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Spin Polarization of Ni_n/Co overlayers with GGA and GGA+U Calculations

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Abstract In this work We have investigated the magnetic ordering, Total Charge and Total Density of State (DOS) of Ni_n/Co systems with a first-principle calculation of the Density Functional Theory (DFT) ferromagnetic (FM) face-centered cubic (fcc) of Nickel Ni on Cobalt Co substrate for n=1-3 overlayers. The relaxed ion, relaxed ion + volume, and non-relaxed electronic structures of the Ni_n/Co (111) crystallographic orientations are determined with generalized gradient approximation (GGA) and generalized gradient approximation + Hubbard (GGA+*U*). The onset of magnetism depends on the faces considered. The magnetism is most favored with GGA+U_{Ni} and GGA+U_{Ni}+U_{Co} than with GGA calculations due to the strong correlations of Hubbard. The observed trends can be explained as in earlier studies in terms of the hybridization between d states of Co substrate, also some interesting specific behavior of the magnetization in the fcc Ni_n/Co (111) overlayers with different layers has been observed.

Keywords Overlayer; magnetic moments; relaxation; Total Charge; DOS; Ni; Co

1. Introduction

Intensive experimental [1-4] and theoretical [5-6] studies of Surface and interface for transition metals have focused on how the magnetic moments are modified in size and/or orientation in such ultrathin films from both fundamental and technological points of view. In our previous study, Nickel (Ni) and Cobalt (Co) are a 3d transition-metal that exhibits a ferromagnetic (Fm) ground state in their bulk form, with magnetic moments of 0.591 and 1.595 μB for GGA, while for GGA+U their magnetic moments are 0.659 and 1.785 μB respectively [7]. Experimentally evidence of the magnetically dead layers of Ni in sputter-grown Ni/Pt multilayers, studied with room-temperature magnetic circular dichroism and temperature-dependent super conducting quantum interference device magnetometry [8]. They found that the magnetic state of Ni/Pt interfaces is quite different from the bulk one due to the changed electronic structure. Also NiMnGa half-Heusler alloy films have been deposited on Si(100) substrates by the pulsed laser deposition technique at temperatures ranging from 450 to 650 ˚C [9]. X-ray diffraction and atomic force microscopy observation show the phase structure and surface morphology of these films are different.

From theoretical points of view, M.K. Husain et al [10] have investigated the exchange bias effect in micron-sized ferromagnetic wires made from Co and $Ni_{80}Fe_{20}$ films. The wires were fabricated using optical lithography, metallization by sputtering and lift-off technique. The onset of exchange biasing effect is found to be 70 and 15 K for the Co and $\mathbf{Ni_{80}Fe_{20}}$ wires, respectively. Also, The Spin polarization of fcc Ni_n (100) and (111) surfaces with GGA and GGA+U investigated for the relaxed and non-relaxed electronic structures [11]. We found that the Ni (100) and (111) surfaces magnetic moments enhancement attributed to the reduced symmetry and coordination number at surfaces, and also when strong correlation is included, the magnetic moments of Ni (100) and (111) surfaces increased. On the other hand, the Magnetization of fcc Co_n (100) and (111) surfaces with GGA and GGA+U also investigated for the relaxed and non-relaxed electronic structures [12]. We obtained that the relaxed and non-relaxed surface local magnetic moments of Co (100) and (111) oscillatory increase with increasing the number of layers, and the local magnetic moments of the atom in the center of the films oscillates decrease towards the bulk value.

In addition to that, Single crystal Co/Ni (111) superlattices with perpendicular magnetic anisotropy interested the magnetic memories switched with a rather small spin-torque current [13]. And they show that the number of the states depends on the Co layer thickness. Also they found that the spin magnetic moment increases at the interfaces or at the surface. In the other hand, F. Gimbert et al [14] used a surface-dedicated first-principles method calculated the electronic structure in Co/Ni (111) overlayers with a Co thickness varying between 1 and 5 monolayers, They found that the energy of the surface states is the same for all the overlayers thicker than 2 Co MLs, while the number of quantum-well (QW) states increases with the Co thickness. Also, the calculated one- and two-atom layers of cobalt on a copper (111) surface was performed in a tight-binding scheme, with single-site, full orbital interactions treated self-consistently [15]. They were examined Antiferromagnetic and ferrimagnetic states with a two-atom periodicity. They found a new type of "spatially modulated" state, and the ferromagnetic state was found to have the lowest total energy. Beside that, A. Ernst et al [16] were reported on Korringa-Kohn-Rostoker Green's function calculations for the ground-state moments of ultrathin Ni films on Cu (001) and on four monolayers (ML) Co/Cu (001). They found that for Ni on a ferromagnetic substrate, such as 4 ML Co/Cu (001), no reduction of the magnetic moment occurs, so that Ni at the interface retains its bulk value. Recently [17], Ferromagnetism of fcc $\mathbf{Co_n}$/Ni (111) overlayers with GGA and GGA+U for n = 1 – 3 overlayers are investigated for the relaxed and non-relaxed electronic structures, we found that the magnetic moment of Co overlayers in Co_n/Ni (111) orientation is found to be larger than that of the Co surface layer in pure semi-infinite surfaces [12] due to the presence of Ni interfacial layer.

Computational Methods

All calculations have been performed with VASP (Vienna ab initio Simulation Package) [18-22], a first principles plane-wave code based on spin-polarized density functional theory. The interaction between ions and valence electrons was described by the projector augmented-wave (PAW) method [23]. The Kohn-Sham equations were solved via iterative matrix diagonalization based on the minimization of the norm of the residual vector to each eigenstate and optimized charge- and spin-mixing routines [24-26].

The generalized gradient corrections added in form of Perdew-Wang functional PW91 [27] were chosen for the exchange correlation function for the GGA. The spin interpolation of Vosko et a1 was also used [28]. To correct the strong electronic correlation, a simple rotationally invariant DFT+U version proposed by Dudarev et a1 [29, 30] and implemented in VASP [31] was used as GGA+U. In this method, the parameters U and J did not enter separately, only the difference U-J was meaningful. Parameters U and J represented on-site Coulomb interaction energy and exchange energy respectively. J was kept to 1 eV for both Ni and Co, with a value of U-J=2.4 and 1.8 eV respectively [7, 32] was used in our calculations. A detailed description of the DFT+U method can be found in Ref. [33].

All results reported in this work were carried out on a surfaces face-central-cubic ferromagnetic supercell including $\mathbf{Ni_n}$/Co (111) orientation for n = 1-3 overlayers. Convergence tests have been checked carefully both for plane wave cutoff energy and k points sample, a plane-wave set expanded in energy cutoff 270 eV and k-points sample with a mesh of points 9x9x1 generated by the scheme of Monkhorst and Pack [33,34] can ensure

the total energies difference is less than 3 meV/atom. For total energy and DOS calculation, the integration over the Brillouin zone was performed using the linear tetrahedron method with blochl corrections [35-37].

Results and Discussion

A number of experimental [1-4, 8, 9] and theoretical [5-7, 10-17] studies of Surface and interface for transition metals have focused on how the magnetic moments are modified in size and/or orientation in such ultrathin films from both fundamental and technological points of view. In our calculations, we investigate the magnetic ordering of Ni_n/Co (111) systems, for n = 1-3 overlayers. We found that the ion relaxation does not change atomic sphere charge and magnetic moments of all our study cases, while the ion + volume relaxation change atomic sphere charge and magnetic moments of our study cases for both GGA and GGA+U respectively. Here we will show the calculated results for relaxed ion + volume and non-relaxed Ni_n/Co (111) surfaces for n = 1–3 overlayers. In this work we used the lattice constants of our previous DFT fcc bulk Ni and Co calculations [7], which produce a ferromagnetic solution. For Ni the lattice constant, magnetic moment are 3.53 Å, 0.591 μB for GGA, while for GGA+U (U-J = 2.4 eV) the obtained values are 3.51 Å, 0.659 μB, respectively. While for Co the lattice constant, magnetic moment are 3.52 Å, 1.595 μB for GGA, while for GGA+U (U-J = 1.8 eV) the obtained values are 3.55 Å, 1.785 μB, respectively. Table 1, show us the Magnetic moments of Ni_n/Co (111) orientation for n = 1-3 non-relaxed and relaxed overlayers with GGA and GGA+U respectively. From this table we see that the magnetic moment of the Co overlayers are Enhanced due to the presence of a Ni interface. However, as the number of Co overlayers increases, the surface local magnetic moments decrease. Also table 1 shows that the magnetic moments for GGA+U_{Ni} and GGA+U_{Co}+U_{Ni} quit similar for non-relaxed and relaxed cases for different Co overlayers.

Table 1: GGA and GGA+U Magnetic moments (in Bohr magnetons, μB) of F Ni_n/Co (111) orientation for n = 1-3 overlayers.

State	n	non-relaxed				relaxed ion+volume			
		Co	Ni			Co	Ni		
		(I)	(S)	(S-1)	(S-2)	(I)	(S)	(S-1)	(S-2)
GGU	**1**	1.784	0.664			1.738	0.664		
	2	1.773	0.615	0.696		1.743	0.630	0.699	
	3	1.701	0.567	0.572	0.614	1.664	0.577	0.577	0.625
GGA+U_{Ni}	**1**	1.755	0.717			1.719	0.710		
	2	1.722	0.702	0.681		1.696	0.693	0.694	
	3	1.674	0.666	0.580	0.634	1.625	0.637	0.551	0.638
GGA+U_{Co}	**1**	1.797	0.660			1.741	0.663		
	2	1.785	0.612	0.691		1.744	0.628	0.701	
	3	1.714	0.570	0.570	0.607	1.671	0.575	0.574	0.625
GGA+U_{Ni}+U_{Co}	**1**	1.775	0.717			1.719	0.710		
	2	1.722	0.702	0.681		1.696	0.693	0.694	
	3	1.674	0.666	0.580	0.634	1.625	0.637	0.551	0.638

The magnetic moments of three overlayers of Ni on Co substrate for (111) orientation with GGA, GGA+U_{Ni}, GGA+U_{Co} and GGA+U_{Ni}+U_{Co} reflected in Fig. 1, which shows that the magnetic moments increases from the surface layer (S) to the interface layer (I) toward the bulk value.

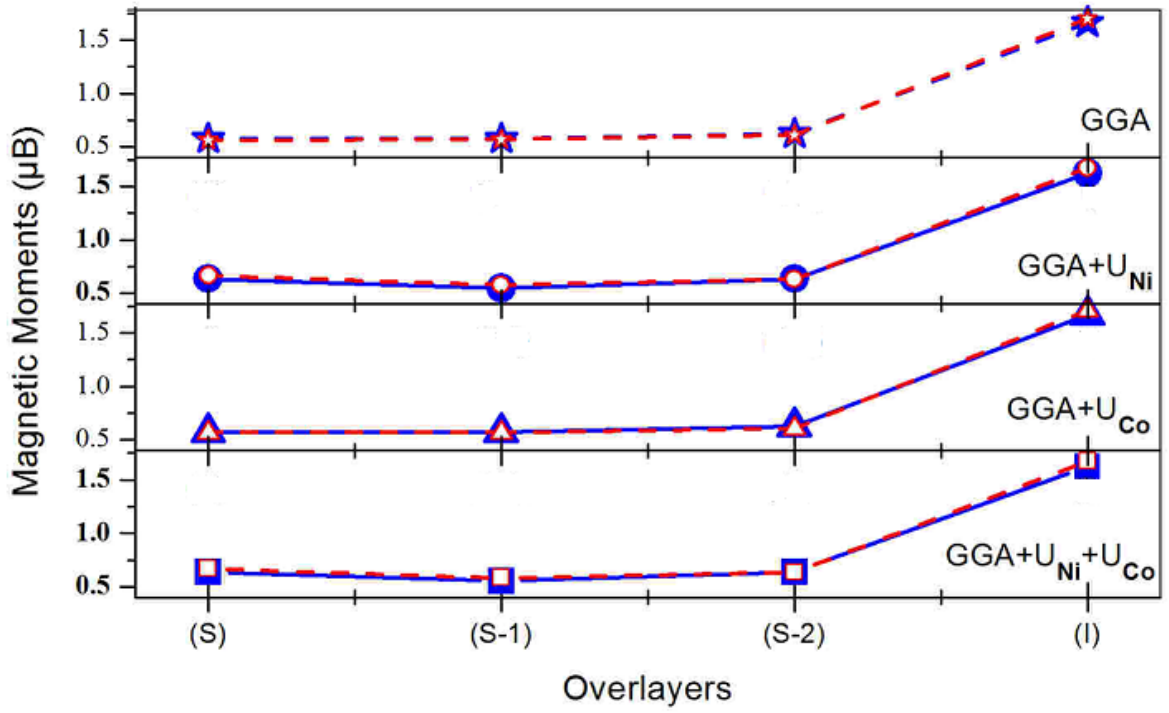

Figure 1: Magnetic moments of three-layers for Ni_n/Co (111) orientation. Solid symbols straight lines for relaxed and open symbols doted lines for non-relaxed. Star for GGA, Circle for GGA+U_{Ni}, triangle for GGA+U_{Co} and Square for GGA+U_{Ni}+U_{Co} respectively.

Table 2, show us the total charge (in coulomb, C) of F Ni_n/Co (111) orientation for n = 1-3 overlayers for relaxed and non-relaxed cases with GGA and GGA+U respectively. From this table we found that the total charge of the Ni overlayers are Enhanced due to the presence of a Co interface. However, as the number of Ni overlayers increases, the surface total charge decrease. In addition to that table 2 shows that the total charge for GGA+U_{Ni} and GGA+U_{Ni}+U_{Co} quit similar for relaxed and non-relaxed cases for different Ni overlayers.

Table 2: GGA and GGA+U Total Charge (in coulomb, C) of F Ni_n/Co (111) orientation for n = 1-3 overlayers.

State	n	non-relaxed				relaxed ion+volume			
		Co	Ni			Co	Ni		
		(I)	(S)	(S-1)	(S-2)	(I)	(S)	(S-1)	(S-2)
GGU	**1**	7.970	9.021			8.085	9.122		
	2	7.979	9.012	9.122		8.061	9.081	9.215	
	3	7.981	9.011	9.118	9.131	8.065	9.075	9.202	9.216
GGA+U_{Ni}	**1**	7.934	9.031			8.031	9.163		
	2	7.945	9.014	9.120		8.074	9.126	9.259	
	3	7.949	9.010	9.114	9.127	8.071	9.120	9.243	9.259
GGA+U_{Co}	**1**	7.938	8.993			8.078	9.122		
	2	7.948	8.984	9.086		8.059	9.080	9.207	
	3	7.951	8.982	9.083	9.095	8.049	9.062	9.192	9.198
GGA+U_{Ni}+U_{Co}	**1**	7.934	9.031			8.081	9.163		
	2	7.945	9.014	9.120		8.074	9.126	9.259	
	3	7.949	9.010	9.114	9.127	8.071	9.120	9.243	9.259

In fig. 2, the total magnetic moments of F Ni_n/Co (111) orientation for n = 1-3 overlayers with GGA, GGA+U_{Ni}, GGA+U_{Co} and GGA+U_{Ni}+U_{Co} was reflected. The figure shows that the total magnetic moments increase with increasing the number of layers for all cases of our study, in addition to that the total magnetic moments GGA+U_{Ni} and GGA+U_{Ni}+U_{Co} they are almost have the same values for different overlayers as shown in table 1.

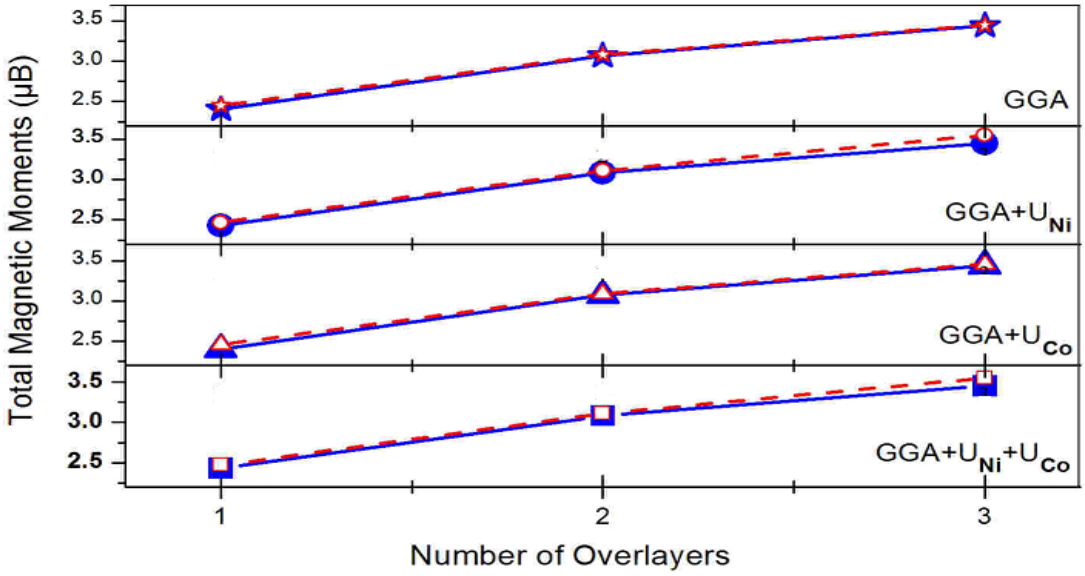

Figure 2: Total magnetic moments of Ni_n/Co (111) orientation for n = 1-3 overlayers. Solid symbols straight lines for relaxed and open symbols dotted lines for non-relaxed. Star for GGA, Circle for GGA+U_{Ni}, triangle for GGA+U_{Co} and Square for GGA+U_{Ni}+U_{Co} respectively.

The total charge of F Ni_n/Co (111) orientation for n = 1-3 overlayers with GGA, GGA+U_{Ni}, GGA+U_{Co} and GGA+U_{Ni}+U_{Co} reflected in Fig. 3, From which we found that the total charge increase with increasing the number of Ni layers for all cases of study.

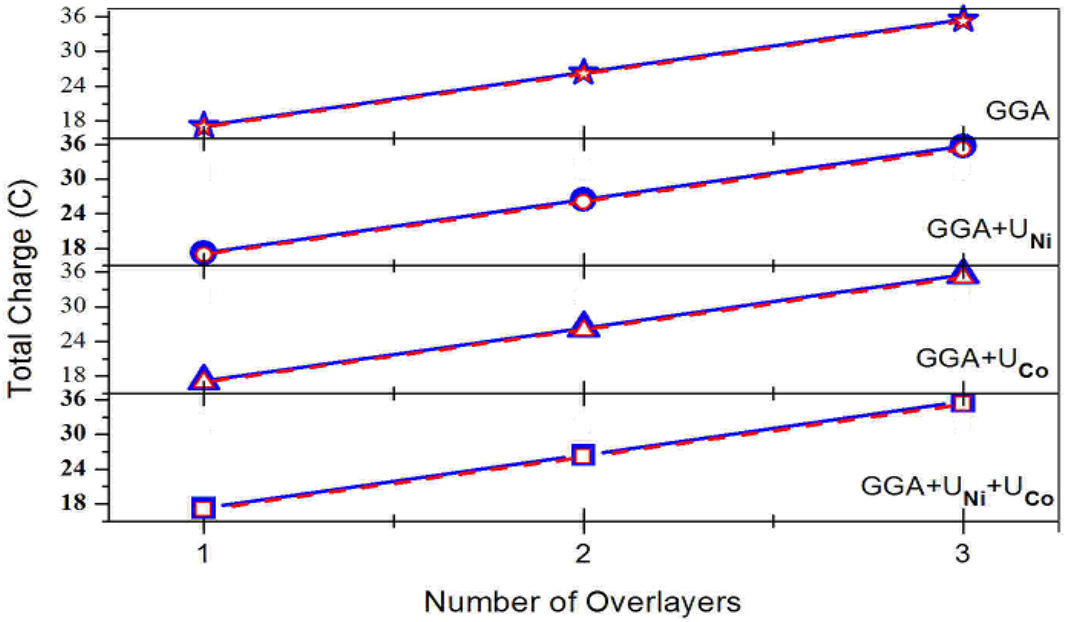

Figure 3: Total Charge of Ni_n/Co (111) orientation for n = 1-3 overlayers. Solid symbols straight lines for relaxed and open symbols dotted lines for non-relaxed. Star for GGA, Circle for GGA+U_{Ni}, triangle for GGA+U_{Co} and Square for GGA+U_{Ni}+U_{Co} respectively.

The Total energy of Ni_n/Co (111) orientation for n = 1-3 overlayers for GGA and GGA+U displayed in table 3 and reflected in Fig. 4. Table 3 and fig. 4 shows that the GGA and GGA+U_{Ni} results are more stable than other cases of our study and they are quite similar. While the relaxed cases for both GGA and GGA+U are more stable than non-relaxed cases for all of our calculations for different numbers of Ni overlayers.

Table 3: GGA and GGA+U Total energy (in electron volt, eV) of F Ni_n/Co (111) orientation for n=1-3 overlayers.

State	n	non-relaxed	relaxed ion+volume
GGU	**1**	-11.07	-11.17
	2	-16.50	-16.58
	3	-21.92	-22.00
GGA+U_{Ni}	**1**	-9.48	-9.65
	2	-13.38	-13.56
	3	-17.23	-17.44
GGA+U_{Co}	**1**	-11.02	-11.18
	2	-16.45	-16.59
	3	-21.86	-22.02
GGA+U_{Ni}+U_{Co}	**1**	-9.48	-9.65
	2	-13.38	-13.56
	3	-17.23	-17.44

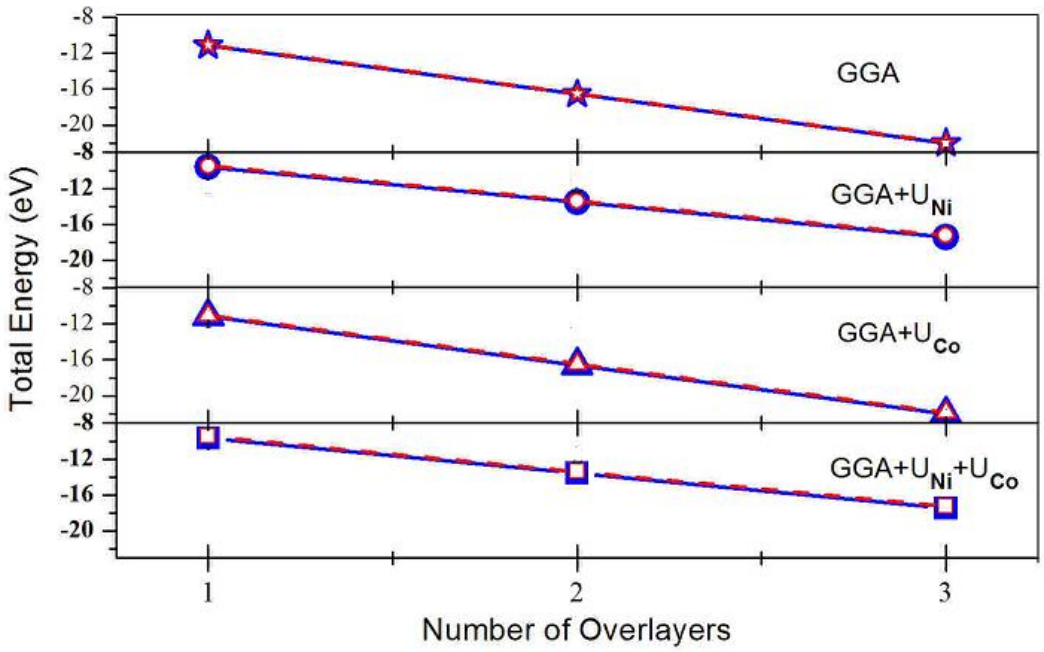

Figure 4: Total Energy of Ni_n/Co (111) orientation for n = 1-3overlayers. Solid symbols straight lines for relaxed and open symbols dotted lines for non-relaxed. Star for GGA, Circle for GGA+U_{Ni}, triangle for GGA+U_{Co} and Square for GGA+U_{Ni}+U_{Co} respectively.

Fig. 5 shows the layer projected total density of states (Total DOS) of Ni_n/Co (111) orientation for n = 2 overlayers for relaxed and non-relaxed GGA and GGA+U calculations respectively. The two overlayers shows that the characteristic narrowing and higher DOS for all of our study cases are quite similar. Also the figure show that the values of Total DOS at Fermi level is higher for non-relaxed cases than the relaxed one for all of our study cases.

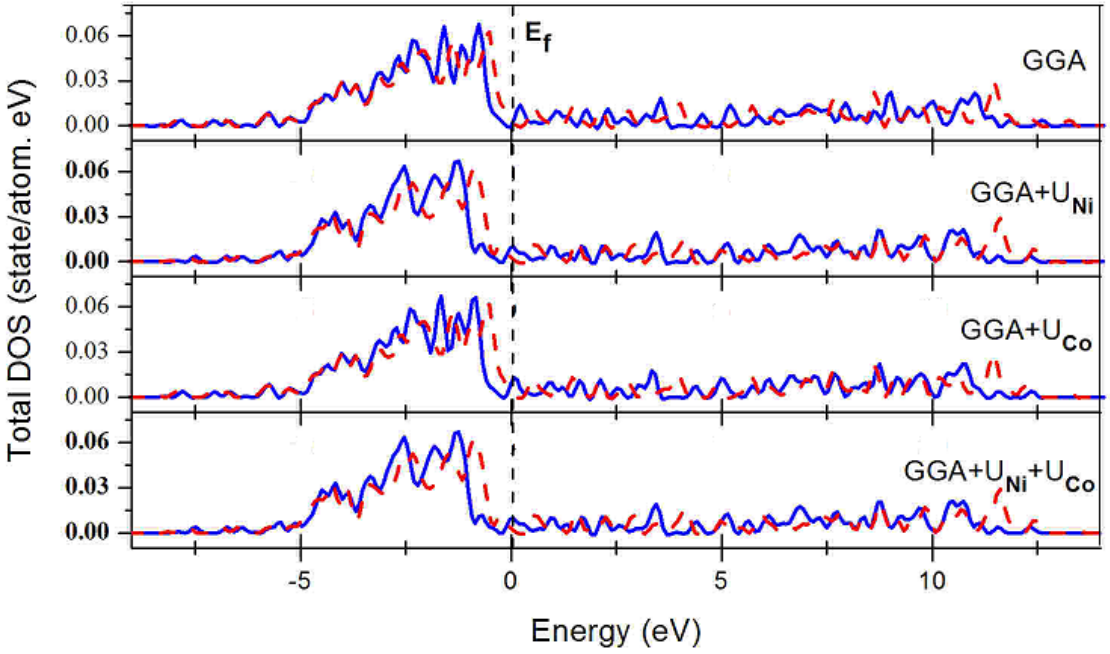

Figure 5: Total DOS of Co_n/Ni (111) orientation for n = 2 overlayers, for GGA, GGA+U_{Ni}, GGA+U_{Co} and GGA+U_{Ni}+U_{Co} respectively. Solid lines for non-relaxed and dashed lines for relaxed cases.

Fig. 6 shows the layer projected total density of states (Total DOS) of Ni_n/Co (111) orientation for n=1 and n=3 overlayers for relaxed and non-relaxed GGA and GGA+U calculations respectively. The one overlayers shows that the characteristic narrowing and the values of Total DOS at Fermi level are lower. While for three overlayers, with the increasing of the number of overlayers, the figure shows that the characteristic is wider and values of Total DOS at Fermi level are higher for all of our study cases. Also the fig. 6 shows that the values of Total DOS at Fermi level are higher for non-relaxed cases than the relaxed one for all of our study cases.

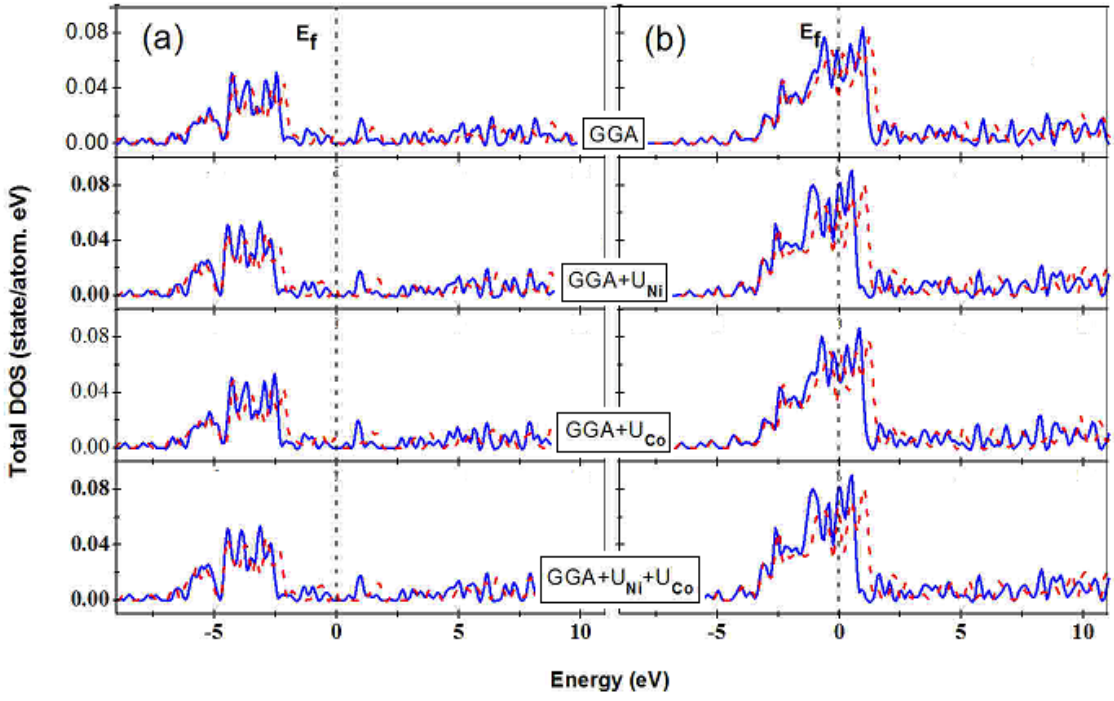

Figure 6: Total DOS of Ni_n/Co (111) orientation for (a) n=1 and (b) n=3 overlayers, for GGA, GGA+U_{Ni}, GGA+U_{Co} and GGA+U_{Ni}+U_{Co} respectively. Solid lines for non-relaxed and dashed lines for relaxed cases.

Conclusion

In this work, the magnetic order, total charge and total DOS are studied for F Ni_n/Co (111) orientation for n=1-3 overlayers. The main results can be summarized as follows:

1- The magnetic moment of Ni overlayers in Ni_n/Co (111) orientation are found to be larger than that of the Ni surface layer in pure semi-infinite surfaces [11] due to the presence of Co interfacial layer.

2- Systems of Ni_n/Co (111) orientation show that the magnetic moments of non-relaxed and relaxed cases increases from the surface layer (S) to the interface layer (I) toward the bulk value.

3- When strong correlation is included, the magnetic moments and the total charge density of Ni_n/Co (111) orientation increased.

4- Total DOS at Fermi level of Ni_n/Co (111) orientation increase with increasing the number of overlayers for relaxed and non-relaxed GGA and GGA+U calculations.

5- Total DOS at Fermi level are higher for non-relaxed cases than the relaxed one for all of our study cases

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