for different μ_{dc} . The optimal $\mu_{\text{dc}} = 37.7$ eV is displayed in red.

Curie-Weiss behavior does not appear in the spin susceptibility shown in Fig. 8(b), which instead remains nearly constant. This situation is quite different from a Kondo behavior where the screening of the moments present at low temperatures vanishes for high temperatures, as, e.g., observed in $\text{CaCu}_3\text{Ru}_4\text{O}_{12}$ [34]. We would like to note that local-moment behavior does not emerge even for μ_{dc} outside the realistic set of parameters as seen in Fig. 8(b). Therefore, the constant local spin susceptibility and rapid loss of the spin moments in NiTe_2 must be connected to the inherent absence of local moments. For completeness, we performed DFT + DMFT calculations under two hypothetical conditions (not shown): (1) by increasing the Hubbard interaction up to $U = 15$ eV and (2) by lifting the degeneracy of the e_g^σ doublet by introducing an artificial crystal-field splitting, thereby allowing orbital polarization, which can enhance correlation effects in some TM compounds. Neither modification alters the observed behavior.

VI. DISCUSSION

In an effort to understand why local moments are not present in NiTe_2 , we perform also LDA calculations, in which the local dynamical correlation effects introduced by DMFT are absent. The results, shown in Fig. 9(a), are not very different from those of the DFT + DMFT as displayed earlier in Fig. 7(a). In both, there is a wide Te 5*p* band spanning from 6 eV below to 2 eV above the Fermi level with the Ni 3*d*

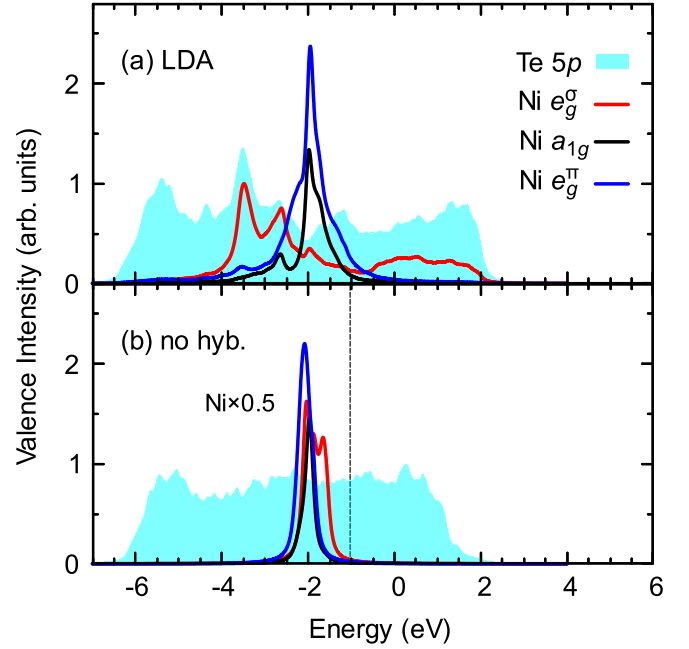


FIG. 9. Valence-band partial density of states obtained from LDA calculations (a) with and (b) without Ni-Te hybridization. In panel (b), the hopping elements between Ni and Te are artificially set to zero in the LDA tight-binding Hamiltonian and the dashed line marks the new chemical potential as given by the charge count.

band peaking at about 2 eV binding energy. This similarity is another indication that electron correlation effects are relatively silent.

To proceed further with our search, we make a breakdown of the Ni 3*d* contribution to the valence band in terms of the local e_g^σ , a_{1g} , and e_g^π states, i.e., the Ni states for a local NiTe_6 cluster with D_{3d} symmetry. Figure 9(a) shows that the a_{1g} and e_g^π states form relatively narrow bands, with a width of about 1.5–2 eV only. The e_g^σ states, in contrast, are part of a very wide band, ranging from 4 eV below to 2 eV above the Fermi level. Correlation effects will not manifest due to the a_{1g} and e_g^π derived bands since they are all below the Fermi level, thus forming a closed subshell. On the other hand, correlations can in principle show up as a result of the e_g^σ bands being partially filled. However, its band width is apparently so large that it supersedes the on-site Coulomb and exchange interactions, with the result that a magnetic state cannot be stabilized.

To elucidate the origin of the e_g^σ , a_{1g} , and e_g^π band widths, we carried out a tight-binding analysis on the LDA results. After having matched the tight-binding bands to the LDA, we switched off the hybridization between the Ni 3*d* and Te 5*p* states. Figure 9(b) shows that the Ni 3*d* bands then become extremely narrow, with a band width of 1 eV or less. This demonstrates that direct Ni-Ni hybridization is considerably weak and that the Ni 3*d* states instead interact predominantly via the Te band. The basics of the electronic structure of NiTe_2 can perhaps be viewed as ordered Ni impurities embedded in the broad Te 5*p* bands. This observation is consistent with the nearest-neighbor interatomic distances—Ni-Ni ~ 3.85 Å and

Ni-Te ~ 2.59 Å—and the more spatially extended nature of the Te 5*p* orbitals.

Very interesting is that in the absence of the Ni-Te hybridization, the entire set of narrow Ni 3*d* states is positioned well below the Fermi level, even when a proper charge count for this artificial NiTe₂ system is taken into account as indicated by the dashed line marking its chemical potential. This suggests that a many-body Anderson-lattice model for NiTe₂ could be constructed using local Ni 3*d*¹⁰ atoms embedded in a Te lattice with 2/3-filled 5*p* bands (5*p*⁴), which after Ni-Te hybridization create holes in the broad Ni-Te composite bands with Ni *e*_g^σ character. These holes can be characterized as “bandlike” or “highly delocalized.” In terms of a configuration-interaction framework, the closed-shell Ni 3*d*¹⁰ ansatz anchors the nonmagnetic state of the material. The 3*d*⁹*L*¹ and 3*d*⁸*L*² configurations are present due to charge transfer from the Ni *e*_g^σ to the unoccupied Te 5*p* ligand states, here denoted as *L*. An average Ni 3*d* count of slightly less than 9 can be achieved provided that the transfer or hopping integrals are indeed large compared to the charge-transfer and Coulomb energies. Yet, NiTe₂ is not a Kondo system since the symmetry determining configuration, namely, the 3*d*¹⁰, is lowest in energy and nonmagnetic.

VII. CONCLUSION

In conclusion, we have presented our investigation on the electronic structure of NiTe₂ using soft x-ray spectroscopy, combined with DFT + DMFT calculations. Core-level photoelectron spectroscopy, x-ray absorption spectroscopy, and resonant photoelectron spectroscopy demonstrate that the Ni 3*d* shell is open and that the *d* hole concentration is not negligible. A value close to one hole per Ni can be estimated already from the experiments. We have been able to obtain accurate simulations of the spectra using DFT + DMFT calculations and determine the configuration distribution as <2% *d*⁷, 23% *d*⁸, 58% *d*⁹, and 18% *d*¹⁰, with $\langle n_d \rangle = 8.91$. Despite the presence of Ni *d* holes and strong on-site Coulomb and exchange interactions, the calculated local spin susceptibility and spin correlation function support a Pauli paramagnetic scenario, consistent with the experimental observations. A Kondo behavior cannot be found from the DFT + DMFT. NiTe₂ could be modeled as local nonmagnetic Ni 3*d*¹⁰ atoms embedded in a Te lattice with 2/3-filled 5*p* bands, which after Ni-Te hybridization create bandlike or highly delocalized holes in the Ni 3*d*. The large Hubbard *U* interaction cannot become operative and correlation effects get silenced.

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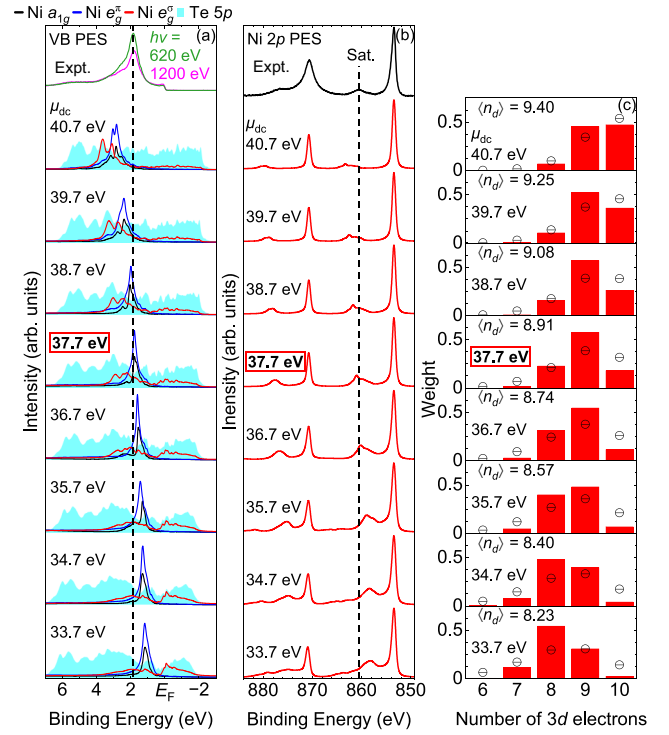


FIG. 10. DFT + DMFT calculations for a range of μ_{dc} values. The Coulomb and exchange parameters are set at $U = 5$ eV and $J = 1$ eV. (a) Ni 3*d* and Te 5*p* spectral functions together with the VB PES spectra taken with $h\nu = 620$ and 1200 eV photons. The dashed line marks the experimental Ni 3*d* peak position. (b) Ni 2*p* spectral functions and Ni 2*p* core-level PES spectrum. The dashed line marks the satellite position in the Ni 2*p* spectrum. (c) Ni 3*d* configuration histograms (in red), average 3*d* shell occupations, and corresponding binomial configuration distributions (in black).

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DATA AVAILABILITY

The data that support the findings of this article are openly available [72].

APPENDIX A: SAMPLE PREPARATION AND CHARACTERIZATION

NiTe₂ single crystals were obtained from chemical vapor transport (CVT). Sample storage and preparation were always performed in an argon atmosphere before the synchrotron experiments.

Crystallinity and composition were confirmed through single-crystal x-ray diffraction, powder x-ray diffraction, and energy-dispersive x-ray spectroscopy. Further details on the growth and the structure are to be found elsewhere [73].

Magnetic susceptibility measurements were carried out using an MPMS3 SQUID magnetometer (Quantum Design) on a 42 mg powder of NiTe₂, which was obtained by grinding the conglomerate that formed on the wall of the quartz ampoule during the CVT process. The data were collected under an applied magnetic field of 0.5 T in both zero-field-cooled and

field-cooled modes over a temperature range from 2 to 300 K, using a brass sample holder.

The elemental Te sample was prepared *in situ* under ultrahigh-vacuum conditions in a molecular beam epitaxy chamber by evaporating Te (ChemPUR, 99.9999%) onto an Al₂O₃ (0001) substrate (CrysTec GmbH) at the MPI-CPFS, Dresden. The nickel metal sample (Johnson Matthey Materials Technology U.K., 99.8%) was cleaned by Ar sputtering at 6×10^{-7} mbar for 1 h in a separate chamber before the measurements.

APPENDIX B: DOUBLE-COUNTING CORRECTION IN DFT + DMFT

Figure 10 shows the double-counting μ_{dc} dependence of the DFT + DMFT results. In panel (a), the calculated Ni 3*d* and Te 5*p* spectral functions are compared to the experimental valence-band spectra taken with 620 and 1200 eV photons. We can observe that the energy position of the

experimental Ni 3*d* main peak, as indicated by the dashed line at about 1.9 eV binding energy, can be well reproduced by the calculations for $\mu_{dc} = 37.7$ eV. In panel (b), the Ni 2*p* spectral function is compared to the measured Ni 2*p* core-level PES spectrum. The peak position of the satellite in the experimental spectrum is indicated by the dashed line.

Also here, we can observe that the energy distance between the main peak and the satellite can be well matched by the calculations for $\mu_{dc} = 37.7$ eV.

The configuration histograms are shown in panel (c) for the various values of μ_{dc} . The average Ni 3*d* shell occupations are also indicated together with the corresponding binomial configuration distribution. A larger value of μ_{dc} means a deeper Ni 3*d* level and favors a higher Ni 3*d* occupation. In all cases, the calculated configuration histograms are somewhat narrower in distribution as compared to the binomial or statistical case, suggesting that correlation effects are present but not strong.

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