Experimental and theoretical study of the electronic structure of AuAl₂

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Abstract

Synchrotron-radiation-excited angle-resolved photoemission spectra for the (100) and (111) faces of AuAl₂ are presented, along with derived experimental dispersion relations. These bands are compared with those obtained from the theoretical band-structure calculation. The density-of-state curves, band hybridization, and charge transfer for AuAl₂ are also calculated. The energy variation of the Au 5d bands for AuAl₂ shows atomic-like behavior in the photon-energy range of 80–200 eV. © 2001 Elsevier Science Ltd. All rights reserved.

1. Introduction

In recent years, much attention has been focused on the band-structure calculation of binary intermetallic compounds containing a noble metal and a group III element, as they provide a system with properties that are interesting from both theoretical and experimental points of view. They are prototype materials for studying the noble-metal d bands in the intermetallic compounds, since group III elements contribute only s–p states to the valence band (VB). This makes it possible to examine the effects of sp–d hybridization and charge transfer in the compounds. One of these compounds AuAl₂ has an unusual purple color, which strongly motivated researchers to study its electronic structure. During the past three decades, the electronic structure of AuAl₂ has been studied by performing band-structure calculations [1–3], X-ray [4–7] and ultraviolet [8] photoemission spectroscopic (XPS and UPS) experiments, angle-integrated photoemission spectroscopic (PES) work [9], X-ray absorption [8,10–12] and emission [5,13–16] studies, and optical reflectivity measurements [17–19]. These electronic-structure studies and numerous other physical-property measurements have been reviewed by Hsu [20]. The

purple color of AuAl₂ results from a reflectance minimum in the green (about 2.2 eV) [17]. Thus, this material absorbs green and reflects purple. It is also concluded that the Au 5d bands lie far below the Fermi level (E_F) and are not responsible for the color of AuAl₂ [17]. The absorption band of AuAl₂ at 2–5 eV is formed by interband transitions between filled Au s–p bands and unoccupied Au p–d/Al p bands [18]. We will later discuss these results based on our angle-resolved photoemission spectroscopic (ARPES) study and relativistic first-principles band-structure calculation of AuAl₂. This unique optical property and the reasonably high metallic conductivity ($\sigma > 10^5 \Omega^{-1} \text{ cm}^{-1}$) of this material promoted its use as radiation sensing devices which require electrodes with reasonable transparency in the visible region [18]. Despite numerous studies performed on this material, there is still no relativistic first-principles band-structure calculation and ARPES study reported for AuAl₂. In contrast, a linear augmented-plane-wave (LAPW) relativistic band-structure calculation [21] and an ARPES study [22] for an isostructural compound AuGa₂ do exist.

There are three non-relativistic band-structure calculations for AuAl₂. Two of them were performed using first-principles augmented-plane-wave (APW) method with the muffin-tin potential approximation [1,3], and the other was done by the mixed-basis band-structure interpolation

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scheme (MBBSIS) [2]. The latter calculation was found to give agreement between the calculated total density of states (DOS) and the XPS data [7]. This agreement is much better than that found from the non-relativistic APW method [1]. The energies of the Au 5d bands of AuGa₂ and AuIn₂ were further checked by the same authors using ARPES [22]. It is noted that the total DOS of AuGa₂ and AuIn₂ calculated by the relativistic MBBSIS method [2] showed three Au 5d bands (Γ_8^1 , Γ_7 , and Γ_8^2), and the middle Γ_7 bands were resolved by the ARPES study [22]. In contrast to the above ARPES work [22], the Γ_7 bands of AuX₂ (X = Al, Ga, In) were not resolved by any of the previous XPS studies [4–7], indicating that even the highest resolution obtained from the work of van Attekum et al. [7] is still too low to resolve the middle Γ_7 bands of these three compounds. Neither angle-integrated PES study [9] was able to resolve the middle Γ_7 band for AuAl₂.

The present ARPES study of the VBs of the (100) and the (111) faces of AuAl₂ was motivated to improve the energy resolution by using synchrotron-radiation-excited photoemission spectroscopy, with the hope to resolve the Γ_7 band for AuAl₂. Furthermore, the VBs along X– Γ –L of AuAl₂ are mapped and compared with those obtained from the first relativistic full-potential band-structure calculation. Quantitative calculations for the degree of band hybridization and charge transfer for AuAl₂ will be presented. Another purpose of this work is to bridge the UPS–XPS energy gap by using a tunable synchrotron radiation photon source, and to study the amplitude-modulation effect of the Au 5d band in AuAl₂. Preliminary results of part of the experimental study of this work have been published [23]. This paper is organized as follows. In Section 2 the experimental and the theoretical methods are described. In Section 3 the results and discussion are presented. The conclusions of this work are contained in Section 4.

2. Methods

2.1. Experimental methods

Procedures for preparation of the (100) and the (111) faces of a AuAl₂ single crystal [24] were reported previously [9]. ARPES experiments were performed at the undulator beam-line 7.0 at the Advanced Light Source. Photon energies in the range of 80–220 eV were selected with a spherical grating monochromator, and a Physical Electronics 137-mm hemispherical analyzer was used in the fixed-analyzer-transmission mode to collect the photoelectron spectra. With 150 lines/mm for grating setting and 3 eV for analyzer pass-energy setting, the energy resolution was less than 80 meV. The angular resolution was less than $\pm 1^\circ$, which corresponds to a momentum resolution of roughly $0.2 \text{ \AA}^{-1}$ at 125 eV kinetic energy. The analysis chamber was also equipped with a low-energy electron diffraction (LEED) system and a dual-anode Mg/Al X-ray source for XPS

and X-ray photoelectron diffraction (XPD) measurements. The chamber pressure during the experiments was 2×10^{-10} Torr.

The sample surfaces were cleaned by repeated cycles of sputtering with Ar ions and annealing to 500°C until photoemission spectra showed no traces of O or C contamination on the sample surfaces. The observed XPD and LEED patterns [23] further confirmed the cleanliness and ordering of the sample surfaces. The two AuAl₂ surfaces after cyclic cleaning contained about 15% less Al atoms than those in the bulk as determined from the area ratio of the Au 4f and Al 2p XPS peaks and the theoretical cross sections [25].

2.2. Theoretical methods

It is well known that the relativistic effects are large in AuAl₂ [2,9]. To interpret the ARPES data, we have calculated the relativistic band structure of AuAl₂ with cubic fluorite (CaF₂) structure and at the experimental lattice constant of 5.99 Å. All the relativistic effects including the mass-velocity and the Darwin terms as well as the spin-orbit coupling were taken into account. The spin-orbit coupling was included in so-called second variational treatment [26,27]. The muffin-tin radii used for the Au and the Al atoms of AuAl₂ are 1.27 Å. The relativistic band structures of Au and Al metals are also calculated for comparison. The lattice constant and the muffin-tin radius used for Au metal are 4.08 and 1.43 Å, respectively, and those values used for Al metal are 4.05 and 1.43 Å, respectively. We used the highly accurate all-electron full-potential linear augmented-plane-wave (FLAPW) method [28]. The calculations are based on the first-principles density functional theory with the standard local density approximation to the exchange-correlation potential [29]. The shallow 5p and 4f core states of Au were also treated as band states by using the so-called local orbitals [28]. The wavefunctions, the charge densities, and the potentials are expanded in terms of the spherical harmonics inside the muffin-tin spheres. The cut-off angular momentum (l_{max}) is 10 for the wave functions and six for the charge densities and the potentials. The Brillouin zone (BZ) integration is carried out by using the improved tetrahedron method [30]. The number of the augmented plane waves (APW) included is about 120 per atom, i.e. $R_{\text{mt}}K_{\text{max}} = 9$ for AuAl₂ and 10 for Au and Al metals [28]. The convergence of the calculated eigenvalues with respect to the number of APW used was checked. In particular, we found that increasing $R_{\text{mt}}K_{\text{max}}$ to 10 changed the relative positions of the eigenvalues at Γ point by up to a couple of meV. We thus believe that 120 APW used per atom is adequate. One should note that in ‘standard’ FLAPW calculations, the number of APW used is between 50 and 100. The number of the k points in the irreducible BZ wedge (IBZW) used in the self-consistent calculations is 72. To calculate the DOS, 165 k points in the IBZW were used.

Fig. 1. Angle-resolved photoemission spectra taken at normal emission for the (100) face of AuAl_2 in the photon-energy range 80–190 eV.

Fig. 2. Angle-resolved photoemission spectra taken at normal emission for the (111) face of AuAl_2 in the photon-energy range 80–200 eV.

3. Results and discussion

3.1. Angle-resolved photoemission spectra and band structure

Figs. 1 and 2 show a set of normal-emission VB photoemission spectra from the (100) and (111) faces of AuAl_2 , respectively. The normals to the sample surfaces were determined from the Au $4f_{7/2}$ XPD polar and azimuth scans [23]. The photon energy ($h\nu$) was varied from 80 to 200 eV so as to probe the third to the fourth BZ for the (100) face and the fourth to the fifth BZ for the (111) face. The E_F was assigned at half height on the onset of a plateau in Figs. 1 and 2. Using a direct-transition model and assuming a free-electron conduction-band structure, we plotted the energy versus momentum dispersion relation for AuAl_2 along $X-\Gamma-L$. It is displayed in Fig. 3 as open circles. The inner potential for AuAl_2 needed for determining the BZ position is estimated to be 12.0 eV. This value was taken to be the difference between the muffin-tin zero of energy (7.4 eV) in the FLAPW calculation and the vacuum level as determined from the work function of AuAl_2 . Here we use the work function of AuGa_2 (4.63 eV) [22] for AuAl_2 . The band structure of AuAl_2 calculated by the FLAPW method is shown in Fig. 4. The band structures along Δ and Λ are also plotted as closed circles in Fig. 3 to compare with the experimentally determined bands. The plateau in Figs. 1 and 2 is caused by photoemission from the smaller binding energy (E_B) Au s–p band. It extends from E_F to $E_B = 3.5$ eV with fairly low intensity except for $h\nu$ between 160 and 190 eV, at which a higher intensity but broader peak starts to move from $E_B = 1.5$ eV towards E_F . In general, s–p bands disperse much more rapidly than the almost flat d bands, thus accounting for the broader feature seen in the photoemission spectra. Another effect responsible for the broad s–p bands comes from the crystal-momentum broadening of the photoelectron final states that results from finite mean-free-path lengths. At $h\nu \geq 160$ eV, more final states are accessible for the Au s–p states, which causes the higher intensity observed in the spectra. The interband transitions from Au s–p band (1–2 eV below E_F) to the flat Au p–d/Al p band

Fig. 3. Band structure of AuAl_2 along $X-\Gamma-L$. Open circles are bands derived from the ARPES data. Closed circles are theoretical band structure calculated by the FLAPW method.

(1–2 eV above E_F) along $X-\Gamma$ are responsible for the purple color of AuAl_2 . In Figs. 1 and 2, a three-peak structure with much higher intensity at higher E_B is due to the Au 5d states. The E_B s of these peaks change less than 0.3 eV by varying $h\nu$. Since dispersion of the Au 5d bands in AuAl_2 is less than 0.3 eV along Δ and Λ in the BZ, the use of DOS peaks as band emissions from the Γ points in our previous angle-integrated photoemission work [9] is justified. We note that the largest- E_B Au 5d band hybridizes with the more dispersed Au s–p band close to the X point along $\Gamma-X$. This hybridization causes more dispersion for this Au 5d band than the other two smaller- E_B Au 5d bands. It should be mentioned here that in the pure fcc transition metals the countervailing symmetry dominates, and hybridization is strongest in the smaller- E_B d bands. Quantitative calculation for the degree of band hybridization for AuAl_2 will be presented in the following.

The E_B values at Γ_8^1 , Γ_7 , and Γ_8^2 for Au metal and for AuAl_2 obtained from various photoemission measurements and band-structure calculations are listed in the second to the fourth columns in Table 1. The spacings of the Au 5d bands at Γ for Au metal and for AuAl_2 can be used to determine the crystal field (10Dq) and the spin-orbit (ξ) parameters in the manner of Wehner et al. [31]. The 10Dq and ξ values for these two materials thus determined are listed in the fifth and sixth columns, respectively, in

Fig. 4. Band structure of AuAl₂ calculated by the FLAPW method.

Table 1. It is worthwhile noting that these parameters are only meaningful at the Γ points in the BZ, where the crystal momentum is zero. In Table 1, the agreement is rather good (within 13%) for Au metal of the three E_B values at the Γ points determined from either the ARPES study [32] or the previous [33,34] and present relativistic band-structure calculations. Worst agreement is found for the $E_B(\Gamma_8^1)$ value of Au metal obtained from the present FLAPW calculation and that obtained from the ARPES data [32]. This disagreement may be inherent for the local density approximation [24] used in the FLAPW calculation. As for AuAl₂, two comparisons are made in Table 1. Firstly, the $E_B(\Gamma)$ values for AuAl₂ obtained from the ARPES and the angle-integrated PES study are compared. The $E_B(\Gamma_8^1)$ and $E_B(\Gamma_8^2)$ values for AuAl₂ obtained from the present ARPES study and those obtained from previous angle-integrated PES work [9] are essentially the same (within the energy resolution of 0.15 eV of the latter experiment). This result implies

that the Au 5d states in AuAl₂ are highly localized. More evidence of the high localization of the Au 5d states in AuAl₂ will be revealed in Section 3.3 below. Secondly, the $E_B(\Gamma)$ values for AuAl₂ obtained from several theoretical and experimental studies are compared. The three $E_B(\Gamma)$ values for AuAl₂ obtained from the FLAPW calculation differ by less than 12% from those obtained from the ARPES data. Again, the major difference in binding energy is found at the Γ_8^1 point. This observation was also found in AuGa₂. The $E_B(\Gamma_8^1)$ value for AuGa₂ obtained from the LAPW calculation [21] is larger by roughly 12% than that obtained from the ARPES data [22], while the theoretical and experimental $E_B(\Gamma_7)$ and $E_B(\Gamma_8^2)$ values have much less disagreement. The theoretical $E_B(\Gamma_8^1)$ value for AuAl₂ is larger by about 0.6 eV than the experimental ARPES value, while the theoretical $E_B(\Gamma_7)$ and $E_B(\Gamma_8^2)$ values for AuAl₂ are larger by roughly 0.4 eV than the respective experimental ARPES values. We need to point out that all

Table 1

The experimental and theoretical binding energies (E_B) of the Au 5d states at Γ , the crystal field parameters (10Dq), and the spin-orbit parameters (ξ) for Au metal and for AuAl₂. All values in eV

	$E_B(\Gamma_8^1)$	$E_B(\Gamma_7)$	$E_B(\Gamma_8^2)$	10Dq	ξ	Reference
Au	3.55	4.45	5.90	1.22	0.71	32 ^a
	3.38	4.33	5.75	1.28	0.70	33 ^b
	3.29	4.34	5.65	1.39	0.66	34 ^c
	3.09	4.34	5.52	1.60	0.61	this work ^d
AuAl ₂	5.05		6.95			9 ^e
	4.90	5.80	6.85	1.18	0.53	this work ^a
	6.1		7.4			5 ^f
	6.31		7.84			7 ^f
	6.88	7.60	7.60	0.72	0.0	1 ^c
	6.33	7.76	7.76	1.43	0.0	2 ^g
	5.47	6.23	7.25	1.02	0.51	this work ^d

^a ARPES study.

^b Linear rigorous cellular calculation.

^c APW calculation.

^d FLAPW calculation.

^e Angle-integrated PES study.

^f XPS study.

^g MBBSIS calculation.

Table 2

Weighting of the Au d and Al p and d character at the three Γ states for AuAl₂

	Au d (%)	Al p (%)	Al d (%)
Γ_8^1	92.0	6.2	1.8
Γ_7	59.3	37.9	2.8
Γ_8^2	69.4	27.6	3.0

the non-relativistic band-structure calculations [1,2] and XPS studies [5,7] produce much larger $E_B(\Gamma)$ values for AuAl₂ than those obtained from the present ARPES data.

The Au d–d overlap integrals, which partly give rise to the crystal-field splittings at Γ , should decrease in the series Au, AuAl₂, AuGa₂, and AuIn₂ as the APW band-structure calculation [1] predicted. It is reported that the experimental 10Dq values for AuGa₂ (1.07 eV) [22] and AuIn₂ (1.06 eV) [22] are much larger than the theoretical ones (0.72 and 0.47 eV, respectively) [1]. Therefore, previous [22,32] and present ARPES data support the theoretically predicted decrease of the 10Dq value in the Au (1.22 eV), AuAl₂ (1.18 eV), AuGa₂ (1.07 eV), and AuIn₂ (1.06 eV) series. Some authors [22] speculated that a larger crystal-field effect in AuGa₂ and AuIn₂ may arise from interactions of the Au 5d orbitals with the Ga 3d or In 4d orbitals, and that the crystal-field splitting is much smaller for AuAl₂ than for AuGa₂ or AuIn₂ since these interactions are essentially nonexistent in AuAl₂ because Al has no occupied d orbitals. This speculation is now proved to be wrong. Next, we notice that the ξ value from atomic calculation for Au metal is 0.72 eV [35]. Our calculated ξ value for both Au metal

and AuAl₂ (0.64 eV) using the FLAPW method is smaller than this atomic value by about 10%, which is expected. We note that the ξ values, which are essentially a property only of the Au 5d orbitals, should be very similar for Au metal and the three AuX₂ compounds. However, the ξ value derived from previous [22,32] and present ARPES data within the crystal-field theory [31] shows some variation in the Au (0.71 eV), AuAl₂ (0.53 eV), AuGa₂ (0.78 eV), and AuIn₂ (0.75 eV). This suggests that the crystal-field theory is oversimplified for compounds where significant hybridization between transition-metal atoms and ligand atoms exists. Nonetheless, the 10Dq and ξ values listed in Table 1 may be treated as empirical parameters to reflect the relative strengths of the d-orbital interactions and also the interactions between the d-orbitals and the p-orbitals of ligand atoms. In order to see the effect of band hybridization on the empirical ξ value in AuAl₂, the weights of the Au d and Al p–d character at the three Γ states calculated from the LMTO-ASA method are listed in Table 2. This calculation shows that there is considerable band mixing of Au d and Al p (mostly) and d (2–3% only) character at the three Γ states in AuAl₂; while in fcc Au metal, purely Au d character exists at the three Γ states. One can immediately see that the Au d weight decreases from 100% in Au metal to 92%, 59%, and 69% at, Γ_8^1 , Γ_7 , and Γ_8^2 , respectively, for AuAl₂. Therefore, the average Au d weight at the three Γ points (roughly 73%) correlates with the percentage decrease of the ξ value from Au metal (0.72 eV) to AuAl₂ (0.53 eV). We thus conclude that AuAl₂ has distinctly smaller Au 5d character at the three Γ states than Au, AuGa₂, and AuIn₂.

The d-band splitting from the ARPES measurement for Au metal [30] and for AuAl₂, as defined by the energy difference between the upper and the lower Γ_8 bands, is 2.35 and 1.95 eV, respectively, which is comparable to that (2.43 and 1.78 eV, respectively) obtained from the relativistic FLAPW calculation. The d-band splitting for AuAl₂ is smaller than that for elemental Au, as one would expect from the consideration that the Au atoms are further apart in the compounds than in the pure metal. However, it is not substantially smaller than that for Au metal, as one would predict by neglecting the spin-orbit effects. The reason for the less narrowing of the Au 5d bands in the compound can be understood from the crystal-field effects, the spin-orbit effects, and band hybridization.

3.2. DOS curves and charge transfer

The total DOS curve for AuAl₂ and for fcc Au metal is shown as a solid line in Fig. 5(a) and (b), respectively. Also shown in Fig. 5(a) are the Au (dotted line) and the Al (thin solid line) site-decomposed partial DOS for AuAl₂. The energy zeroes are the Fermi energies of the respective materials. The apparent gap of about 0.25 eV around $E_B = 6.5$ eV in the AuAl₂ DOS curve is a pseudo gap with rather low DOS. The high DOS at 1–2 eV below E_F and at 1.5–3.5 eV above E_F increases the probability of interband transitions

Fig. 5. (a) Total and site-decomposed density of states for AuAl_2 , and (b) total density of states for Au metal calculated by the FLAPW method. In (a), the dotted line denotes the Au site-decomposed density of states and the thin solid line, the Al site-decomposed density of states.

from Au s–p bands to Au p–d/Al p bands (symmetry-projected DOSs are not shown). These interband transitions are responsible for the purple color of AuAl_2 . The DOS at E_F ($n(E_F)$) value for AuAl_2 is 0.92 states/eV-cell, which is comparable to that calculated by using the MBBSIS method (1.08 states/eV-cell) [2] or the nonrelativistic APW method (1.19 states/eV-cell) [1]. The (E_F) value obtained from the specific-heat measurement (1.28 states/eV-cell) [36] is this ‘band-structure’ DOS enhanced by a factor $1 + \lambda$, where λ is the electron-phonon mass enhancement parameter. The λ value thus determined for AuAl_2 is 0.39. We note that this λ value is 34% larger than the value (0.29) [37] calculated by using McMillan’s formula [38] with critical temperature of 0.095 K and Debye temperature of 297 K. Here we assume that the effective Coulomb repulsion between electrons (μ^*) in McMillan’s formula to be 0.1, which is a reasonable value for metals. We also note that small changes in μ^* should not affect the λ value.

One should note that it is difficult to quantify the charge transfer from FLAPW band-structure calculation. This is because there is no unique way to assign the charge distribution in the interstitial region (i.e. outside the muffin-tin spheres) to individual atoms in the solid. We therefore have performed relativistic electronic-structure calculations for fcc Au, fcc Al, and AuAl_2 using the linear muffin-tin orbital method with the atomic sphere approximation (LMTO-ASA) [39]. In this latter method, there is no interstitial region and thus it is possible to estimate charge transfer. The same atomic radius of Au was used for both fcc Au

Table 3

Total integrated number of electrons per atom for the valence orbitals from the LMTO-ASA calculations at the Au sites for Au metal and for AuAl_2 , and at the Al sites for Al metal and for AuAl_2

	n_s	n_p	n_d	n_f	n_{total}
Au site (Au metal)	0.81	0.78	9.27	0.14	11.00
Au site (AuAl_2)	0.57	0.80	9.05	0.28	10.70
Al site (Al metal)	1.10	1.48	0.42		3.00
Al site (AuAl_2)	1.25	1.70	0.20		3.15

metal and Au in AuAl_2 . The atomic radius of Au (1.594 Å) was determined by the experimental unit cell volume of fcc Au metal. The atomic radius of Al (1.637 Å) in AuAl_2 was determined by the experimental unit cell volume of AuAl_2 minus the atomic volume of Au. The atomic radius of fcc Al (1.583 Å) was determined by the experimental unit cell volume of fcc Al metal. Listed in Table 3 are the total integrated number of electrons per atom for the valence orbitals at the Au sites for Au metal and for AuAl_2 , and at the Al sites for Al metal and for AuAl_2 . From these calculated numbers, one concludes that the total charge transfer from Au to Al when forming the AuAl_2 compound is 0.3 electrons per atom, and that the larger Au-site s and d charge loss is partially compensated by the smaller gain in the Au-site p and f charges. We also note that charge neutrality is maintained. This observation agrees with the conclusion drawn from the experimental X-ray absorption near-edge spectra [12] and core-level shift data [9] of AuAl_2 .

3.3. Photon-energy dependence of the Au 5d-band intensity

The photon-energy dependence of the Au 5d-band intensity for the (111) and the (100) face of AuAl_2 in the range $80 \leq h\nu \leq 200$ eV is shown in Fig. 6 as filled squares and crosses, respectively. Also shown in Fig. 6 as a solid line is the atomic cross section of the Au 5d states calculated by

Fig. 6. Photon-energy dependence of the Au 5d-band intensity for the (111) and the (100) faces of AuAl_2 . The solid line is the atomic cross section calculated by Yeh and Lindau [40] of the Au 5d states for elemental Au.

Yeh and Lindau [40] for elemental Au. The data points were obtained by correcting the photoemission spectra for a Shirley-type inelastic background [41], measuring the area under the photoemission energy distribution curve in the range $3.5 \leq E_B \leq 9$ eV, and correcting this area with respect to the incident photon flux. They were then normalized to the atomic cross-section value at $h\nu = 80$ eV. It is well known that the Au 5d atomic cross section shows a 100-fold decrease as the Cooper minimum [42] ($h\nu \sim 210$ eV for the Au 5d band) is approached from low photon energy. We note that in this photon-energy range, the Au 5d states of AuAl₂ show atomic-like behavior, which is in sharp contrast to the solid-state effect observed for the Au 5d states in Au metal [43].

4. Conclusions

The spacings of the three Au 5d bands at the Γ points for AuAl₂ were determined for the first time. The binding energies at the Γ point for AuAl₂ determined from the ARPES study agree with those obtained from the FLAPW band-structure calculation and the angle-integrated PES work to within 12%. The Au 5d bands do not actively participate in the coloring and optical property of AuAl₂. The total charge transfer from Au to Al when forming the AuAl₂ compound is 0.3 electrons per atom. The Au d and Al p–d states hybridize most at the Γ_8^1 point, less at the Γ_7 point, and least at the Γ_8^1 point for AuAl₂. The energy variation of the Au 5d photoemission-peak intensities for AuAl₂ shows atomic-like behavior.

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