Influence of correlation and temperature on the electronic structure of bulk and thin film GdN

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Abstract

The influence of correlation and temperature on the electronic structure of bulk and thin film GdN have been studied using the $s-f$ model, which combines the one electron band structure with a many body procedure. The TB-LMTO method was used to obtain the one electron band structure of the system. The $s-f$ exchange coupling constants for each band were obtained from the spin polarized band structure of the system using a mean field model. The correlation effects are found to be present in the system. However they are not sufficiently strong to bring a correlation induced splitting in the spectrum. Some bands of the thin films of GdN exhibit splitting at $T = T_c$ and it is due to the combined effect of correlation and temperature. The conduction bands of both the bulk and the thin films of GdN exhibit red shift with respect to temperature.

I. INTRODUCTION

There has been a lot of interest in this decade towards the understanding of ground state properties of rare earth monopnictides. The prime reason for the interest in these systems is due to the rich variety of their properties. Some of the rare earth monopnictides RX(R=rare earth; X=N, P, As, Sb and Bi) show anomalous physical properties such as dense Kondo behavior, valence fluctuation behavior, heavy fermion state etc[1,2]. Half-metallic behavior is found in many rare earth pnictides by C.M. Aerts et.al.[3] using the SIC-LSD method. The electronic structure of GdX and ErX (X=N,P,S) is studied by A.G. Petukhov et.al.[4] using the LMTO method. It is known that in these systems the 4f electrons are strongly correlated and hence the LSDA can't provide an adequate description of these electrons. However treating these localized electrons as the core like electrons in the atomic limit, convincing results for some equilibrium properties are obtained by Petukhov et.al. Estimated quasiparticle corrections to the band structure of GdN were provided by Lambrecht et.al[10] and the optical properties of GdN were also studied by them. However the calculations were done at T=0K and the influence of correlation effects was not considered. In the rare earth systems, the exchange interaction between the conduction electrons and the local moments ($s-f$-exchange) is crucial and it will have strong influence on the electronic structure of these systems. Further, the temperature effects in these systems will also be significant as they are mostly either ferromagnetic or antiferromagnetic systems.

In this work, we study the influence of temperature and correlation on the electronic structure of GdN. Our interest is primarily on the GdN thin films. However, as there are no such studies on bulk GdN, we consider the case of bulk GdN also. GdN crystallizes in the simple NaCl structure. The magnetism of GdN originates from the 4f orbitals of Gd. The magnetic structure of GdN is controversially discussed in the literature[5,6]. However from the recent studies it is understood that it is a ferromagnetic system with Curie temperature of 58K[7]. The reported electronic properties seem to be controversial as well. Again, from the recent studies it is known to be a semiconductor. It should be pointed out here that the experimental results on the magnetic and electronic properties are very sensitive to the stoichiometry of the system. In the present work we have calculated the quasiparticle band structure (QBS) of bulk as well as thin films of GdN and we have used the $s-f$ model for our calculations. This model allows to combine a many-body model with a one electron

band structure results. We have used the TB-LMTO method to obtain the one electron band structure. We present our results on the QBS of the bulk and thin films of GdN in this paper. We have considered thin films with thickness of two, three and four monolayers in our studies. We organise the paper as follows. In section II we give a brief outline of the $s-f$ model, and in section III we describe the geometry of the films and the film Green's functions. The method of evaluation of $s-f$ exchange constants are mentioned in the section IV. We discuss our results in section V and the conclusions are given in section VI.

II. THE $s-f$ MODEL

The theory of the s-f model is discussed in many other papers[11,12]. However for the sake of completeness, we give a brief outline here. This model explicitly takes into account the exchange interaction between the localized moments present at the lattice sites and the conduction electrons. The model consists of three partial operators.

$$H = H_s + H_f + H_{sf} \tag{1}$$

Here H_s stands for itinerant conduction electrons, which are treated as 's' electrons without explicit Coulomb interaction.

$$H_s = \sum_{ij\sigma} T_{ij}\ c^{\dagger}_{i\sigma}\ c_{j\sigma} \tag{2}$$

$c^{\dagger}_{i\sigma}$ and $c_{i\sigma}$ are respectively the creation and annihilation operator of an electron with spin $\sigma(\sigma =\uparrow,\downarrow)$ at the lattice site $\mathbf{R_i}$. The spin system is described by the Hamiltonian

$$H_f = -\sum_{ij} J_{ij}\ \mathbf{S_i}\cdot\mathbf{S_j} \tag{3}$$

The interaction between the conduction electrons and the localized moments is given by

$$H_{sf} = -J_{sf} \sum_{i} \mathbf{S_i}\cdot\sigma_{\mathbf{i}}\ = -1/2\ J_{sf}\ \sum_{i\sigma}\ (z_\sigma\ S^z_i\ n_{i\sigma} + S^{\sigma}_i\ c^{\dagger}_{i-\sigma}\ c_{i\sigma}) \tag{4}$$

Where z_σ is 1 for $\sigma = \uparrow$ and it is -1 for $\sigma = \downarrow$

$$S^{\sigma}_i = S^x_i + i z_\sigma S^y_i$$

All the information concerning the quasiparticle electronic structure of the system described by the above said Hamiltonian may be obtained from the retarded single electron Green's

function

$$G_{ij\sigma} =<<\ c_{i\sigma}\ ;\ c^{\dagger}_{j\sigma}\ >>_E = -i\int_0^{\infty} e^{-iEt/\hbar}\ [c_{i\sigma}(t), c^{\dagger}_{j\sigma}(0)]_+\ dt \tag{5}$$

The evaluation of this Green's function starts with it's equation of motion which is written as

$$\sum_m (E\delta_{im} - T_{i,m})\ G_{mj\sigma}(E) =\ \hbar <\ [c_{i\sigma}, c^{\dagger}_{j\sigma}] > +\ << [c_{i\sigma}, H_{sf}]; c^{\dagger}_{j\sigma} >> \tag{6}$$

Here we have neglected the direct spin-spin interaction term H_f of the Hamiltonian which carries the information of the magnon energies. As our interest is on the electronic quasiparticle spectrum, the magnon energies which are very small compared to the electron energies are neglected. However, implicitly a spontaneous magnetic order is assumed. Introducing the self-energy $M_{ij\sigma}(E)$ as

$$<< [c_{i\sigma}, H_{sf}]; c^{\dagger}_{j\sigma} >> \ \ =\ \ \sum_r\ M_{ir\sigma} G_{rj\sigma}(E) \tag{7}$$

and making a Fourier transformation, we get the Green's function as

$$G_{\mathbf{k}\sigma}(E) = \hbar[E - \epsilon(\mathbf{k}) - M_{\mathbf{k}\sigma}(E)]^{-1} \tag{8}$$

where $\epsilon(\mathbf{k})$ is the Bloch energy and $M_{\mathbf{k}\sigma}(E)$ is the self-energy. The determination of the self-energy is a lengthy procedure and it may be found in the other papers[11,12]. The self energy is temperature dependent and the temperature enters in the self-energy through the f-spin magnetisation $< S^z >$ and other spin correlation functions. The spectral density is given as

$$S_{\mathbf{k}\sigma}(E) = -\frac{1}{\pi}\ Im\ G_{\mathbf{k}\sigma}\ (E)$$

and the quasiparticle density of states is given as

$$\rho_{\sigma}(E) = \frac{1}{N}\sum_{\mathbf{k}}\ S_{\mathbf{k}\sigma}(E)$$

In the case of a film the Bloch dispersion $\epsilon(\mathbf{k})$ can be written in a matrix form and for a film with N monolayers it may be written as

$$\hat{\epsilon}(\mathbf{k}) = \begin{pmatrix} \epsilon^{11}(\mathbf{k}) & \epsilon^{12}(\mathbf{k}) & .. & .. & .. \\ \epsilon^{21}(\mathbf{k}) & \epsilon^{22}(\mathbf{k}) & \epsilon^{23}(\mathbf{k}) & .. & .. \\ .. & .. & .. & .. & .. \\ .. & .. & .. & .. & .. \end{pmatrix}_{N\times N}$$

Where $\epsilon^{\alpha,\alpha}(\mathbf{k})$ is the intralayer Bloch energy and $\epsilon^{\alpha,\beta}(\mathbf{k})$ is the interlayer Bloch energy. $\mathbf{k}$ is a vector in the two dimensional Brillouin zone. The $\epsilon^{\alpha,\alpha}(\mathbf{k})$s and $\epsilon^{\alpha,\beta}(\mathbf{k})$s are related to hopping matrix elements through the Fourier transforms

$$\epsilon^{\alpha,\alpha}(\mathbf{k}) = \sum_{i,j} T_{i,j}^{\alpha,\alpha}\ e^{i\mathbf{k}.(\mathbf{R_i}-\mathbf{R_j})}$$

$$\epsilon^{\alpha,\beta}(\mathbf{k}) = \sum_{i,j} T_{i,j}^{\alpha,\beta}\ e^{i\mathbf{k}.(\mathbf{R_i}-\mathbf{R_j})}$$

$T_{i,j}^{\alpha,\alpha}$ and $T_{i,j}^{\alpha,\beta}$ are respectively intralayer and interlayer hopping matrix elements. The Green's function for the film can also be written in a matrix form as

$$\hat{G}_{\mathbf{k}\sigma}(E) = \hbar[E\hat{\mathbb{1}} - \epsilon(\hat{\mathbf{k}}) - \hat{M}_{\mathbf{k}\sigma}(E)]^{-1} \tag{9}$$

$\hat{M}_{\mathbf{k}\sigma}(E)$ is the self-energy matrix which again has the same structure as $\epsilon(\hat{\mathbf{k}})$.

III. GEOMETRY, BLOCH ENERGIES AND GREEN'S FUNCTION OF THE FILM

In the present work, we consider thin films with two, three and four monolayers and they are derived from the (100) planes of bulk GdN. In order to obtain the two, three and four layer films, we constructed appropriate supercells using the unit cell of bulk GdN. For the two layer film, the supercell consists of seven atomic planes with two adjacent planes in the supercell having real atoms and the remaining five layers having empty spheres. For three-layer film the supercell consists of eight atomic planes where three adjacent planes in the supercell contain real atoms and the remaining five layers contain empty spheres. Similarly we obtained the four-layer film by constructing a supercell having 10 atomic planes where four adjacent planes in the supercell contain real atoms and the remaining six layers contain empty spheres. The band structures of the supercells are then calculated using the TB-LMTO method[13,14]. Collecting the eigenvalues at all the k-points having only k_x and k_y components yields the band structure of the two, three and four layer films. The band structure of the two-layer film is shown in Fig.1. The low-lying six bands are due N-3p orbitals. The 4f bands of Gd lies above these bands and the top twelve bands are the conduction bands and these arise from the (5d,6s) orbitals of Gd. When the band structure of the system obtained from the TB-LMTO method is used as the one electron input in the

many body calculation, a double counting of the $s-f$ interaction once explicitly through the many body procedure and once in an averaged way through the band structure calculation occurs. We circumvent this problem in the following way. The spin polarised band structure calculation is quite compatible with the Stoner model[16]. When the 4f- induced magnetic behaviour is absent in the system, the Stoner quasiparticle energies will be identical to the free paramagnetic band structure. It obviously means that the spin polarised band structure will exhibit a shift with respect to the paramagnetic band structure. As our concern is on the conduction band of GdN which is constituted by the Gd 5d and 6s orbitals, we believe that all the 4f induced magnetic behaviour of the conduction band is absent in the paramagnetic state and hence we used the paramagnetic band structure of the system as the necessary one-particle input for the many body procedure.

The calculation of QBS of the film needs the evaluation of the Bloch energy matrix $\hat{\epsilon}(\mathbf{k})$. We used the following procedure to calculate the diagonal ($\epsilon^{\alpha,\alpha}(\mathbf{k})$-intralayer) and off -diagonal ($\epsilon^{\alpha,\beta}(\mathbf{k})$-interlayer) elements of the Bloch energy matrix. The eigen values of the conduction bands are arranged in the ascending order at every $\mathbf{k}$-point and the first value at every $\mathbf{k}$-point is assumed to constitute the first band, the second value at every $\mathbf{k}$-point to constitute the second band and so on. In the case of two-layer film, there will be 12 conduction bands, 18 bands in the case of three-layer film and 24 bands for the four-layer film. The conduction bands are arranged into six sections consisting of two bands in each section in case of two-layer film, three bands in each section for the three-layer film and the analogous for the four-layer film. Using the fact that the Bloch energy values in each section are the eigen values of the Bloch energy matrix described above, we obtain the $\epsilon^{\alpha,\alpha}(\mathbf{k})$ and $\epsilon^{\alpha,\beta}(\mathbf{k})$ of the two, three and four-layer films by numerical procedure. In the case of ferromagnetic GdN film the intralayer Bloch energies $\epsilon^{\alpha,\alpha}(\mathbf{k})$s are identical and the Green's function for the ferromagnetic film with N layer is

$$\hat{G}_{\mathbf{k}\sigma}(E) = \begin{pmatrix} E-\epsilon^{11}(\mathbf{k})-M_{\mathbf{k}\sigma}(E) & -\epsilon^{12}(\mathbf{k}) & -\epsilon^{13}(\mathbf{k}) & .. & .. \\ -\epsilon^{21}(\mathbf{k}) & E-\epsilon^{22}(\mathbf{k})-M_{\mathbf{k}\sigma}(E) & -\epsilon^{23}(\mathbf{k}) & .. & .. \\ .. & .. & .. & .. & .. \\ .. & .. & .. & .. & .. \end{pmatrix}^{-1}_{N\times N}$$

Where the off-diagonal components of the self-energy are not considered since these play

very mionor role. The layer dependent spectral density of the film is given as

$$S^{\alpha\alpha}_{\mathbf{k}\sigma}(E) = -\frac{1}{\pi}\ Im\ G^{\alpha\alpha}_{\mathbf{k}\sigma}\ (E)$$

and the layer dependent quasiparticle density of states is given as

$$\rho_{\alpha\sigma}(E) = \frac{1}{N}\sum_{\mathbf{k}}\ S^{\alpha\alpha}_{\mathbf{k}\sigma}(E) \tag{10}$$

Our results for the films are described in terms of the sub-layer spectral density and the sub-layer quasiparticle density of states.

IV. EVALUATION OF J_{sf}

The experimental information on the magnitude of J_{sf} is not available in the literature. Hence we used the following procedure to obtain J_{sf}. The spin-polarized LDA-Bloch band structure is quite compatible with the mean field ansatz[15,16]. Hence the J_{sf} may be obtained from the spin-polarized band structure results as

$${J^{(m)}}_{sf} = \frac{1}{NS}\ \sum_{\mathbf{k}}\ ({\epsilon(\mathbf{k})^{(m)}}_{\downarrow} - {\epsilon(\mathbf{k})^{(m)}}_{\uparrow}) \tag{11}$$

Where m is the band index. We have evaluated J_{sf} for all the bands using this procedure. The spin-polarized LMTO band structure results are employed in the calculation. The values of J_{sf} for the first three bands obtained from this model for the bulk GdN are respectively 0.42eV, 0.28eV and 0.3eV. For GdN films the values of J_{sf} for the first three bands obtained from this model are respectively 0.37eV, 0.27eV and 0.28eV.

It should be noted here that in a standard LSDA calculation, the unoccupied 4f and occupied 4f states lie close to the Fermi level. Hence, the influence of these bands on the conduction bands will be larger in LSDA than in reality. This may lead to the overestimation of the value of J_{sf}. Hence the experimental estimation of J_{sf} is very much desirable.

V. DISCUSSIONS OF RESULTS

Bulk GdN

We shall first discuss the results of the bulk GdN. Inorder to understand the influence of correlation effects on the electronic structure of this system it is advantageous to consider

the quasiparticle band structure (QBS) of a model system already published[11]. At T=0K, the ↑-spin spectrum is identical to the Bloch dispersion except for a shift of $-\frac{1}{2}J_{sf}S$. The ↓-spin spectrum consists of two parts. The upper part is referred as a polaron part and the lower part is called as a scattering part. At finite temperature, the ↑-spin spectrum also gets an additional branch due to spin flip processes. The splitting of the band into two branches persists even at $T = T_c$ and such a splitting is not at all obtainable from a one electron picture.

The above said points can be used to understand the QBS of bulk and thin film GdN. First we intend to demonstrate the influence of correlation effects on the electronic structure of GdN and hence we have plotted in Fig.2 the QBS of the first three conduction bands of bulk GdN at $T = T_c$ along with the Bloch band structure obtained from LMTO calculation. In the right panel we have plotted the spectral density in the form of density plot. The degree of blackening measures the magnitude of the spectral density. Both spectra correspond to paramagnetic states except temperature. It may be seen from the figure that the correlation effects are indeed present in the system. However the splitting of the bands into two branches is not explicitly seen as the correlation effects are not sufficiently strong (small J_{sf}/W ratio, W being the band width) to split the spectrum. However indications of the splitting is visible in certain regions of the **k**-space and it obviously means that the splitting is **k** dependent. Other features of the quasiparticle spectrum may be understood from the analysis of the quasiparticle density of states (QDOS).

The QDOS of the first three bands at three different temperatures is shown in Fig.3. At T=0K ($< S^z > /S = 1.0$) the exchange splitting between the ↑-spin band the ↓-spin band dominate the spectrum. As the temperature increases, the redistribution of spectral weight occurs. It can be seen from Fig.3 that the increase of temperature is accompanied with the shifting of spectral weight towards higher energies for the ↑-spin spectrum and lower energies for the ↓-spin spectrum. Both the spectra approach each other in a non-rigid manner and at $T = T_c (< S^z > /S = 0.0)$ the two spectra become identical. It may be seen from the figure that all the bands exhibit redshift with respect to temperature. The conduction band edge shows a redshift of 0.483eV with respect to temperature. The redshift is shown in the Fig.4. Here the ↑-spin QDOS of the lowest band of the bulk GdN at $T = 0K$ is compared with the QDOS of the same band at $T = T_c$. The redshift is expected to be overestimated as the J_{sf} obtained from spin polarized band structure may be overestimated. This fact should be

considered while making a comparison with the experimental measurements.

Thin film GdN

We shall now discuss the results of the thin films of GdN. In order to visualize the correlation effect on the electronic structure, we have plotted in Fig.5, the QBS of the first layer of the two-layer film at $T = T_c$ along with the Bloch dispersion obtained from LMTO calculation. The two branches seen in the band structure is a consequence of the two layer film. Here again we have shown the results for the first three bands. Both panels in Fig.5 correspond to the paramagnetic phase. The splitting of the bands seen in right panel is clearly a consequence of the combined effect of correlation and temperature. The QDOS of the first three bands at three different temperatures (f-spin magnetisations) are shown in Fig.6. At T=0K ($< S^z > /S = 1.0$) the exchange splitting between the $\uparrow$-spin band and the $\downarrow$-spin band dominate the spectrum. However, a correlation induced splitting is observed in band 3. As the temperature increases, the redistribution of spectral weight makes the $\uparrow$-spin band and $\downarrow$-spin coincide at $T = T_c (< S^z > /S = 0.0)$. The correlation induced split gap is found to increase with increasing temperature and a split gap appears in band 2 at $T = T_c$.

In a thin film, the surface layers and the interior layers will exhibit different QBS due to the differences in their interlayer hopping. Inorder to visualise it we have shown in Figs. 7 and 8 the layer dependent QDOS of the three layer and four layer films. The QDOS of the first and second layer of a three-layer film is shown in Fig.7 while the same for a four layer film is shown in Fig.8. For the sake of compactness, we have shown the QDOS of the first band alone at three different temperatures. The three and four layer films exhibit in general the same temperature dependent effects as found in the two-layer film. Considerable difference in the QDOS of the first layer and the second layer is observed and it is a consequence of the additional interlayer hopping experienced by the electrons in the second layer. For a two-layer film, the conduction band edge shows a redshift of 0.416 eV, for a three-layer film the shift is 0.440 eV and for a four-layer film it is 0.472 eV.

VI. CONCLUSIONS

We have studied the influence of correlation and temperature on the electronic structure of both bulk and thin film GdN using the $s - f$ model. The $s - f$ exchange constants were obtained using a mean field model employing spin- polarized TB-LMTO band structure

results. We have demonstrated the presence of correlation effects in the bulk as well as thin films of GdN. We found that the correlation effects are not sufficiently strong to split the spectrum. However at $T = T_c$ some bands exhibit splitting and it is due to the combined effect of correlation and temperature. Both the bulk and the thin films of GdN exhibit red shift of the conduction band edge with respect to temperature and the magnitude of the red shift is rather large.

Acknowledgments

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FIG. 1: Paramagnetic band structure of a two layer GdN film obtained from the TB-LMTO method

FIG. 2: Quasiparticle band structure of bulk GdN at $T = T_c$ (right panel) and the corresponding Bloch band structure obtained from the LMTO calculations (left panel). The first three bands are shown in the figure. (The degree of blackening is a measure of the magnitude of the spectral density)

FIG. 3: Quasiparticle density of states (QDOS) of the first three bands of bulk GdN at different temperatures (different f-spin magnetisations)

FIG. 4: Redshift of the lowest conduction band for bulk GdN. The solid line corrresponds to the $\uparrow$-spin QDOS at T=0 K while the dashed one corresponds the QDOS at $T = T_c$.

FIG. 5: Quasiparticle band structure of the two layer GdN film at $T = T_c$ (right panel) and the corresponding Bloch band structure obtained from LMTO calculations (left panel). The first three bands are shown in the figure. (The degree of blackening is a measure of the magnitude of the spectral density)

FIG. 6: Quasiparticle density of states (QDOS) of the first three bands of the two layer GdN film at different temperatures (different f-spin magnetisations)

FIG. 7: QDOS of the first and second layer of a three layer GdN film at different temperatures (different f-spin magnetisations). The first band alone is shown in the figure.

FIG. 8: QDOS of the first and second layer of a four layer GdN film at different temperatures (different f-spin magnetisations). The first band alone is shown in the figure.

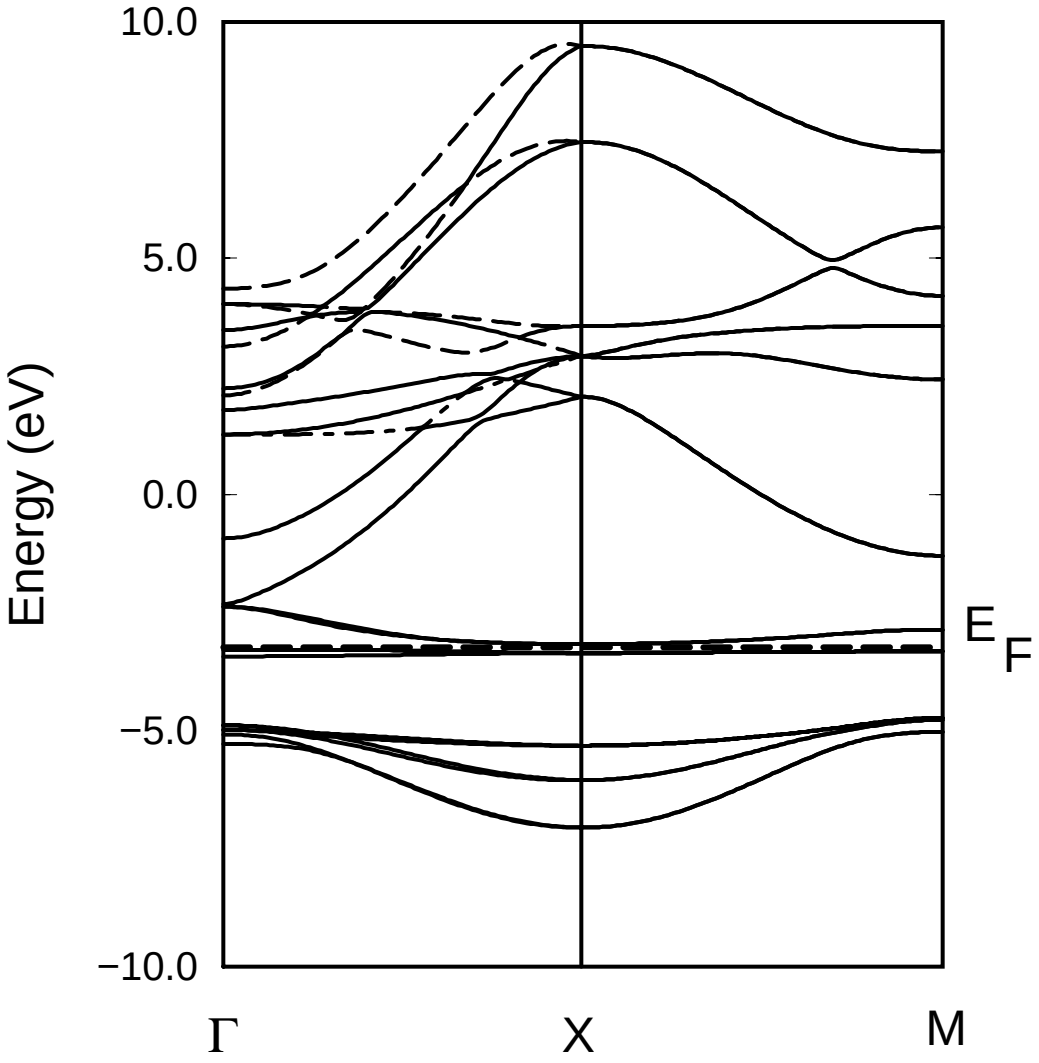


Fig.1

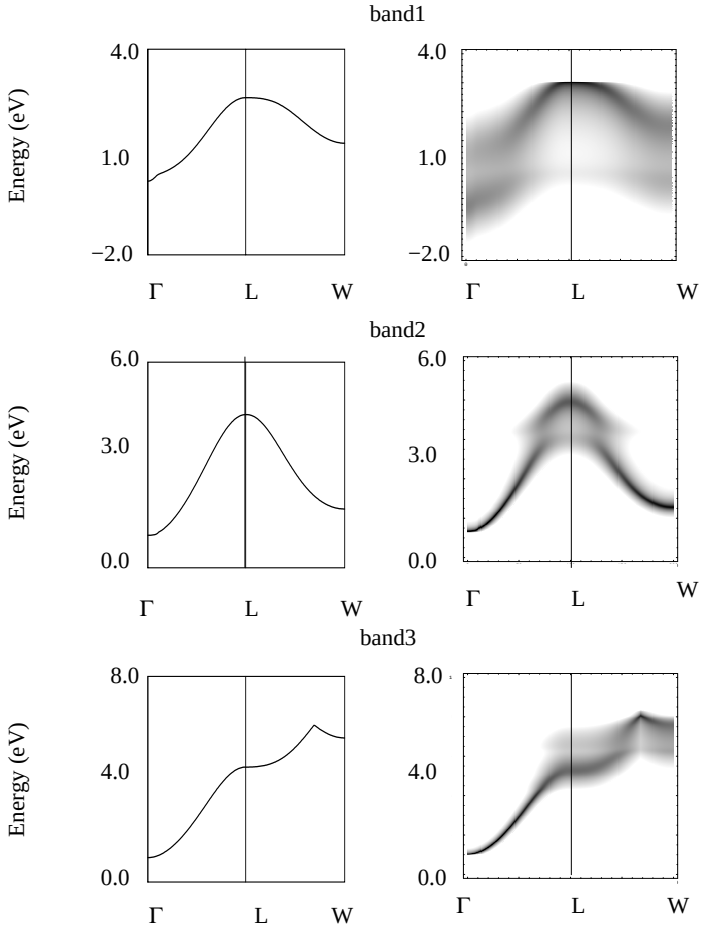


Fig.2

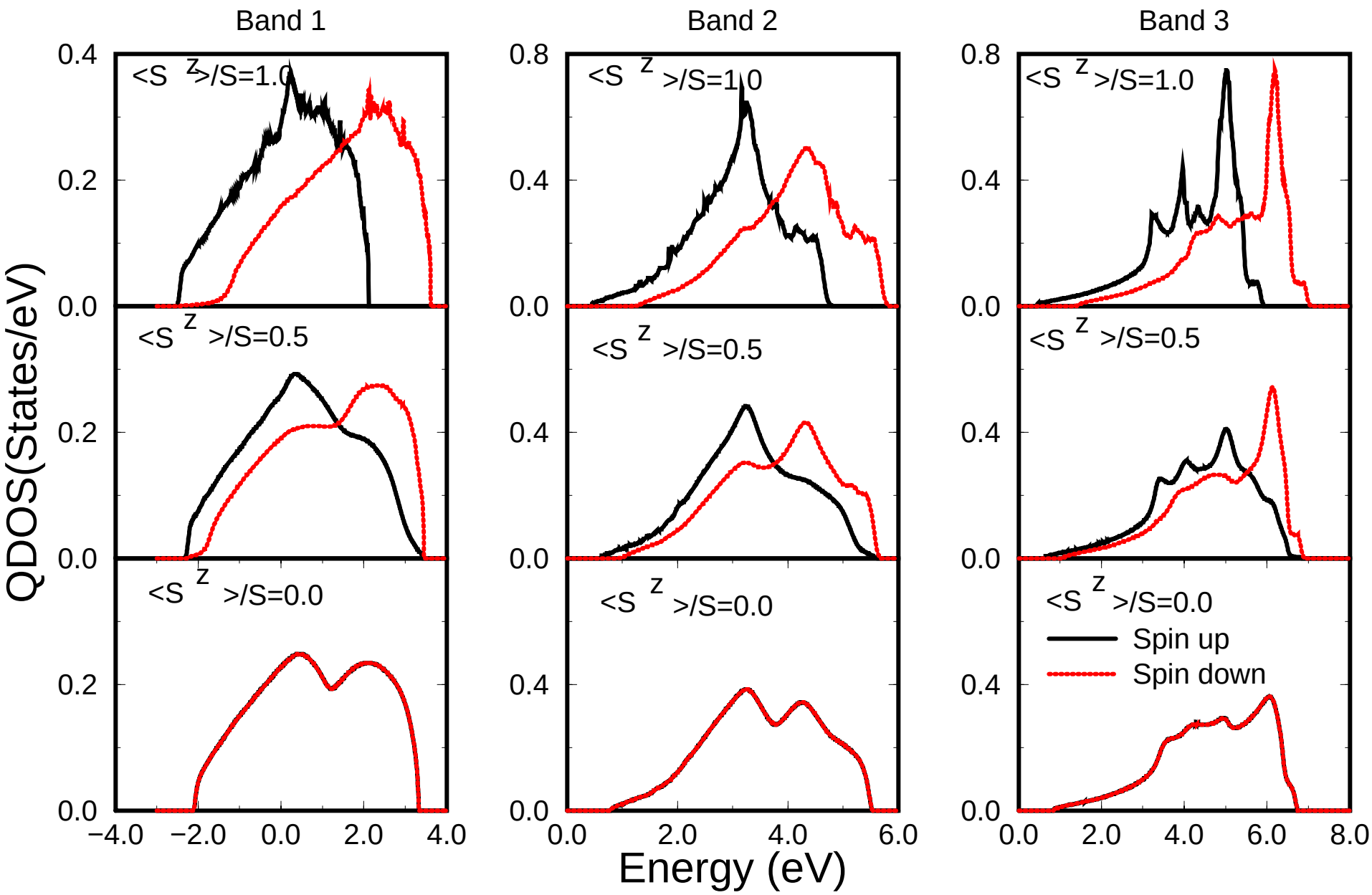
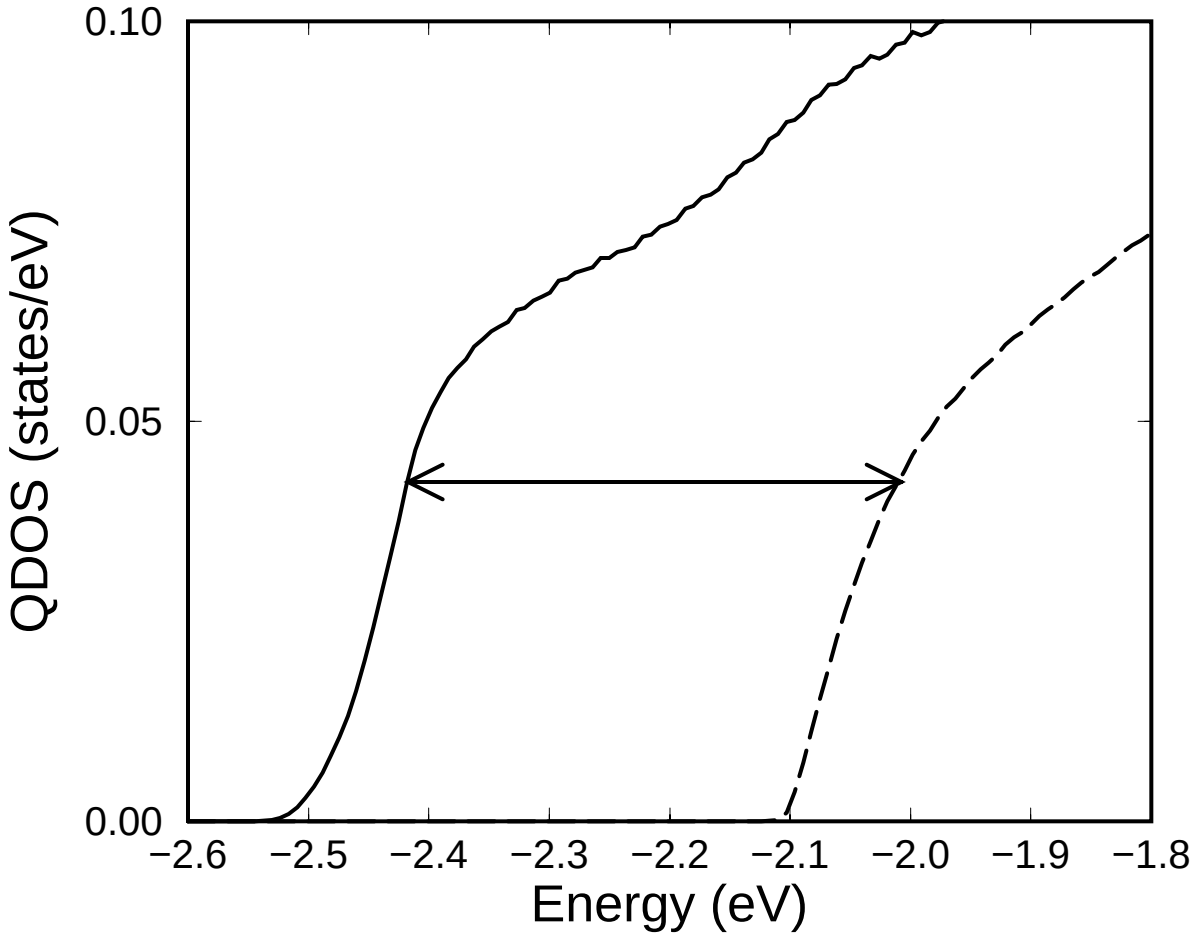

Band 1
Band 2
Band 3
<S z>/S=1.0
<S z>/S=0.5
<S z>/S=0.0
QDOS(States/eV)
Energy (eV)
Spin up
Spin down
0.0
0.2
0.4
0.8
−4.0
−2.0
2.0
4.0
6.0
8.0

Fig.3


0.10
0.05
0.00
QDOS (states/eV)
−2.6
−2.5
−2.4
−2.3
−2.2
−2.1
−2.0
−1.9
−1.8
Energy (eV)

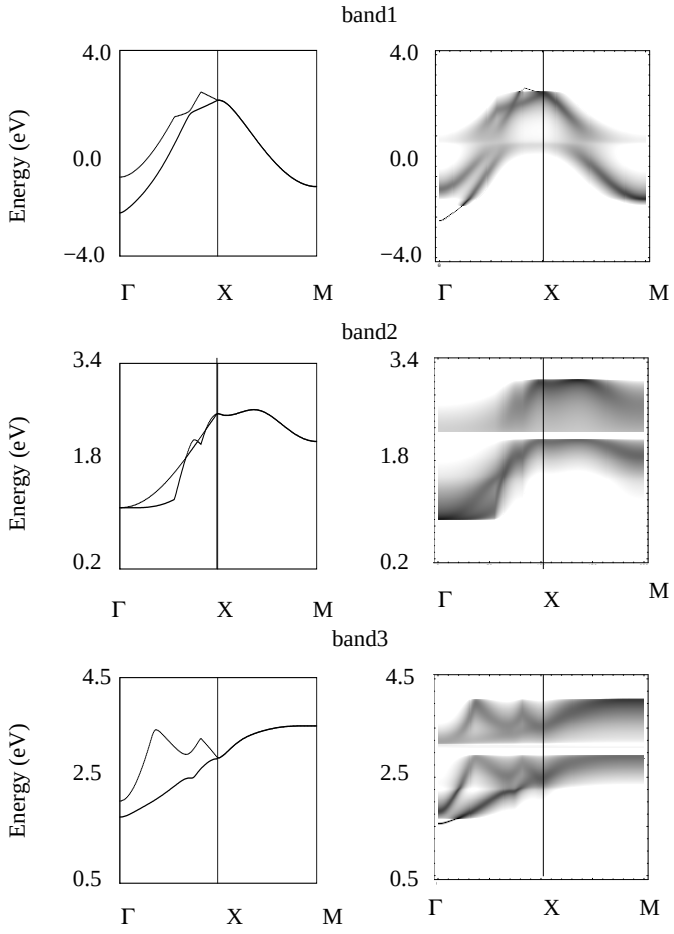
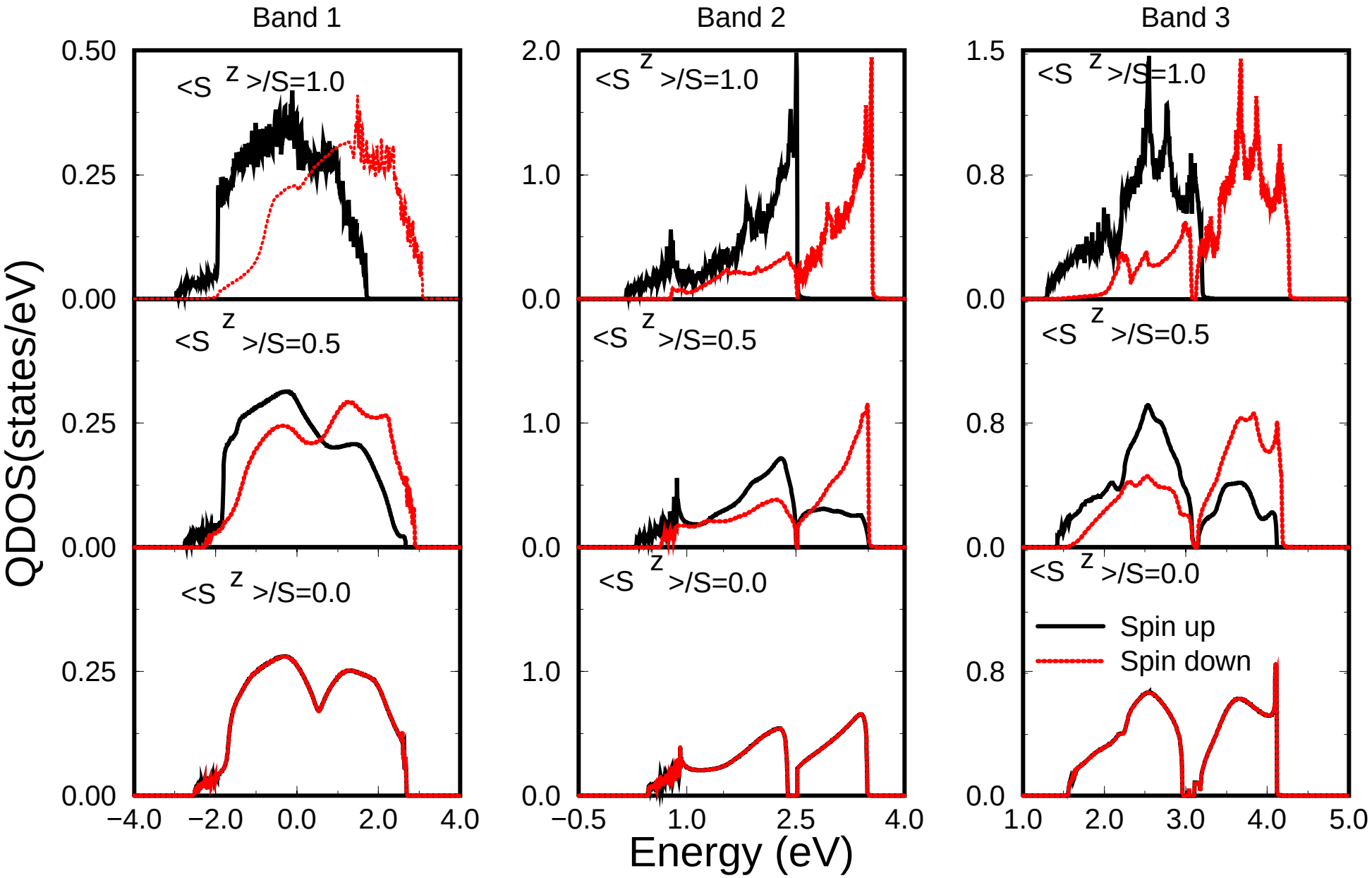


Fig.5


Band 1
Band 2
Band 3
QDOS(states/eV)
Energy (eV)
<S z >/S=1.0
<S z >/S=0.5
<S z >/S=0.0
Spin up
Spin down
0.50
0.25
0.00
2.0
1.0
0.0
1.5
0.8
−4.0
−2.0
0.0
2.0
4.0
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1.0
2.5
4.0
1.0
2.0
3.0
4.0
5.0

Fig.5

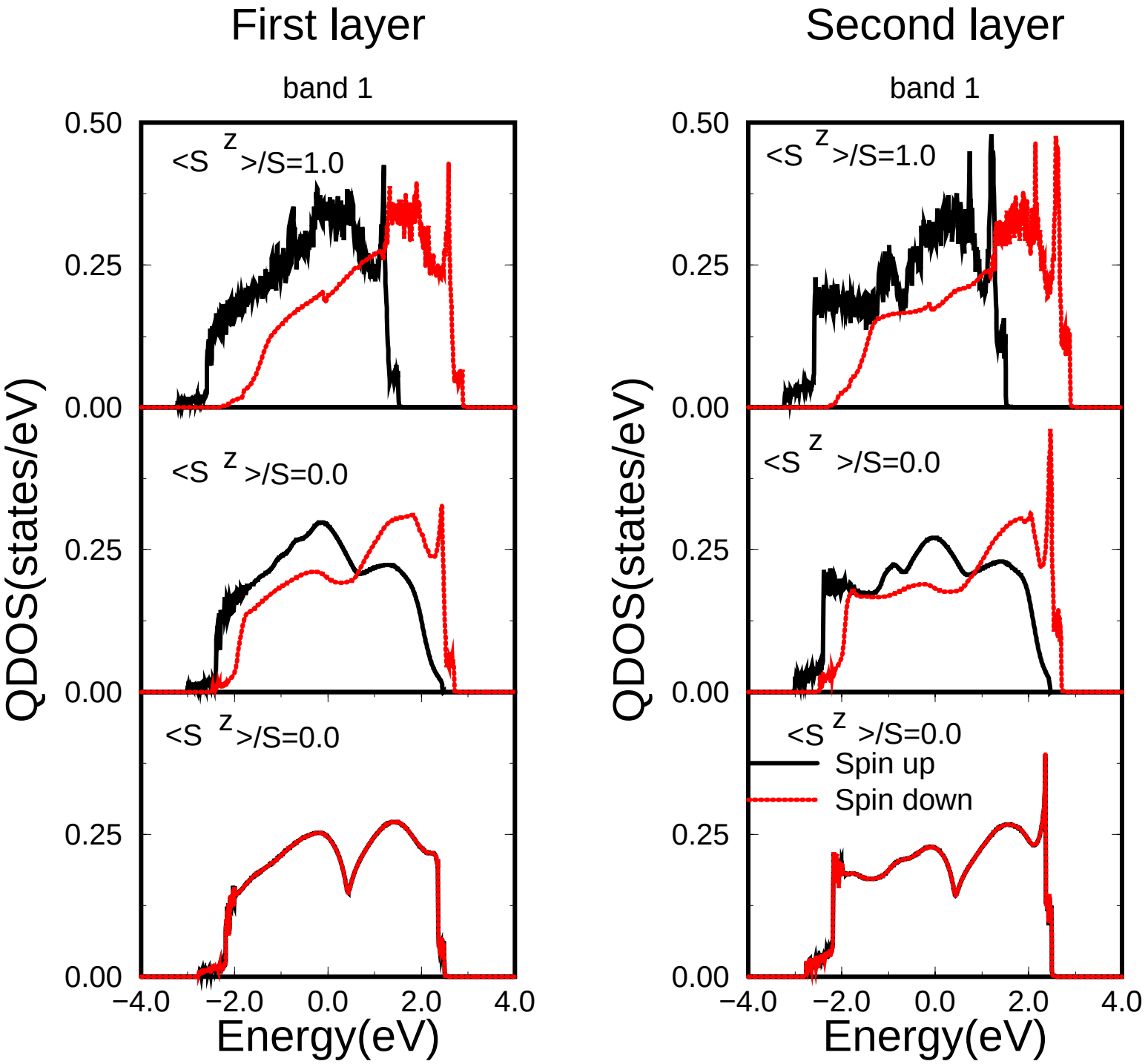
First layer
band 1
<S z>/S=1.0
<S z>/S=0.0
<S z>/S=0.0
QDOS(states/eV)
0.50
0.25
0.00
−4.0
−2.0
0.0
2.0
4.0
Energy(eV)
Second layer
band 1
<S z>/S=1.0
<S z>/S=0.0
<S z>/S=0.0
Spin up
Spin down

Fig.6

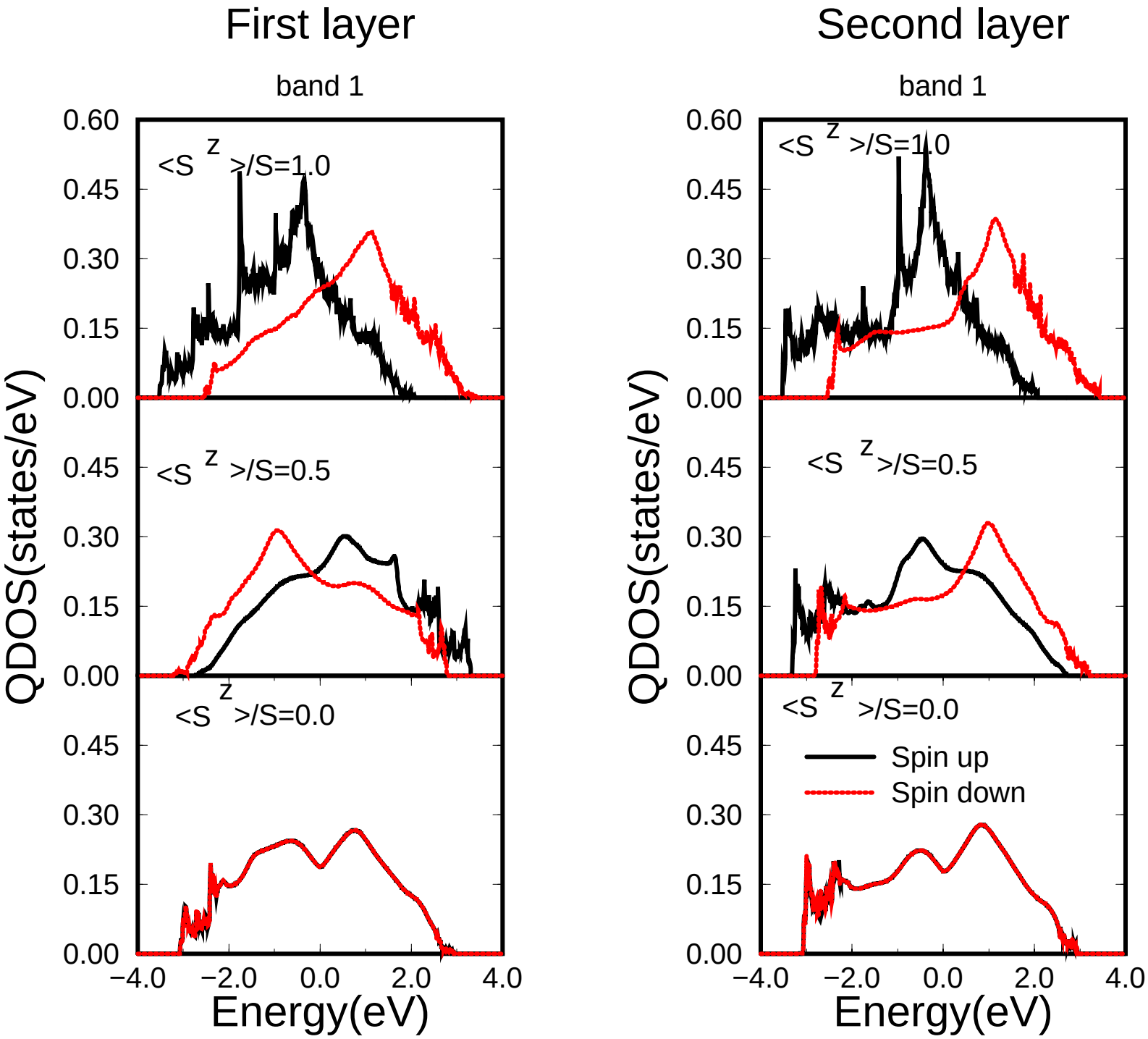
First layer
band 1
<S z >/S=1.0
<S z >/S=0.5
<S z >/S=0.0
QDOS(states/eV)
Energy(eV)
0.60
0.45
0.30
0.15
0.00
−4.0
−2.0
0.0
2.0
4.0
Second layer
band 1
<S z >/S=1.0
<S z >/S=0.5
<S z >/S=0.0
Spin up
Spin down
QDOS(states/eV)
Energy(eV)

Fig.8