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Half-metallic ferromagnetism in Sc doped in NiO; by first principles calculations

Nazir Ahmad Teli[1*], M. Mohamed Sheik Sirajuddeen[2]

[1,2]Department of Physics,

B. S Abdur Rahman Crescent Institute of Science and Technology, Vandalur Chennai-600048

ABSTRACT

Using first principles calculation, structural, electronic and magnetic properties of NiO were studied by substitution of 3d transition metal atom Sc. 3d transition metal atom Sc is doped in the host compound of NiO in doping concentration of 25% by replacing the Ni atoms to form the compound $Sc_{0.25}Ni_{0.75}O$. The resulting compound $Sc_{0.25}Ni_{0.75}O$ shows the half-metallic ferromagnetism. For determining the equilibrium energy and lattice constant of the supercell $Sc_{0.25}Ni_{0.75}O$, the volume optimization was carried out for both ferromagnetic and non-magnetic phase and is found more stable in ferromagnetic phase. The band gap of spin up direction was found to be 1.13 eV for $Sc_{0.25}Ni_{0.75}O$ at Fermi level. The compound $Sc_{0.25}Ni_{0.75}O$ is predicted to exhibit the half-metallic ferromagnetism with 100% spin polarization at the Fermi level. Therefore, the compound is a good candidate for spintronics devices. The magnetic moment per supercell is equal to 10.00616μ_B.

Keywords : First principles calculations, NiO, Structural, electronic and magnetic properties, Half-metallic ferromagnetism

I INTRODUCTION

To investigate the structural, electronic and magnetic properties of Sc doped in NiO is the main aim of this work. On doping Sc in the host compound NiO, the half-metallic ferromagnetism was investigated. The half-metallic ferromagnetism was first predicted in some Heusler alloys by De-Groot et al [5, 6]. The transition metal oxides like ZnO and CrO are reported to exhibit half-metallic ferromagnetism [7, 8, 9]. It is reported that NiO was doped with transition metals Cu, Zn and Cd and half-metallic ferromagnetism was observed [4]. In half-metallic ferromagnetism, one spin direction is conducting and the other spin direction is semiconducting. Half-metallic ferromagnetic materials are the best candidates for spintronic devices.

NiO has a rock salt structure with lattice constant equal to 4.155Å which shows the metallic character. Terakura et al and Shen et al reported that the LDA failed to describe NiO as an insulator and predicted it to be a metal [1, 2].

Transition metal mono-oxides like NiO are predicted to have vibrational and antiferromagnetic property [19, 20]. The electronic and optical properties have been investigated of NiO with the Coulomb repulsion parameter U and the band gap becomes charge transfer type at higher values of U [3, 17, 18]. Using the GGA+U method the NiO is predicted to be semiconductor [10] but in this work, GGA method is used which shows NiO as metallic. On the basis of this result from GGA NiO is doped with transition metal Sc predicting half-metallic ferromagnetism (HMF).

II. METHODS

Based on density functional theory (DFT), a spin-polarized Full Potential Linearised Augmented Plane Wave (FP-LAPW) was used for the first principles calculations [11, 12]. The electronic properties were studied using WIEN2k code [13,14] which employs the full potential linearised augmented plane wave plus local orbitals. The generalized gradient approximation (GGA) [15] usually favors magnetism more than the local spin density approximation [16] and the properties of transition metals have been greatly improved by GGA. GGA is used as the exchange-correlation potential for all calculations. The full relativistic calculations are implemented for core states and scalar approximation was used for the valence states. The FP-LAPW+lo method expands the Kohn-Sham orbitals in atomic-like orbitals inside the muffin-tin (MT) atomic spheres and plane waves in the interstitial region with a cut-off $R\text{-}K_{max}=7$. The energy cut-off was chosen as -6 Ry, which defines the separation of valance and core states.

To study the electronic structure of Sc doped in NiO a supercell was created. The NiO has a NaCl rock salt structure which belongs to cubic (Fm3m) space group. The doped NiO was modeled in 2×2×2 supercell. Supercell of NiO was created by replacing two Ni atoms with two Sc atoms and the other atoms were left in their respective places. A doping concentration of 25% of Sc atoms achieved as 12.5% doping did not yield the desired result. The number of k points in the whole brillouin zone is chosen as 63 k-points and the total energy of the crystal converges to less than 10^{-4} Ry.

III RESULTS AND DISCUSSION

3.1. Structural Properties

For determining the equilibrium energy and lattice constant the volume optimization for compound $Sc_{0.25}Ni_{0.75}O$ was carried out in GGA method as shown in Figure 1. The calculated lattice constant and the minimum equilibrium energy of the supercell $Sc_{0.25}Ni_{0.75}O$ and the unit cell NiO are given in Table 1. The crystal structure of $Sc_{0.25}Ni_{0.75}O$ compound was plotted as shown in Figure 2 using the Vesta software [17].

NiO has a rock salt structure with the space group 225 (Fm3m) and the positions of atoms as Ni (0, 0, 0) and O (½, ½, ½). Supercell was created by doping two atoms of Sc into the host compound NiO. Two atoms of Ni are replaced with two atoms of Sc and their effect causes half-metallic property in the supercell.

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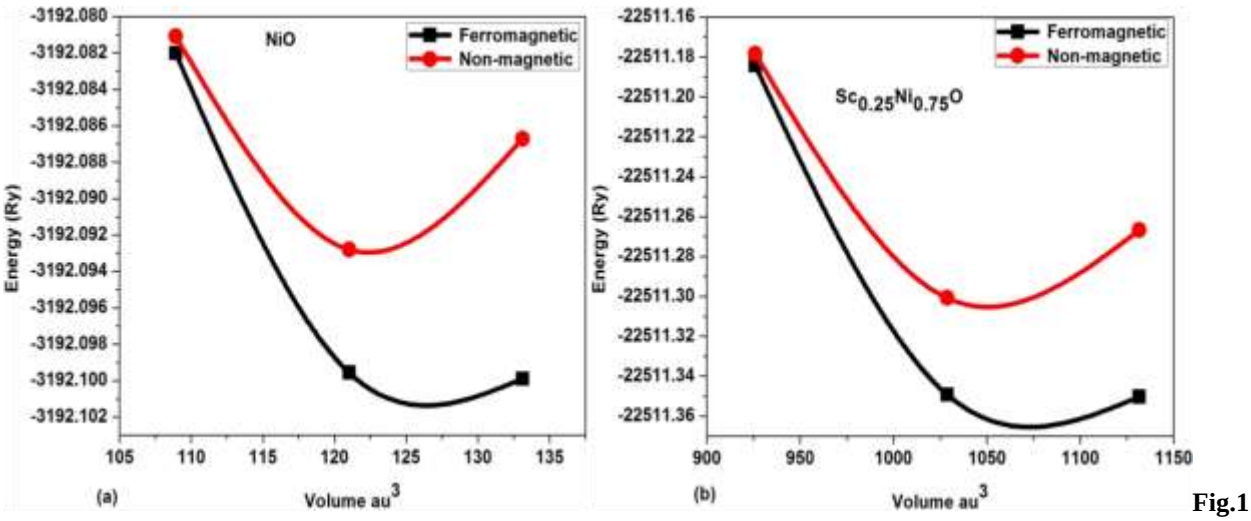

Fig.1

Volume Optimization Curves (a) NiO (b) $Sc_{0.25}Ni_{0.75}O$

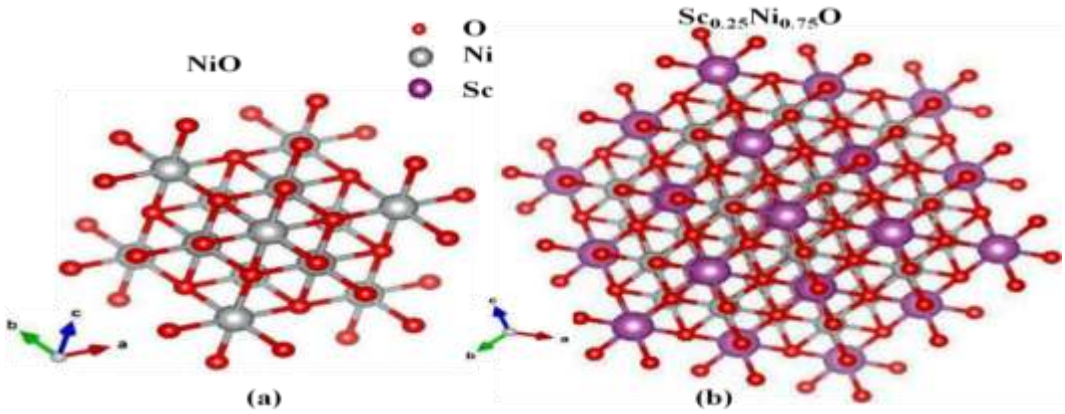

Fig. 2 Crystal structure for (a) NiO (b) $Sc_{0.25}Ni_{0.75}O$

Table 1. Minimum equilibrium energy and calculated lattice constant

S. No.	Compound	Phase	Equilibrium Energy (Ry)	Lattice Constant (Å)
1	NiO	Ferromagnetic	-3192.101383	4.24 per formula unit
		Non-magnetic	-3192.092790	4.18 per formula unit
2	$Sc_{0.25}Ni_{0.75}O$	Ferromagnetic	-22511.365266	8.66 per super cell
		Non-magnetic	-22511.303596	8.58 per super cell

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3.2 Band structure and density of states (DOS)

The host compound NiO appears to be metallic with the bands crossing the Fermi level (E_F) in both the spin up and spin down direction with the GGA calculation. The supercell was created using calculated lattice constant equal to 4.24Å for plotting the density of states and electronic band structure. Figure 3 shows the total spin density of states (TDOS) and partial spin density of states (PDOS) of the host compound NiO and Figure 4 shows the band structure of NiO which also confirms the metallic character of NiO. Partial dos of NiO show that contribution of oxygen (O) is responsible for making the host compound metallic. After replacing the Ni atoms with the Sc atoms this metallic property of NiO changes and the new doped compound $Sc_{0.25}Ni_{0.75}O$ show half-metallic property.

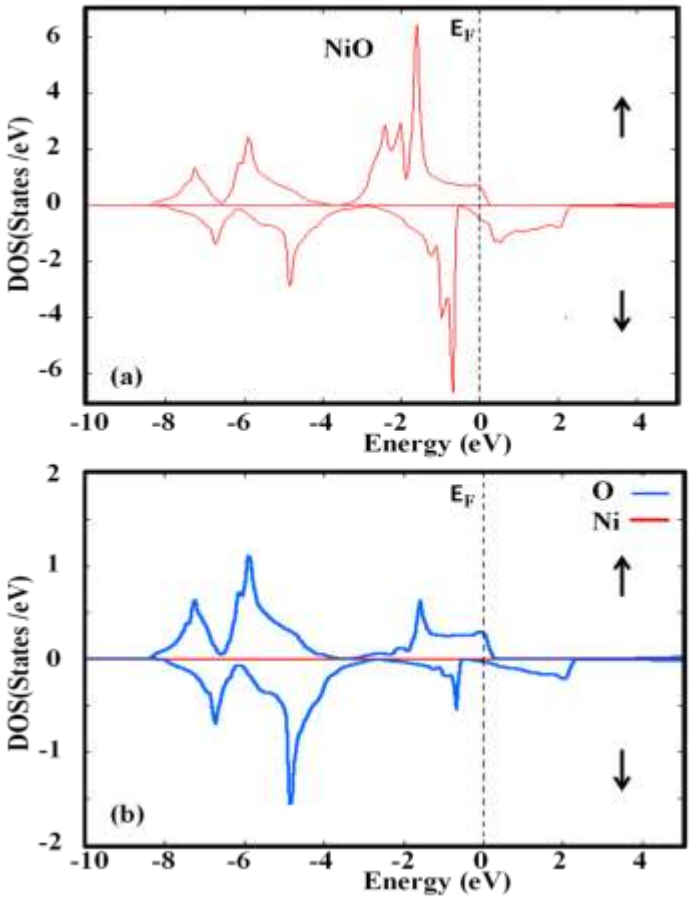

Fig. 3 (a)Total DOS of NiO and (b) Partial DOS of NiO

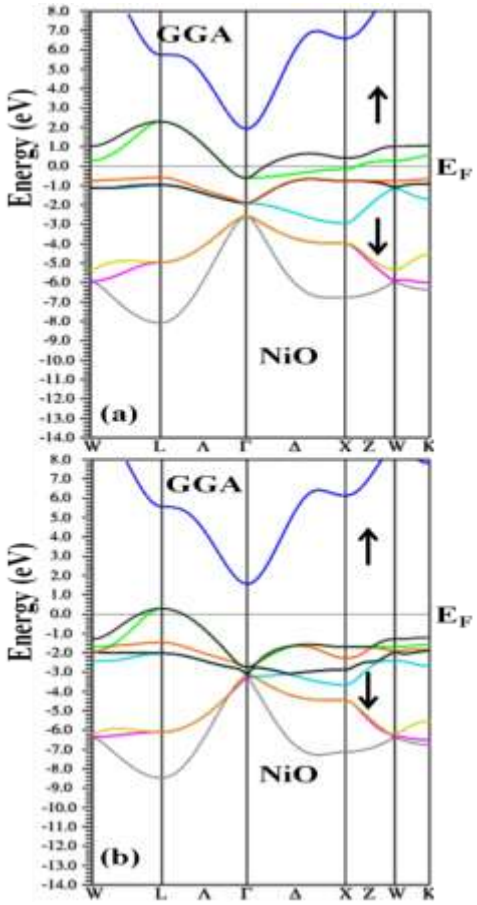

Fig. 4 Bandstructure of NiO

Figure 5 shows the total spin density of states (TDOS) and partial spin density of states (PDOS) of the resulting compound $Sc_{0.25}Ni_{0.75}O$ and Figure 6 shows the band structure of the compound $Sc_{0.25}Ni_{0.75}O$. In the spin up direction, the Sc-3d orbitals hybridize with the Ni-3d orbitals and O-2p orbitals. Due to the hybridization, the 3d-bands of Sc are pushed across the Fermi level and form a band gap in spin up direction. The band gap is equal to

1.13 eV which is measured between the conduction and valence band at the Γ point. The band gap is evidenced in both Total DOS and bandstructure of the resulting compound. Hence, the compound $Sc_{0.25}Ni_{0.75}O$ in spin up direction exhibits the semiconductor character. The partial spin density of states shows that there is the contribution of all the three elements in creating a band gap at Fermi level but more contribution is of doping atom Sc.

In the spin-down direction of the compound $Sc_{0.25}Ni_{0.75}O$, there is a weak hybridization between the orbitals of Sc-3d, Ni-3d, and O-2p. So, the bands Sc-3d, Ni-3d and O-2p disperse linearly across the Fermi level which shows the metallic character. Therefore, the compound $Sc_{0.25}Ni_{0.75}O$ exhibits semiconducting character in spin up direction and conducting in spin down direction and hence half-metallic ferromagnetism is predicted in this compound.

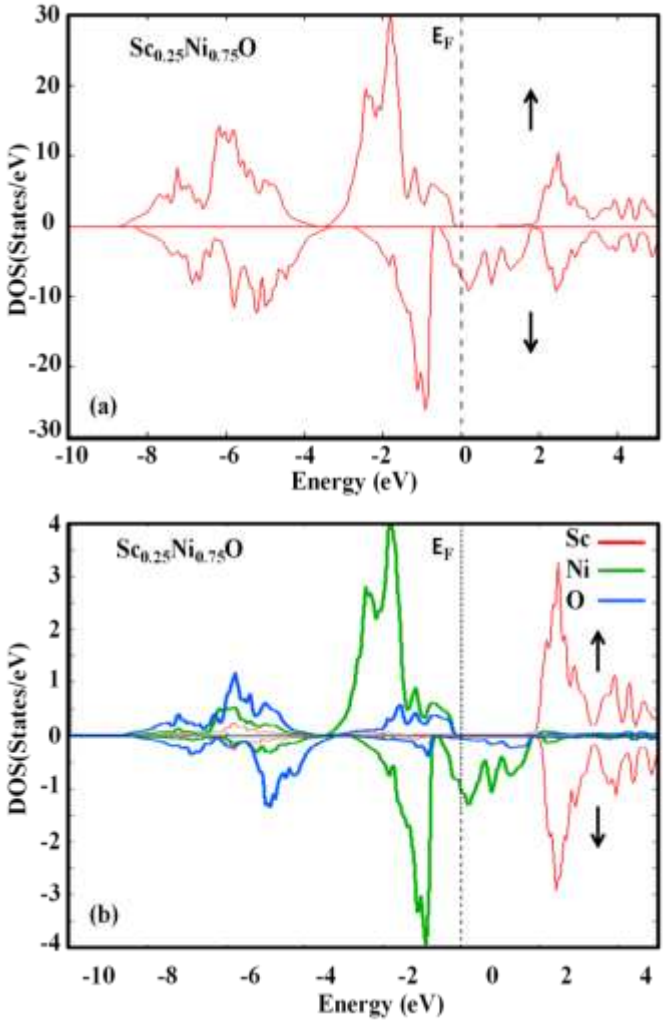

Fig. 5 (a) Total DOS of $Sc_{0.25}Ni_{0.75}O$ and (b) Partial dos of $Sc_{0.25}Ni_{0.75}O$

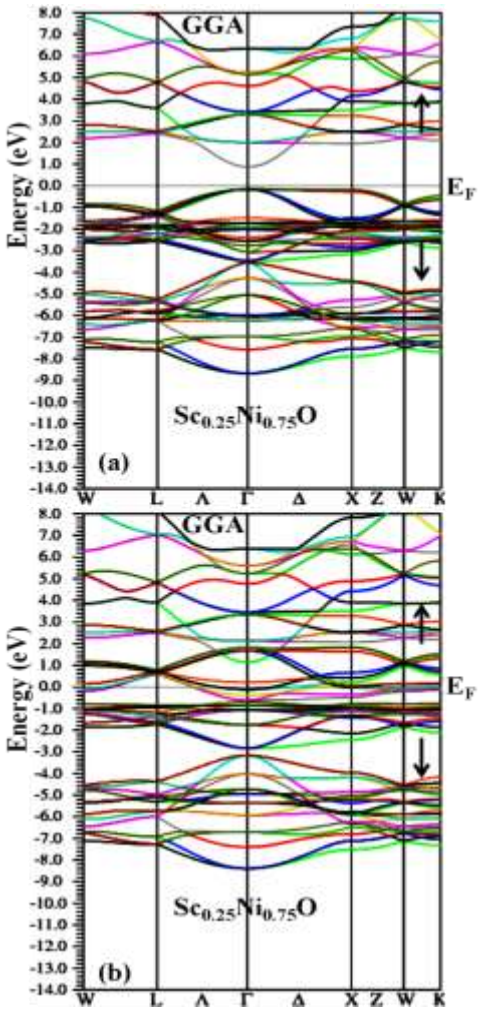

Fig.6 Bandstructure of $Sc_{0.25}Ni_{0.75}O$

IV MAGNETIC PROPERTIES

The magnetic moment of the compound $Sc_{0.25}Ni_{0.75}O$ is given in Table 2. The spinning of electrons creates the spin magnetic moment in the supercell. The total spin magnetic moment in the supercell is equal to 10.00616 μ_B. The Sc-3d transition metal atoms have less contribution in creating the magnetism in the supercell but Ni 3d transition metal atoms have a great influence in creating the magnetic moment in the supercell. Also, the O atoms are creating a more magnetic moment as compared to doping atoms Sc but less than Ni atoms. So, the maximum magnetic moment produced in the supercell is due to the Ni and O atoms. The valence electrons have the capability to induce the magnetic moment in the supercell.

Table 2. Spin Magnetic Moment of supercell

Atoms in Supercell	**$Sc_{0.25}Ni_{0.75}O$ (μ_B)**
Interstitial	0.06401
Sc1	-0.02626
Sc2	-0.02626
Ni3	1.39396
Ni4	1.39399
Ni5	1.39170
Ni6	1.39130
Ni7	1.39165
Ni8	1.39147
O9	0.29958
O10	0.29958
O11	0.17348
O12	0.17348
O13	0.17359
O14	0.17359
O15	0.17366
O16	0.17366
Total Spin Magnetic Moment	**10.00616**

V. CONCLUSION

Half-metallic property of Sc doped in NiO was investigated using the full potential linearised augmented plane wave plus local method and GGA method. In this work electronic, structural and magnetic properties were studied. The total density of states (TDOS) and band structure of the compound $Sc_{0.25}Ni_{0.75}O$ show that it exhibits half-metallic ferromagnetism. The total density of states and band structure of the compound $Sc_{0.25}Ni_{0.75}O$ shows it clearly that the band gap is visible in spin up direction and no gap in spin down direction. The compound is more stable in ferromagnetic phase which was observed after volume optimization. It has been found that the total magnetic moment of the supercell is $10.00616\mu_B$ and the compound has 100% spin polarization. So, the present work has a good advantage in using spintronics applications.

VI ACKNOWLEDGMENTS

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REFERENCES

[1.] Terakura, K., T. Oguchi, A. R. Williams, and J. Kübler. "Band theory of insulating transition-metal monoxides: Band-structure calculations." *Physical Review B* 30, no. 8 (1984): 4734.

[2.] Shen, Z-X., R. S. List, D. S. Dessau, B. O. Wells, O. Jepsen, A. J. Arko, R. Barttlet et al. "Electronic structure of NiO: Correlation and band effects." *Physical Review B* 44, no. 8 (1991): 3604.

[3.] Bengone, O., M. Alouani, P. Blöchl, and J. Hugel. "Implementation of the projector augmented-wave LDA+ U method: Application to the electronic structure of NiO." *Physical Review B* 62, no. 24 (2000): 16392.

[4.] Mi, Wenbo, Hua Yang, Yingchun Cheng, and Haili Bai. "Ferromagnetic half-metallic characteristic in bulk Ni0. 5M0. 5O (M= Cu, Zn and Cd): A GGA+ U study." *Solid State Communications* 152, no. 13 (2012): 1108-1111.

[5.] De Groot, R. A., F. M. Mueller, P. G. Van Engen, and K. H. J. Buschow. "New class of materials: half-metallic ferromagnets." *Physical Review Letters* 50, no. 25 (1983): 2024.

[6.] De Groot, R. A., F. M. Mueller, P. G. Van Engen, and K. H. J. Buschow. "Half-metallic ferromagnets and their magneto-optical properties." *Journal of applied physics* 55, no. 6 (1984): 2151-2154.

[7.] Li, Ai-Yu, Xiao-Dan Li, Qiu-Bao Lin, Shun-Qing Wu, and Zi-Zhong Zhu. "Half-metallic ferromagnetism in Ag-doped ZnO: An ab initio study." *Solid State Sciences* 14, no. 7 (2012): 769-772.

[8.] Lewis, Steven P., Philip B. Allen, and Taizo Sasaki. "Band structure and transport properties of CrO 2." *Physical Review B* 55, no. 16 (1997): 10253.

[9.] Li, Ai-Yu, Xiao-Dan Li, Qiu-Bao Lin, Shun-Qing Wu, and Zi-Zhong Zhu. "Half-metallic ferromagnetism in Ag-doped ZnO: An ab initio study." *Solid State Sciences* 14, no. 7 (2012): 769-772.

[10.] Li, Yujie, Fan Yang, and Ying Yu. "LSDA+ U study on the electronic and anti-ferromagnetic properties of Ni-doped CuO and Cu-doped NiO." *Chinese Journal of Catalysis* 38, no. 5 (2017): 767-773.

[11.] Hohenberg, Pierre, and Walter Kohn. "Inhomogeneous electron gas." *Physical review* 136, no. 3B (1964): B864.

[12.] Kohn, Walter, and Lu Jeu Sham. "Self-consistent equations including exchange and correlation effects." *Physical review* 140, no. 4A (1965): A1133.

[13.] Blaha, P. "k. Schwarz, GKH Madsen, D. Kvasnicka, J. Luitz." *Wien2k An Augmented Plane Wave Plus Local Orbital Program for Calculating the Crystal Properties, Vienna University of Technology, Austria* (2001).

[14.] Schwarz, Karlheinz, Peter Blaha, and Georg KH Madsen. "Electronic structure calculations of solids using the WIEN2k package for material sciences." *Computer Physics Communications* 147, no. 1-2 (2002): 71-76

[15.] Perdew, John P., Kieron Burke, and Matthias Ernzerhof. "Generalized gradient approximation made simple." *Physical review letters* 77, no. 18 (1996): 3865.

[16.] Perdew, John P., and Yue Wang. "Accurate and simple analytic representation of the electron-gas correlation energy." *Physical Review B* 45, no. 23 (1992): 13244.

[17.] Cinquini, Fabrizio, Livia Giordano, Gianfranco Pacchioni, Anna Maria Ferrari, Cesare Pisani, and Carla Roetti. "Electronic structure of Ni O⁄ Ag (100) thin films from DFT+ U and hybrid functional DFT approaches." *Physical Review B* 74, no. 16 (2006): 165403.

[18.] Bredow, Thomas, and Andrea R. Gerson. "Effect of exchange and correlation on bulk properties of MgO, NiO, and CoO." *Physical Review B* 61, no. 8 (2000): 5194.

[19.] Floris, Andrea, Stefano de Gironcoli, E. K. U. Gross, and Matteo Cococcioni. "Vibrational properties of MnO and NiO from DFT+ U-based density functional perturbation theory." *Physical Review B* 84, no. 16 (2011): 161102.

[20.] Rohrbach, A., and J. Hafner. "Molecular adsorption of NO on NiO (100): DFT and DFT+ U calculations." *Physical Review B*71, no. 4 (2005): 045405.