Energy Functional dependence of exchange coupling and magnetic properties of Fe/Nb multilayers

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Abstract

We present an ab initio calculation of the exchange coupling for Fe/Nb multilayers using the self-consistent full-potential linearized augmented-plane wave (FLAPW) method. The exchange correlation potential has been treated in the local spin density approximation (LSDA) as well as generalized gradient approximation (GGA). We find that for the LSDA as well as the GGA the exchange coupling oscillates with a period of 6.0 Å of Nb spacer thickness which is close to the experimental value in the preasymptotic region. This is also close to the earlier calculated period (i.e. 4.5 Å) by augmented spherical wave (ASW) method. The LSDA shows antiferromagnetic coupling for 2 and 5 Nb monolayers (ML) but the GGA shows the ferromagnetic coupling for all Nb spacer layers. The period of oscillation is found to be in good agreement with the period calculated using the Ruderman-Kittel-Kasuya-Yosida (RKKY) and quantum well (QW) models. The magnetic moment of Fe is found to be higher in the GGA than the LSDA. Fe magnetic moment also shows strong oscillations as a function of the spacer layer thickness, in agreement with the experimental results. We find that the GGA results show better agreement with the experiment than the LSDA results.
I. INTRODUCTION

During the last decade, magnetic multilayers have received a lot of attention due to their interesting properties like oscillating interlayer exchange coupling (IEC) between antiferromagnetic (AF) and ferromagnetic (FM) ordered layers\cite{1, 2, 3} and giant magnetoresistance (GMR) apart from their industrial applications. Such oscillations in interlayer exchange coupling and the saturation magnetoresistance were reported by Parkin et al.\cite{2} with a period 15-20 Å in Fe/Cr, Co/Cr and Co/Ru multilayers. Purcell et al.\cite{4} showed that the coupling oscillates with a smaller period of 3.0-4.0 Å in Fe/Cr/Fe sandwich structure because of the high degree of perfection of Fe whisker substrate and the sharpness of Fe/Cr interfaces. The first theoretical explanation was provided by Bruno et al.\cite{5}, who explained the oscillations as a function of spacer layer thickness due to the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction between the magnetic layers. They expressed the period of oscillations in terms of nesting vectors of the spacer’s Fermi surface. However, the coupling strength $J$ was described by an adjustable parameter in their work. There are several other explanations of this phenomenon based on electronic Fabry-perot-like interference effects\cite{6} or quantum-well (QW) theories\cite{7}. In order to understand this phenomenon, first-principles techniques have also been employed which are more transparent and parameter free but require considerable computational effort. The first-principles calculations of the exchange coupling $J$ have been reported for various systems such as Fe/Cr, Fe/Cu, Fe/Mo, Co/Cu\cite{8, 9, 10, 11}. Recently, the combined theoretical-experimental work on Fe/Au supercells, with only 2 monolayers of Fe\cite{12}, showed that the exchange coupling $J$ exhibits oscillatory behaviour. However, this was found to be ferromagnetic for all layers. Some results have also been reported for the oscillatory behaviour of magnetic moments as a function of spacer layer thickness\cite{9}.

Fe/Nb is an interesting system as it provides a way of exploring the coexistence of ferromagnetism and superconductivity. This is one of the main interests of experimental studies of Fe/Nb/Fe multilayers\cite{13, 14, 15, 16}. Mühge et. al.\cite{15} studied the magnetism and superconducting properties of Fe/Nb trilayer system. They have found a strong dependence of the superconducting transition temperature $T_c$ on Fe layer thickness. They also studied the magnetic properties using the magneto-optical Kerr effect, ferromagnetic resonance and magnetization measurements by SQUID magnetometer.
Although a large number of studies exist for Fe/Cr, Fe/Au, Co/Cr etc., there are only a few theoretical studies for Fe/Nb system. The difficulty one faces with Fe/Nb is that the lattice parameter of Fe and Nb differ by 13% and thus it presents an additional complication for theoretical as well as experimental studies. The Fe/Nb multilayers show strong interlayer exchange coupling [13] which changes in continuous and reversible way by introducing hydrogen into the sample [14]. This system has not been explored much theoretically and therefore needs a detailed study. The experimental results for Fe/Nb multilayers [13, 15, 16] show oscillatory interlayer exchange coupling as a function of Nb spacer layer thickness within a period of 9.0 Å to 12.8 Å. Sticht et al. [17] showed the oscillating exchange coupling in Fe/Nb multilayers as a function of Nb spacer layer thickness using the augmented spherical wave (ASW) method [18].

To study the exchange coupling in Fe/Nb multilayers, we have used a self-consistent full-potential linearized augmented plane-wave (FLAPW) method [19] that treats crystal potential accurately and makes no shape approximation for the crystal potential. In this paper we report the energy functional dependence of exchange coupling and magnetic properties of Fe/Nb multilayers. Some preliminary results of our work have been reported earlier [20]. Our results show that the interlayer exchange coupling for both the local spin density approximation (LSDA) and the generalized gradient approximation (GGA) oscillates with a period of 6.0 Å which is close to the ASW result of 4.5 Å [17]. Our calculated period is close to the experimental result in the preasymptotic region. We find that the GGA favors FM coupling for all Nb monolayers while the LSDA gives FM as well as AF coupling. We have also studied the change in magnetic moment of Fe and Nb as a function of Nb spacer layer thickness within the LSDA and the GGA. We find that Nb develops induced magnetic moments which oscillate as a function of Nb spacer layer. The magnetic moment on Fe gets reduced appreciably from its bulk value and depends on Nb spacer layer thickness. The Fe magnetic moment shows strong oscillations as a function of Nb thickness in agreement with the experimental results [13, 15].

The organization of the paper is as follows. In Sec. II we provide the details of our calculation. In Sec. III we present our results and discuss them. Finally, we give our conclusions in Sec. IV.
II. COMPUTATIONAL DETAILS

A. Method

All calculations reported in this paper have been carried out using the self-consistent full-potential linearized augmented plane-wave (FLAPW) method \[^{19}\] in a scalar relativistic version without spin-orbit coupling. We have used the LSDA as well as GGA for our calculations. The muffin-tin radii are 1.33 Å for Fe and Nb. The maximum value in the radial sphere expansion is \(l_{\text{max}} = 10\), and the largest \(l\) value for the non-spherical part of the Hamiltonian matrix is \(l_{\text{max,ns}} = 4\). The cutoff parameters are \(R_{mt}K_{\text{max}} = 8\) for the plane wave and \(R_{mt}G_{\text{max}} = 14\) for the charge density. The number of plane waves ranges from 1400 to 5475, depending on the number of Nb layers. An improved tetrahedron method has been used for the Brillouin-zone integration \[^{21}\].

B. Supercell geometry

To perform the calculations we have constructed tetragonal supercells consisting of bcc Fe and Nb monolayers and in each supercell the number of Nb monolayers (ML) range from 1ML to 7ML. The schematic geometry of FeNb\(_4\) multilayers is shown in Fig. 1. The lattice constants of bulk Fe and Nb are very different with 13% lattice mismatch. To reduce the lattice mismatch we started with a multilayer whose lattice constant is average of bulk Fe and Nb and then relaxed the lattice parameter. The relaxed parameter was found to be 3.067 Å. All calculations are performed with this relaxed lattice constant. The lattice parameter along (001) direction changes from 3.067 Å to 12.269 Å in supercells. The atomic positions have not been relaxed.

C. Interlayer exchange coupling and k-point convergence

The total energy is calculated for ferro and antiferromagnetic ordering of Fe atoms for each Nb spacer layer thickness. To obtain reliable energy differences between ferromagnetic and antiferromagnetic ordering, the unit cell of AF structure is also used for FM structure. The exchange coupling, \(J\), is calculated by taking the energy difference

\[
J(d) = E^{\uparrow\uparrow}_{\text{tot}}(d) - E^{\uparrow\downarrow}_{\text{tot}}(d)
\]  

(1)
where $d$ is the thickness of the spacer layer and $E_{\text{tot}}^{\uparrow \downarrow}(d)$ and $E_{\text{tot}}^{\uparrow \uparrow}(d)$ are the total energies of the system in antiferromagnetic and ferromagnetic arrangements. For the calculation of the IEC, a sufficiently large number of $k$ points are needed. The convergence of the IEC as a function of $k$ points in the irreducible Brillouin zone (IBZ) is shown in Fig. 2 for the LSDA and GGA potentials. We find that the convergence is reached if we use about 200 $k$ points in the IBZ and the IEC converges faster than the total energy as a function of $k$ points in the IBZ.

### III. RESULTS AND DISCUSSION

#### A. Interlayer exchange coupling

The total energies of the Fe/Nb multilayers have been calculated for para, ferro and antiferromagnetic ordering of Fe atoms for each Nb spacer layer thickness within the LSDA and the GGA exchange correlation potentials. It is found that the total energy for paramagnetic multilayers is always higher than the total energy of the other two magnetic configurations in both the LSDA and GGA potentials.

The interlayer exchange coupling of Fe/Nb multilayer is shown in Fig. 3 for the LSDA and GGA potentials, as a function of Nb spacer layer thickness. The IEC flips from ferromagnetic to antiferromagnetic at around 2.5 Å and 8.0 Å and then to ferromagnetic coupling at around 4.0 Å and 10.5 Å for the LSDA. The period of oscillation is found to be 6.0 Å which is in good agreement with the experimental value in the preasymptotic region. In the experiment, the preasymptotic value is about 6.5 Å while the asymptotic period is found to be 9.0 Å \[13\]. The IEC has similar trends as in the ASW work \[17\] except the period of oscillation is slightly larger than the ASW work. We have taken an optimized lattice constant which is smaller than the ASW work as well as we have considered only 1ML of Fe in our calculation while Sticht et al. \[17\] have taken 2ML of Fe. This may be a possible reason for getting a different period from the ASW work \[17\].

The IEC also shows the oscillations for the GGA potential but it does not change to antiferromagnetic coupling and the period of oscillation is found to be the same i.e. 6.0 Å. This indicates that the GGA favors ferromagnetic ordering in this system and it is in good agreement with the experimental results \[13\] where the IEC is found to be ferromagnetic for
Nb thickness less than 14.0 Å. Our calculations are restricted upto 11.0 Å of Nb thickness. Similar behaviour has been seen in Fe/Au system where it was found that 2ML of Fe showed FM coupling only \(^{12}\) while for higher number of Fe ML, FM as well as AF coupling \(^{22}\) was observed. This is consistent with the fact that in pure Fe, GGA gives the ferromagnetic ground state while the LSDA gives the paramagnetic ground state. The magnitude of IEC is 4.45 mJ/m\(^2\) for the LSDA and 22.64 mJ/m\(^2\) for the GGA potential, which is very large compared to the experimental value of 0.034 mJ/m\(^2\). Similar trend has been reported earlier in \textit{ab initio} works \(^9, 10, 22\) on Fe/Cr, Fe/Au, Co/Cu multilayer systems where the theoretical value of the IEC has been found to be 2 to 3 orders of magnitude higher than the experimental value. The GGA gives higher value of the IEC than the LSDA which is related to the fact that the GGA favors ferromagnetic ordering in this system. This is further supported by our calculation of energy difference between ferromagnetic and antiferromagnetic states in bcc Fe using the GGA and LSDA. Using the GGA we get the energy difference of 0.49 eV while in the LSDA the energy difference is 0.39 eV.

The higher magnitude of the IEC as compared to the experimental results can be attributed to the following reasons: (1) The roughness at interface has been neglected in our calculations. Bruno \textit{et al.} \(^5\) studied the effect of interfacial dislocations, interfacial roughness and lattice strain on the period and the amplitude of the IEC within the RKKY approach. They found that the interfacial dislocations reduce amplitude of the IEC. The reduction was more in (111) direction than (001) direction in Cu/Co and Au/Co cases. The interface roughness causes fluctuations in the spacer layer thickness and also breaks in-plane translational symmetry. As a result the IEC is strongly reduced and the period is increased. In Fe/Nb multilayers, which have about 13% lattice mismatch at the interfaces, this effect is probably larger compared to the multilayers, which have matched interfaces such as Fe/Cr, Co/Cu, Fe/Au etc. The interdiffusion and intermixing at the interface causes formation of FeNb alloy at the interface \(^{13}\). This will further contribute to roughness and suppress the IEC. (2) The magnitude of the IEC in experimental study \(^{13}\) has been reported for higher thickness of Nb layer but our calculations are limited to 11.0 Å Nb layer thickness.
B. Magnetic properties

We find that the Fe layers induce the magnetic moments on Nb atoms. The induced moment on Nb atoms at interface layer is opposite to that of Fe atoms. In Fig. 4, we show the induced magnetic moments per atom on Nb spacer layers using the GGA when Fe atoms are ferromagnetically ordered in $FeNb_7$ multilayers system. The induced magnetic moments show oscillations although the amplitude of the oscillations away from the interface is quite small. The induced magnetic moments at the interface is 0.17 $\mu_B$ while at the middle layer it is 0.01 $\mu_B$ in $FeNb_7$ multilayer. We notice that the amplitude of the oscillations increases with the increase in number of Fe layers. This is similar to the nature of induced magnetic moment in the spacer layer seen in other systems [23]. It is also seen that the Nb atoms have higher magnetic moments on the interfacial Nb spacer layer. These induced magnetic moments are reduced in the LSDA calculations. The magnetic moment at the interface changes to 0.09 $\mu_B$ and zero magnetic moment at the middle layer of Nb in the LSDA. The explanation is given in next section for the difference of magnetic moments of Nb for both the LSDA and GGA functionals.

In Fig. 5, we plot the change in the magnetic moment per atom in Fe layers as a function of Nb spacer layer and find that it also shows oscillations in the LSDA as well as GGA. Also shown in the inset are the experimental results of Fe/Nb multilayers [13]. The magnetic moment of Fe is reduced at the interface as compared to the bulk value, in agreement with the experimental results. In case of the GGA potential, the magnetic moment of Fe varies from 1.32 $\mu_B$ to 0.90 $\mu_B$ while in LSDA, it varies from 1.12 $\mu_B$ to 0.46 $\mu_B$ depending on the Nb layers in the system. In both cases the magnetic moment of Fe is smaller than the magnetic moment in bulk Fe (2.24 $\mu_B$). Our GGA calculations show that the magnetic moment of Fe at the interface decreases rapidly with Nb thickness till 5.0 Å and is almost constant between 5.0 Å to 10.0 Å and then shows a sharp increase around 10.0 Å. We note that the GGA results show much better agreement with the experiment. In particular, the sharp rise of the magnetic moment around 10.0 Å is well reproduced by the GGA results.

We also find the magnetic moment of Fe, in case of $Fe_2Nb_2$, varies from 2.16 $\mu_B$ to 2.00 $\mu_B$ and the induced magnetic moment on Nb layer also changes from 0.54 $\mu_B$ to 0.22 $\mu_B$. Thus the reduction in magnetic moment of Fe atoms at interface depends on Nb spacer thickness and magnetic moments of Nb spacer layer also depends on Fe layer thickness.
C. Electronic structure

To understand the behaviour of the magnetic moments of Fe and Nb, we have examined the d-band density of states (d-DOS) of Fe and Nb in $Fe/Nb_4$ multilayer system. The ferromagnetic d-DOS for Fe in bulk and $Fe/Nb_4$ multilayers are shown in Fig. 6. This figure shows that the difference between up and down electrons in bulk Fe is more compared to the corresponding difference in $Fe/Nb_4$ multilayers. Thus the magnetic moment of Fe in $Fe/Nb_4$ multilayers is smaller compared to the bulk value. Also we note from the figure that the down spin d-DOS in $Fe/Nb_4$ is shifted to lower energy compared to the corresponding d-DOS in bulk Fe. This shows that the exchange splitting in $Fe/Nb_4$ is smaller than that in bulk Fe. The figure also shows a comparison between the LSDA and GGA d-DOS. We see from the figure that exchange splitting in the GGA is larger compared to the LSDA.

In Fig. 7, we have shown the d-DOS of Nb layers at the interface and at the middle layer for ferromagnetic $Fe/Nb_4$ multilayers using the GGA. The bulk d-DOS of Nb is also shown. The layer at interface is denoted by Nb1 and the middle layer by Nb2. The interface and middle layers have different d-DOS compared to the bulk d-DOS of Nb. The d-DOS at the interface layer has peaks between -3.0 eV to 2.0 eV while the middle layer has much smaller d-DOS in this energy range. This shows some hybridization of d-states of Nb and Fe at the interface layer while this hybridization is almost absent in the middle layer. This is consistent with the result in Fig. 4 which shows that the Nb interface layer near the Fe layer has higher magnetic moment as compared to the layers far from Fe layers. Thus the induced magnetic moment on Nb layer is a consequence of the hybridization between Fe and Nb d-states. Nb magnetic moment shows oscillations as shown in Fig. 4 because Fe layer induces a spin polarization in Nb layers which oscillates due to Friedel oscillations [24]. This is consistent with the earlier result for Fe/Mo multilayers where magnetic moment on Mo also shows Friedel oscillations [10]. Mirbt et al. [10] have also found the reduction in the Fe magnetic moments which is same in our case. The mechanism of the oscillation of Fe magnetic moments is not clear and open for further work.
D. Comparison with Models

Several models \cite{5,10,25,26} have been presented to explain the period of oscillations of the IEC. The RKKY and QW models express the period in terms of the nesting vectors at the Fermi surface. The RKKY and the QW models give the same period because of the dependence on the dimensions of the Fermi surface of the space material. We shall now discuss the results of these models and compare them with our results.

1. RKKY Model

In the RKKY theory, one magnetic layer polarizes the spacer layer and the other magnetic layer interacts with this. Since the spin polarization is oscillatory as a function of spacer layer thickness, the IEC also oscillates. The period of oscillation is given by \( \frac{2\pi}{k} \), where \( k \) is the spanning vector \cite{27} across the Fermi surface of the spacer layer. Therefore, to calculate the period of oscillation of the IEC we have calculated the Fermi surface of Nb which has many critical spanning vectors corresponding to many oscillation periods. The calculated values of spanning vectors in [100] plane are 0.79, 0.63, 0.53, 0.46, 0.35, 0.20 and 0.15 in unit of \( \pi/d \), where \( d \) is the distance between the lattice planes along (001) direction. The corresponding oscillation periods for these spanning vectors are 4.20 Å, 5.43 Å, 6.20 Å, 7.24 Å, 9.31 Å, 16.29 Å and 21.73 Å which are in good agreement with earlier calculations \cite{27}. The oscillation period of one of these spanning vector is 6.20 Å, which is in good agreement with our FLAPW calculation. Because our FLAPW calculations are restricted up to 7ML of Nb spacer layer thickness, we could find only one period of oscillation.

2. QW Model

We have also calculated the period of oscillation of the IEC using the quantum well (QW) model \cite{27} even though within first order perturbation theory the RKKY and QW models are equivalent. In this model the Fermi energy oscillates as a function of the well thickness. The period of the oscillation is given by the wave vector at the Fermi energy in the well. We consider the free electron model where the standing wave form in QW if \( \lambda = \frac{2L}{n} \), where \( \lambda \) is the wavelength, \( L \) is the thickness of the well and \( n \) specifies the energy level. \( L \) is defined as \( 2L = Nd \), where \( N \) is the number of spacer ML and \( d \) is the interlayer spacing.
Thus using the above relations and \( k = 2\pi/\lambda \), we get the condition \( k = 2\pi/Nd \). For a free electron in the well, the energy can be written as

\[
E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m} \left( \frac{2\pi n}{Nd} \right)^2
\]  

(2)

As shown in Ref. [27], energy \( E \) shows oscillation as a function of \( N \). Since the density of states (DOS) for this case varies as \( E^{1/2} \), it will also show oscillation as a function of \( N \) at Fermi level. The period of oscillations can be predicted by analyzing the peak positions of QW states in the electronic density of states [25, 27]. In Fig. 8, we have plotted the variation in s and p DOS in the Nb spacer layer at Fermi energy as a function of Nb spacer layer thickness, which shows a peak at 3.0 Å and at 9.0 Å. This gives period of oscillation to be 6.0 Å which is in good agreement with the result obtained from our FLAPW calculation and the RKKY model.

Since both of these models gives the same results for the period of the IEC, the comparison of our results with the model results gives no clue regarding the mechanism of IEC. This question has been addressed by Schilfgaarde and Harrison [26] and Mirbt et al. [10] in connection with Fe/Cr/Fe and Fe/Mo/Fe layers. In the RKKY theory, the amplitude of the coupling is bilinear in the magnetic moments on two sides while in QW model the amplitude does not depend on the magnetic moments. To analyze this, the calculated IEC was fitted to the asymptotic limit of the RKKY expression and the amplitudes were calculated. For the fit, results for spacer layer thickness less than 5ML were ignored as the expression used for the fit corresponded to the asymptotic limit. Since the electronic structures of Nb and Mo are similar [10, 28, 29], Fe/Nb system may show a behaviour similar to Fe/Mo system. For the Fe/Mo system, Mirbt et al. [10] fitted their results up to 20ML and found that the amplitude is proportional to the magnetic moments squared of Fe for 3ML, 4ML and 10 ML caliper while the IEC has no dependence on magnetic moments for 2ML caliper. Thus their analysis does not favor either the RKKY or the QW model. In our case the maximum thickness is 7ML and therefore this kind of fit to the asymptotic expression is not possible at present and will be taken up in future work.
IV. CONCLUSIONS

We have calculated the interlayer exchange coupling between Fe layers when separated by Nb spacer layers using the self-consistent FLAPW method with the LSDA and GGA exchange correlation potentials. We observe an oscillating exchange coupling as a function of Nb spacer layer thickness with a period of 6.0 Å for the LSDA as well as GGA in good agreement with the preasymptotic value observed in the experiment. It is close to earlier calculated period 4.5 Å by the ASW method. Our calculated period is also in good agreement with the period calculated using the RKKY and QW models. The LSDA calculations show an AF coupling at 2.5 Å and 8.0 Å thickness of Nb space layer but the GGA calculations favor ferromagnetic coupling for all Nb spacer layers. We find that the induced magnetic moments on Nb atoms show oscillatory behaviour. The Fe magnetic moment also shows strong oscillations as a function of Nb spacer layer thickness. The GGA gives higher magnetic moments for Fe and Nb compared to the LSDA. The GGA results show better agreement with the experiment than the LSDA results. The reduction in magnetic moments of Fe and the induced magnetic moment on Nb atoms is found to be a consequence of the hybridization between Fe and Nb d-bands.

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FIGURE CAPTIONS

Fig. 1. Supercell used for FeNb₄ multilayer.

Fig. 2. Interlayer exchange coupling, J(meV) for FeNbₙ multilayers as a function of k-points in the IBZ for different number of Nb layers for (a) LSDA and (b) GGA. The calculated results are shown by filled squares, circles and stars.

Fig. 3. Interlayer exchange coupling, J (meV) for FeNbₙ multilayers as a function of Nb spacer layer thickness (Å) for the LSDA and GGA.

Fig. 4. Induced magnetic moment on Nb spacer layer in ferromagnetic FeNb₇ multilayer. The Fe atoms are placed at positions 0 and 8. The filled squares show the calculated results.

Fig. 5. Magnetic moments on Fe atoms in FeNbₙ multilayers as a function of Nb spacer layers. The dots correspond to the GGA and filled squares to the LSDA results. The experimental results of Mattson et al. [13] are shown in the inset.

Fig. 6. The top panel shows the partial density of states of spin-up and spin-down d-bands for ferromagnetic bulk Fe using the GGA. The bottom panel shows the partial density of states of spin-up and spin-down d-bands for Fe in ferromagnetic Fe/Nb₄ system using the LSDA and GGA.

Fig. 7. The top panel shows the partial density of states of spin-up and spin-down d-bands for Nb in ferromagnetic Fe/Nb₄ system. Nb1 denotes the d-DOS at the interface while Nb2 denotes the d-DOS at the middle layer. The bottom panel shows the d-DOS for bulk Nb using the GGA.

Fig. 8. Density of states of s and p states of Nb at Fermi level as a function of Nb spacer layer thickness.
Interlayer Exchange Coupling (meV)

Number of \( k \)-points in IBZ

LSDA

FeNb\(_n\)

- \( n=1 \)
- \( n=4 \)
- \( n=5 \)
Interlayer Exchange Coupling (meV) vs Nb spacer layers thickness (Å)

- LSDA
- GGA
Magnetic Moments on Nb ($\mu_B$) vs. Number of Nb spacer layers.

GGA
Fe Up

DOS (States/eV)

Energy (eV)

Fe Dn

LSDA

GGA

FM

Fe/Nb₄

FM

GGA

LSDA

Dn

Up

DOS (States/eV)

Energy (eV)
