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RESEARCH ARTICLE

Deciphering the evolution of electronic and magnetic properties in alkali doped nickel oxide: An In-silico approach

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ABSTRACT: In this study, we employed the DFT+U method to systematically explore the electronic, and magnetic properties of nickel oxide doped with alkali metal atoms (Li, Na, K). The Hubbard potential-U was judiciously applied to all doped compound resulting from alkali doping, and were found to exhibited half-metallic properties. A noteworthy observation was the half-metallic band gap in the spin-down channel, which exhibited a linear variation with the increasing value of the Hubbard potential. Furthermore, the total magnetic moment was discernible in the supercells, with all supercells demonstrating 100% spin polarization at the Fermi level. Consequently, the findings from this study hold significant potential for applications in spintronics, thereby paving the way for future research in this domain.

Keywords: DFT+U calculations, NiO, Alkali metals, Electronic and magnetic properties, Half-Metallic

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1. INTRODUCTION

Spintronics, or spin electronics, represents a promising frontier in the realm of information technology, offering potential advancements in data storage, processing, and transfer. Unlike traditional electronics that rely solely on the charge of electrons, spintronics exploits both the charge and the intrinsic spin of electrons to encode and process information [1, 2]. The electron spin, which can adopt one of two states - up or down, serves as a binary data carrier, thereby doubling the data capacity compared to conventional electronics. This unique property of electron spin has opened up new avenues for the development of high-speed, low-power, and non-volatile memory devices. Moreover, the advent of spin-polarized currents, where the majority of electrons share the same spin state, has led to the discovery of phenomena such as Giant Magnetoresistance (GMR) and Tunnel Magnetoresistance (TMR). These phenomena have revolutionized the field of data storage, leading to the development of high-density hard drives and non-volatile magnetic random-access memory (MRAM).

The injection of spin polarized electrons plays a key role in spintronics. The discovery of half-metallic materials has led to a significant enhancement in spin current, surpassing that induced by the injection of spin from ferromagnetic material to semiconductor [3-7]. The inception of half-metallicity was first reported in Heusler alloys by De Groot et al. in 1983 [6], and subsequent studies have predicted the emergence of half-metallic ferromagnetism in transition metal oxides, nitrides, and phosphides [8-15].

Certain oxides such as NiO, MnO, FeO, and CoO, traditionally classified as wide band gap antiferromagnetic insulators, have been reported to exhibit metallic or semiconducting behavior under the density functional theory with local spin density approximations (DFT-LSDA) [16-20]. This discrepancy is attributed to the strong correlation effects that disrupt the accurate description of the electronic properties of these compounds. To address this issue, the Mott-Hubbard model has been implemented, providing a more robust description of these correlation effects [21].

Nickel oxide (NiO) has been reported to exhibit half-metallic behavior in both wurtzite (w-NiO) and zinc blende

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structures [10, 22, 23]. Studies by R. Long et al. have demonstrated that NiO doped with carbon and nitrogen exhibits enhanced photo-catalytic efficiency, as determined by first-principles calculations [24]. Further research has indicated that doping transition metals in NiO predicts half-metallic ferromagnetism, as evidenced by DFT calculations [25-27]. Optical properties of these doped materials have also been explored [28]. Experimental studies by G. Bharathy et al. have observed the emergence of ferromagnetism in pure NiO and Co-doped NiO, synthesized using the sol-gel technique [29]. These magnetic properties were found to increase gradually with the concentration of the dopant. Comprehensive investigations into the electrical, structural, and optical properties of Na and K-doped NiO films have also been reported [30-31].

In the current research endeavor, alkali metals (Li, Na, and K) were doped into a wide band gap NiO semiconductor, where the concentration of dopant is 12.5%. The GGA+U method was employed to investigate the electronic and magnetic properties of these doped compounds. Notably, all the doped compounds exhibited half-metallic properties, underscoring their potential for further exploration in spintronics applications via experimental approaches. Monoxide.

2. COMPUTATIONAL APPROACH

We have used WIEN2k [32-34] code to conduct an in-depth analysis of the electronic and magnetic properties of alkali doped NiO. The Full Potential Linearized Augmented Plane Wave (FPLAPW) method was utilized within the framework of Density Functional Theory (DFT) [35-37]. The Generalized Gradient Approximation (GGA) method, proposed by Perdew et al. was employed for the treatment of exchange and correlation potentials [38-39] to account for the exchange and coulombic interactions of the electrons. Hubbard Model was employed into our methodology to account for the on-site coulomb interactions of d-orbitals. The Hubbard Model method has been recognized as one of the most accurate methods for the calculation of electronic structure and magnetic properties. In FPLAPW method, the Kohn-Sham orbitals are expanded in atomic orbitals inside the Muffin-Tin (MT) spheres and plane waves in the interstitial region [40, 41]. The core and valence states were differentiated by an energy cut-off of -6 Ry. The host compound (NiO) which is stable in a cubic rock salt structure with space group Fm-3m (225), was doped with alkali atoms (Li, Na, and K) to study the electronic structure and magnetic properties. Using a lattice constant equal to 4.22 Å, a supercell Ni_8O_8 of 16 atoms was created. Doped supercells were generated by replacing Ni atom with alkali metal atom. The Hubbard potential was applied to all the supercells to account for the strong correlation effect. The iterative process was deemed complete when the energy converged and reached a threshold of 10^{-4} Ry. This rigorous approach ensures the reliability and accuracy of our findings.

3. RESULTS AND DISCUSSION

3.1. Structural Properties

Fig. 1 shows the crystal structure of bulk NiO and alkali doped compound in the supercell configuration. We first computed the lattice constant of bulk NiO with Hubbard potential. The calculated lattice constant is 4.22 Å, which is comparable to the measured value 4.17 Å [43], showing agreement with the experimental results. In order to find the effect of alkali metal doping on the bulk NiO, we constructed a 2x2x2 super cell from the primitive bulk cell. The supercell has 16 atoms (8 Ni and 8 O), and was used for all subsequent calculations. To create a doped structure, one of the Ni atoms was replaced by the alkali metal (yellow ball in Fig. 1(b)). The lattice parameter of the supercell used in the calculations was 8.373 Å. The resulted doped structure was then relaxed to ground state by minimizing the energy for electronic structure and magnetic calculations as will be discussed in the coming sections.

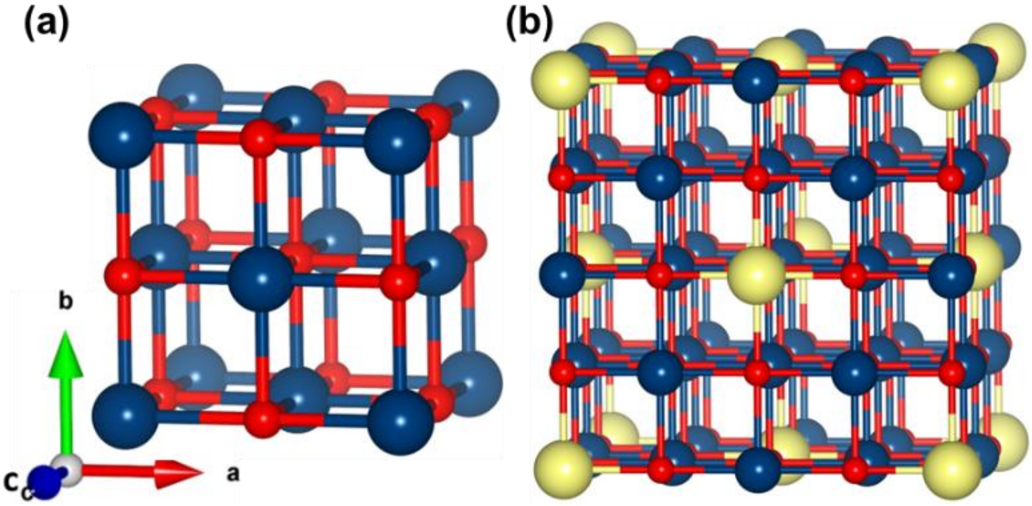

Fig. 1. Optimized crystal structures of (a) pristine, and (b) alkali doped bulk NiO. The atomic color code is as: Oxygen:Red, Ni:Teal and alkali metal:Yellow.

3.2. Electronic Properties

3.2.1. Band Structure and Density of States

The Fig. 2(a) shows the density of states (DOS) of pristine NiO calculated using GGA+U method. The pristine NiO is a wide band gap semiconductor and exhibits anti-ferromagnetic behavior. The band gap of NiO was calculated 3.0 eV as shown in Fig. 2(a), which is consistent with the value as reported by Ru-song Li et al. [19]. This wide band gap semiconductor character of NiO is changed into half-metallic with doping of alkali metal atoms. The Pristine NiO was doped with alkali metal atoms (Li, Na, K) to envisage to tailor its electronic and magnetic behavior in the doped configuration. The doping was performed by replacing one of the alkali metals one by one in the supercell (2x2x2) of NiO making doping concentration of 12.5%. Thereafter, to investigate the effect of the Hubbard potential on the electronic band gap of doped compounds, different U values were considered. Fig. (3, 4, and 5) shows the total DOS, partial DOS (PDOS) and band structure of the doped supercells. It is found that the doped compounds display half-metallic band gap in spin up channel. Half-metallic band gaps were seen increasing gradually as U value increases up to 6 eV, and then it saturates as shown in Fig. 2(b). The calculated band gaps at different U values for different compounds are shown in Table 1.

Partial DOS of each supercell predicts the orbital contribution to the band edges. Fig. 3 shows the total DOS, PDOS and band structure of Li-doped NiO. For each compound, we found that Li doping changes the electronic nature of NiO from wide band gap semiconductor to to the desired half metallic behavior. It is apparent from Fig. 3 that Li-doped NiO exhibits metallic behavior for spin-up electrons and semiconducting nature for spin-down electrons. Na and K doped NiO show a similar variation of band gap as a function of U value (see Fig. 4 and 5). It is important to note the PDOS shows here that this behavior is seen for U values up to 5 eV for Li and Na doped NiO. When U is 6 and 7 eV, the band gap opens for both spin up and down channels and the compound no longer remains half-metallic. This discrepancy arises due to the fact that to obtain PDOS, a projection on spherical harmonics on TDOS is done. In this procedure, one loses part of the information. So, the sum of the parts of PDOS is lower than the total DOS, which contains the essential information. Thus, total DOS band gaps are more reliable and are chiefly considered here. From PDOS, we found that chiefly Ni-d orbitals contribute to band edge in spin-down channel with a small contribution of O-p orbitals to the conduction band. On the other hand, O-p orbitals show a significant contribution to the valence band of spin-up electrons. The dopant bands (Li-s) have no contribution to the band edges, only Ni-d and O-p bands are visible at the Fermi level of each and every Li-doped NiO for different U values. Ni-d orbitals and O-p orbitals hybridize each other in spin up channel and cross the Fermi level but they push each other at Fermi level in spin down channel and give rise a band gap in spin down channel. This varying character of band gaps predicts direct dependency on the applied Hubbard potential up to a specific range. Different dopants show different band gaps but the variation for all is linear up to U = 6 eV (Fig 2(b)) after that the linear increase stops and the gap remains constant.

3.3. Effect of U-term on band gap and magnetic moment

The alkali metal atoms were doped in place of Ni 3d transition metal atom in NiO to examine their effect on electronic and magnetic properties. Hubbard potential was applied only to Ni atoms for correlation effect because Ni is 3d transition metal. In Fig. 2(b), a relationship between band gap and Hubbard potential of doped supercells is shown. An increment in band gap is noticed with applied Hubbard potential up to U = 6 eV and then curves show saturation behavior. In the first compound $Li_{0.125}Ni_{0.875}O$, when U=1eV the value of band gap is 0.5 eV and magnetic moment of dopant Li is 0.013 μ_B.

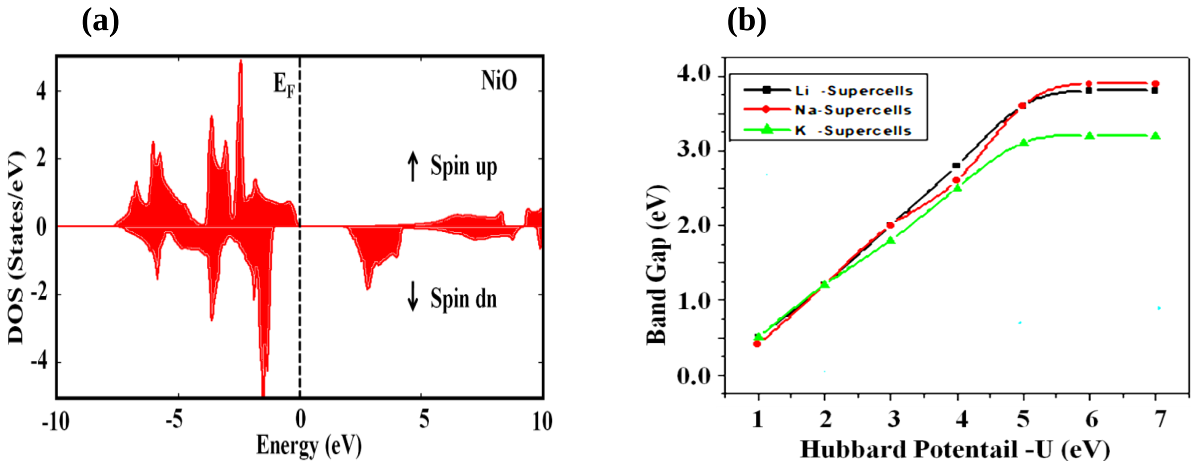

Fig. 2. (a) The spin-polarized total DOS of NiO compound, vertical dashed line represents the Fermi level. (b) Effect of Hubbard potential (U) on band gap for Li, Na and K doped NiO.

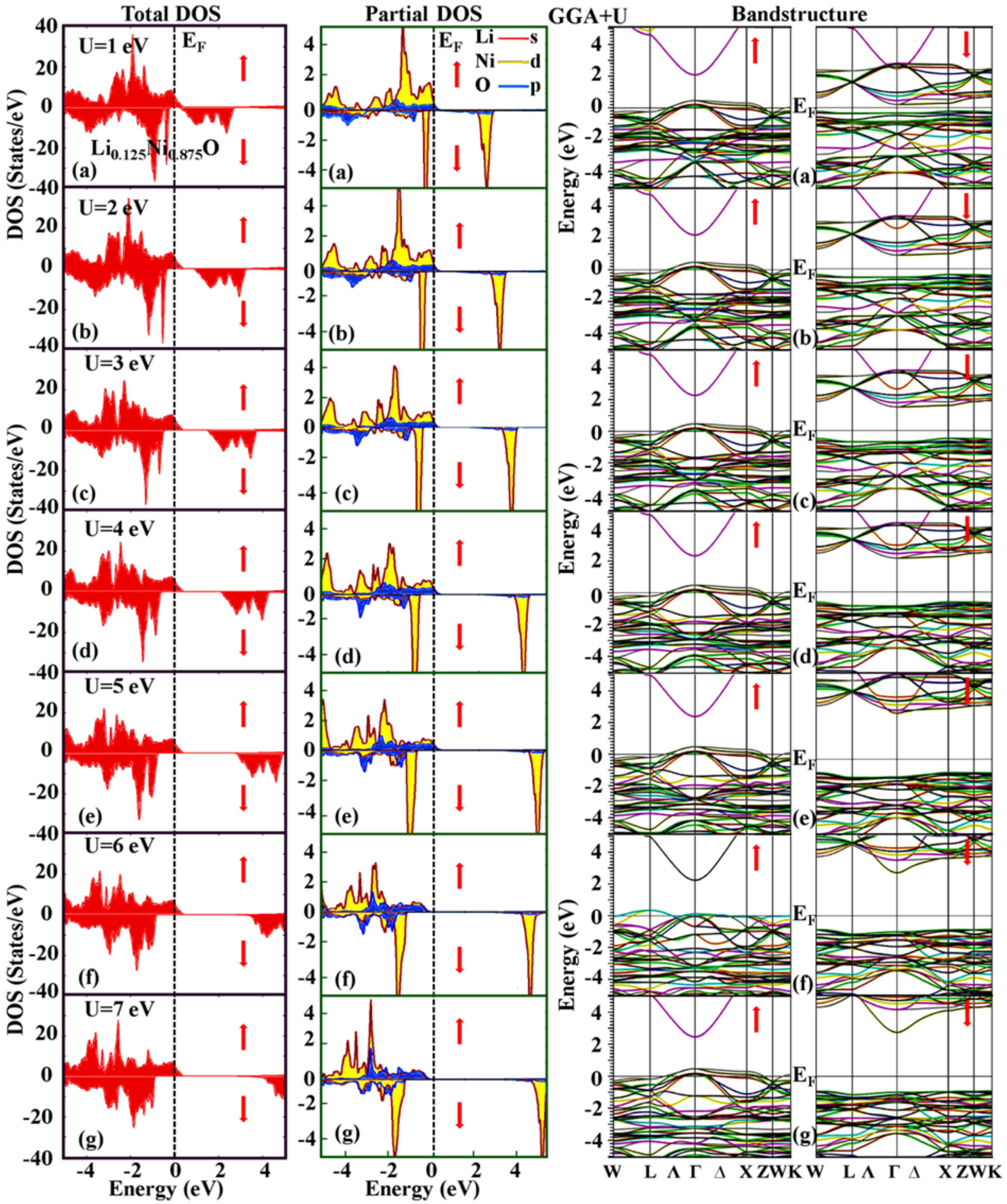

Fig. 3. The total DOS, Partial DOS and Band structure of Li Doped NiO compounds for different U values. In these subplots, up and down arrows indicates the spin-up and spin down electron.

For U = 2 eV, the value of band gap is increased to 1.2 eV but the value of magnetic moment of Li decreased to 0.012 μB. A linear progression has been seen in band gap up to U = 6 eV but in magnetic moment a reversal is observed. In other compounds like $Na_{0.125}Ni_{0.875}O$ and $K_{0.125}Ni_{0.875}O$ same trend is observed in band gap and also in magnetic moment of dopants with respect to Hubbard potential as depicted in Table 1. This predicts a relationship of Hubbard potential with band gaps and magnetic moment of dopants. In general, all the compounds doped with alkali metal atoms exhibit a linear relationship between their band gaps and Hubbard potential. Also, a linear variation in magnetic moment values of dopants was found with respect to Hubbard potential.

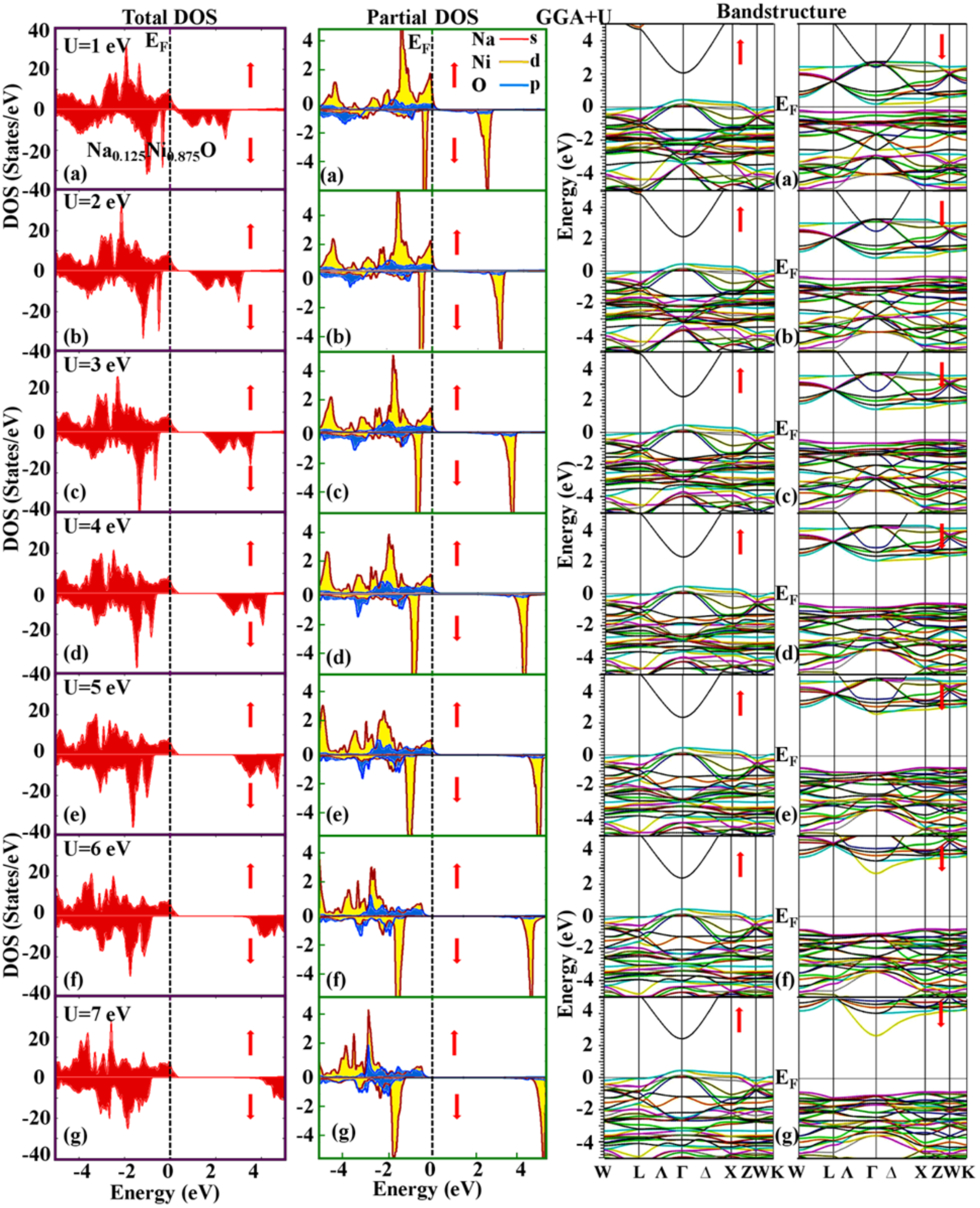

Fig. 4. The total DOS, Partial DOS and Band structure of Na-doped NiO compounds for different U values. In these subplots, up and down arrows indicates the spin-up and spin down electron.

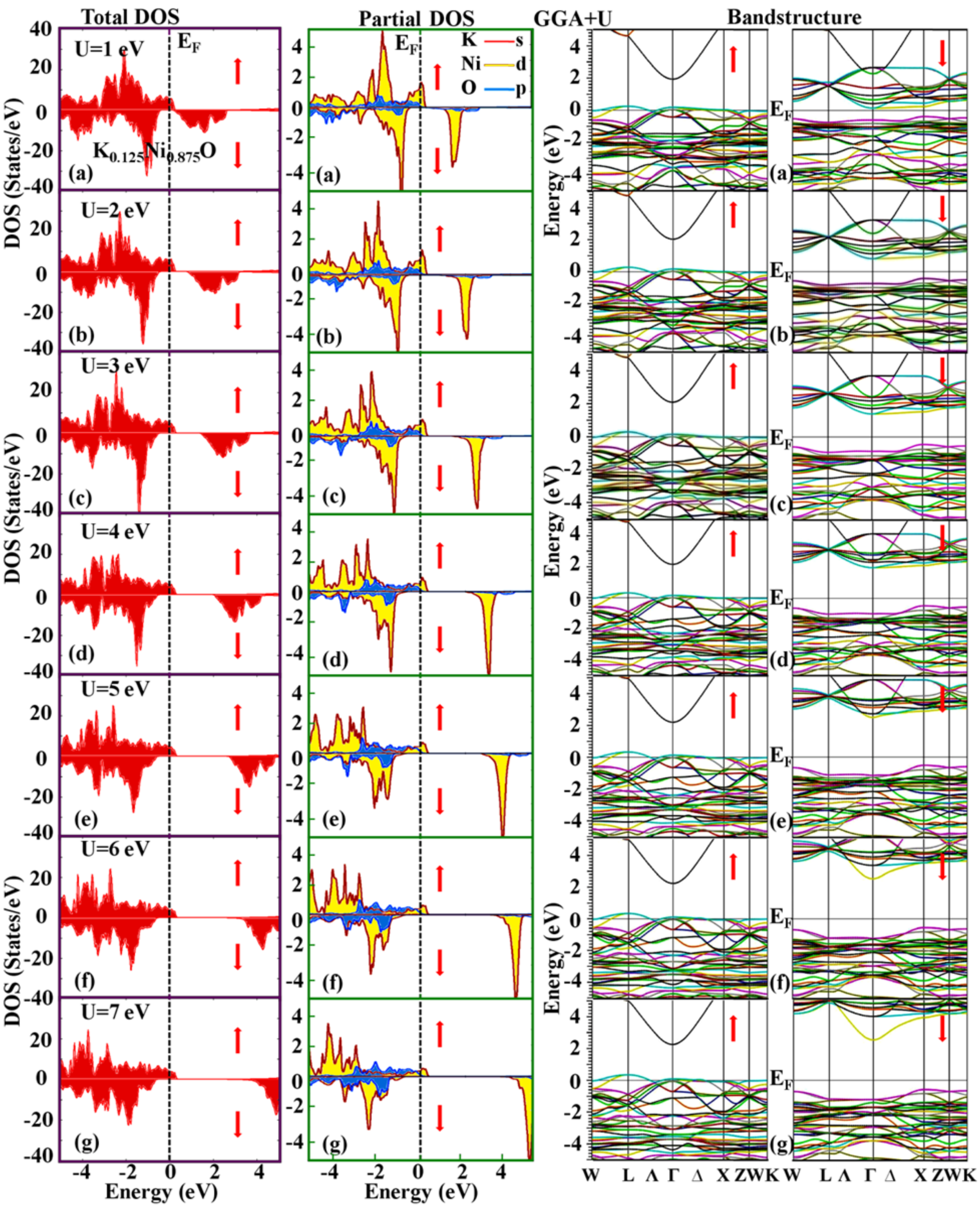

Fig. 5. The total DOS, Partial DOS and Band structure of K-doped NiO compounds for different U values. In these subplots, up and down arrows indicates the spin-up and spin down electron.

3.4 Magnetic properties

The calculations were based on the GGA+U method which predicts the magnetic moment in ground state of the $X_{0.125}Ni_{0.875}O$ (X = Li, Na and K) compounds. The total magnetic moment of the supercells is shown in Table 1. Nickel and oxygen atoms are the main source for spin magnetic moment in the supercells. It is noticed that dopants like Li and Na contain positive values but K dopant contain negative value of magnetic moment in a super cell.

Interesting evidence has been observed that with increasing Hubbard potential magnetic moment of Ni atoms increases but for O atoms and dopant atoms was seen decreasing. The electronic configuration of all participating elements in supercells is as Ni-($1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^8$), O-($1s^2\ 2s^2\ 2p^4$), Li-($1s^2 2s^1$), Na-($1s^2 2s^2 2p^6 3s^1$), and K-($1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$). An electronic configuration provides the valence electrons of the elements. Those valence electrons originate the magnetic moment in the supercells.

3.5. Half-metallicity with 100% spin polarization

Half-metallicity is the property of a compound to exhibit metallic and semiconducting /insulator behaviors in their respective spins (spin up and spin down). The DOS and band structures of all the supercells exhibit a band gap at Fermi level in spin down channel which evidences the half-metallicity. Half-metallic devices work on spin of the electron due to which they are more efficient. To understand the spin of an electron in half-metals spin polarization is the property that explains it. So, spin polarization can be measured by using the below formula to explain the half-metallicity of the compounds [42].

$$P_s = \frac{n(E_F)\uparrow\ -\ n(E_F)\downarrow}{n(E_F)\uparrow\ +\ n(E_F)\downarrow}$$

According to the above formula the spin polarization (Ps) is the difference of electronic states in numerator and addition of electronic states in denominator of both the spins.

Table 1: Hubbard potential U (eV), Band gap (eV) and Total spin magnetic moment (in μB unit) of the alkali doped NiO.

Supercell	**Hubbard potential (U)**	**Band Gap**	**Mag. moment**			**Interstitial mag. moment**	**Total spin mag. moment**
			Li/Na/K	**Ni**	**O**		
Li$_{0.125}$Ni$_{0.875}$O	1	0.5	0.013	10.974	1.8	0.214	13.001
	2	1.2	0.012	11.385	1.401	0.203	13.001
	3	2.0	0.011	11.699	1.096	0.194	13.001
	4	2.8	0.011	11.975	0.823	0.192	13.001
	5	3.6	0.01	12.24	0.558	0.19	12.998
	6	3.8	0.009	12.439	0.36	0.19	12.998
	7	3.8	0.008	12.608	0.189	0.194	13
Na$_{0.125}$Ni$_{0.875}$O	1	0.4	0.009	10.955	1.827	0.208	12.999
	2	1.2	0.008	11.371	1.423	0.199	13
	3	2.0	0.007	11.668	1.136	0.191	13.002
	4	2.6	0.006	11.966	0.843	0.186	13.001
	5	3.6	0.006	12.235	0.575	0.185	13
	6	3.9	0.005	12.435	0.374	0.185	12.999
	7	3.9	0.005	12.604	0.204	0.187	13
K$_{0.125}$Ni$_{0.875}$O	1	0.5	-0.005	10.915	1.904	0.186	13
	2	1.2	-0.018	11.351	1.491	0.177	13.001
	3	1.8	-0.029	11.694	1.166	0.17	13
	4	2.5	-0.039	11.995	0.876	0.166	12.999
	5	3.1	-0.048	12.287	0.594	0.167	13
	6	3.2	-0.055	12.499	0.388	0.168	13.001
	7	3.2	-0.06	12.676	0.213	0.172	13

Spin polarization of all the supercells were measured and found 100%. Therefore, all supercells Ni0.875OX0.125 (X=Li, Na and K) are exhibiting half-metallicity with 100% spin polarization and can be applicable for spintronics.

4. CONCLUSION

The DFT+U method was applied to calculate the electronic, magnetic and half-metallic properties of NiO doped with alkali metal atoms (Li, Na, K) within the treatment of full potential linearized augmented plane wave approach. The host compound (NiO) was doped by Li/Na/K with 12.5 percent of concentration. Total DOS and band structure plots of the compounds $X_{0.125}Ni_{0.875}O$ (X = Li, Na, K) display half-metallic character. The half–metallic gap was seen in spin down channel. This band gap shows a linear variation with application of U values. Also, the magnetic moment of dopants decreases by increasing the value of U. Spin polarization was measured and found 100% for all half-metallic compounds. Therefore, the proposed compounds can be useful for future investigations. Hubbard potential U was applied with energy range 1eV to 7eV to all supercells doped by Li/Na/K.

CONFLICT OF INTEREST

The authors declare that there is no conflict of interests.

REFERENCES

[1] Wolf, S.A., Awschalom, D.D., Buhrman, R.A., Daughton, J.M., von Molnár, V.S., Roukes, M.L., Chtchelkanova, A.Y. and Treger, D.M., 2001. Spintronics: a spin-based electronics vision for the future. *Science*, *294*(5546), pp.1488-1495.

[2] Li, X. and Yang, J., 2016. First-principles design of spintronics materials. *National Science Review*, *3*(3), pp.365-381.

[3] Zhu, H.J., Ramsteiner, M., Kostial, H., Wassermeier, M., Schönherr, H.P. and Ploog, K.H., 2001. Room-temperature spin injection from Fe into GaAs. *Physical Review Letters*, *87*(1), p.016601.

[4] Schmidt, G., Ferrand, D., Molenkamp, L. W., Filip, A. T. and Wees, B. J. V. 2000. Fundamental obstacle for electrical spin injection from a ferromagnetic metal into a diffusive semiconductor. *Physical Review B*, 62(8), pp. R4790 - R4793.

[5] Galanakis, I., Dederichs, P.H. and Papanikolaou, N., 2002. Slater-Pauling behavior and origin of the half-metallicity of the full-Heusler alloys. *Physical Review B*, *66*(17), p.174429.

[6] De Groot, R.A., Mueller, F.M., van Engen, P.V. and Buschow, K.H.J., 1983. New class of materials: half-metallic ferromagnets. *Physical Review Letters*, *50*(25), p.2024.

[7] Kervan, N. and Kervan, S., 2013. Half-metallic properties in the Fe_2TiP full-Heusler compound. *Intermetallics*, *37*, pp.88-91.

[8] Lewis, S.P., Allen, P.B. and Sasaki, T., 1997. Band structure and transport properties of CrO_2. *Physical Review B*, *55*(16), p.10253.

[9] Li, A.Y., Li, X.D., Lin, Q.B., Wu, S.Q. and Zhu, Z.Z., 2012. Half-metallic ferromagnetism in Ag-doped ZnO: an ab initio study. *Solid State Sciences*, *14*(7), pp.769-772.

[10] Chen, Z., Miao, L. and Miao, X., 2011. Half-metallicity of wurtzite NiO and w-NiO/ZnO (0001) interface: First principles simulation. *AIP Advances*, *1*(2), p. 022124.

[11] Liu, J., Wang, X.Q., Liu, Y. and Dong, H.N., 2007. First principle calculation of electric and magnetic properties for new half-metal Fe_2ScO_4. *Chinese Journal of Chemical Physics*, *20*(3), p.291.

[12] Coey, J.M.D. and Chien, C.L., 2003. Half-metallic ferromagnetic oxides. *MRS Bulletin*, *28*(10), pp.720-724.

[13] Houari, A., Matar, S.F. and Eyert, V., 2010. Semiconducting (half-metallic) ferromagnetism in Mn (Fe) substituted Pt and Pd nitrides. *Physical Review B*, *82*(24), p.241201.

[14] Sirajuddeen, M.M.S. and Banu, I.S., 2016. An ab initio study on electronic and magnetic properties of Cr, V doped Cd and Zn nitrides for spintronic applications. *Journal of Magnetism and Magnetic Materials*, *406*, pp.48-59.

[15] Zhang, W.B., Yu, N., Yu, W.Y. and Tang, B.Y., 2008. Stability and magnetism of vacancy in NiO: A GGA+ U study. *The European Physical Journal B*, *64*, pp.153-158.

[16] Terakura, K., Oguchi, T., Williams, A.R. and Kübler, J., 1984. Band theory of insulating transition-metal monoxides: Band-structure calculations. *Physical Review B*, *30*(8), p.4734.

[17] Bengone, O., Alouani, M., Blöchl, P. and Hugel, J., 2000. Implementation of the projector augmented-wave LDA+ U method: Application to the electronic structure of NiO. *Physical Review B*, *62*(24), p.16392.

[18] Messick, L., Walker, W.C. and Glosser, R., 1972. Direct and temperature-modulated reflectance spectra of MnO, CoO, and NiO. *Physical Review B*, *6*(10), p.3941.

[19] Li, R.S., Xin, D.Q., Huang, S.Q., Wang, Z.J., Huang, L. and Zhou, X.H., 2018. A full potential all-electron calculation on electronic structure of NiO. *Chinese Journal of Physics*, *56*(6), pp.2829-2836.

[20] Gillen, R. and Robertson, J., 2013. Accurate screened exchange band structures for the transition metal monoxides MnO, FeO, CoO and NiO. *Journal of Physics: Condensed Matter*, *25*(16), p.165502.

[21] Qin, M., Schäfer, T., Andergassen, S., Corboz, P. and Gull, E., 2022. The Hubbard model: A computational perspective. *Annual Review of Condensed Matter Physics*, *13*, pp.275-302.

[22] Wu, R.Q., Feng, Y.P., Ouyang, Y.F., Zhou, P. and Hu, C.H., 2008. Half-metallic NiO in zinc-blende structure from ab initio calculations. *Journal of Applied Physics*, *104*(4).

[23] 23. Xu, H.B., Fan, S.W., Yang, X.B., Pan, L.Q. and Yao, K.L., 2014. Bulk, surfaces and interfaces half-metallicity for zinc blende NiO: Modified Becke–Johnson potential investigation. *Japanese Journal of Applied Physics*, *53*(12), p.125801.

[24] Long, R., English, N.J. and Mooney, D.A., 2010. Electronic structures of N-and C-doped NiO from first-principles calculations. *Physics Letters A*, *374*(9), pp.1184-1187.

[25] Zhou, N., Cheng, Y., Huang, B. and Liao, X., 2019. Effect of nonmagnetic dopants (Ag, Cu or Mg) on ferromagnetic half-metallic properties of NiO. *Physica B: Condensed Matter*, *557*, pp.6-11.

[26] Mi, W., Yang, H., Cheng, Y. and Bai, H., 2012. Ferromagnetic half-metallic characteristic in bulk $Ni_{0.5}M_{0.5}O$ (M= Cu, Zn and Cd): A GGA+ U study. *Solid State Communications*, *152*(13), pp.1108-1111.

[27] Teli, N.A. and Sirajuddeen, M.M.S., 2019. Investigation of half-metallic ferromagnetism in hafnium and tantalum doped NiO for spintronic applications: a DFT study. *Current Applied Physics*, *19*(4), pp.357-362.

[28] Petersen, J.E., Twagirayezu, F., Scolfaro, L.M., Borges, P.D. and Geerts, W.J., 2017. Electronic and optical properties of antiferromagnetic iron doped NiO–A first principles study. *AIP Advances*, *7*(5), p. 055711.

[29] Bharathy, G. and Raji, P., 2018. Pseudocapacitance of Co doped NiO nanoparticles and its room temperature ferromagnetic behavior. *Physica B: Condensed Matter*, *530*, pp.75-81.

[30] Wang, N., Liu, C.Q., Wen, C.L.B., Wang, H.L., Liu, S.M., Jiang, W.W., Ding, W.Y. and Chai, W.P., 2016. Structural, electrical and optical properties of K-doped NiO films prepared by rapid pyrolysis sol-gel technique. *Thin Solid Films*, *616*, pp.587-593.

[31] Denny, Y.R., Lee, K., Park, C., Oh, S.K., Kang, H.J., Yang, D.S. and Seo, S., 2015. Electronic, electrical and optical properties of undoped and Na-doped NiO thin films. *Thin Solid Films*, *591*, pp.255-260.

[32] Blaha, P., Schwarz, K., Sorantin, P. and Trickey, S.B., 1990. Full-potential, linearized augmented plane wave programs for crystalline systems. *Computer Physics Communications*, *59*(2), pp.399-415.

[33] Schwarz, K., Blaha, P. and Madsen, G.K., 2002. Electronic structure calculations of solids using the WIEN2k package for material sciences. *Computer Physics Communications*, *147*(1-2), pp.71-76.

[34] Kohn, W. and Sham, L.J., 1965. Self-consistent equations including exchange and correlation effects. *Physical Review*, *140*(4A), p.A1133.

[35] Hohenberg, P. and Kohn, W., 1964. Inhomogeneous electron gas. *Physical Review*, *136*(3B), p.B864.

[36] Madsen, G.K., Blaha, P., Schwarz, K., Sjöstedt, E. and Nordström, L., 2001. Efficient linearization of the augmented plane-wave method. *Physical Review B*, *64*(19), p.195134.

[37] Wu, Z. and Cohen, R.E., 2006. More accurate generalized gradient approximation for solids. *Physical Review B*, *73*(23), p.235116.

[38] Perdew, J.P. and Zunger, A., 1981. Self-interaction correction to density-functional approximations for many-electron systems. *Physical Review B*, *23*(10), p.5048.

[39] Perdew, J.P., Burke, K. and Ernzerhof, M., 1996. Generalized gradient approximation made simple. *Physical Review Letters*, *77*(18), p.3865.

[40] Schwarz, K., 2003. DFT calculations of solids with LAPW and WIEN2k. *Journal of Solid State Chemistry*, *176*(2), pp.319-328.

[41] Gao, S., 2003. Linear-scaling parallelization of the WIEN package with MPI. *Computer Physics Communications*, *153*(2), pp.190-198.

[42] Sirajuddeen, M.M.S. and Banu, I.S., 2016. An ab initio study on electronic and magnetic properties of Cr, V doped Cd and Zn nitrides for spintronic applications. *Journal of Magnetism and Magnetic Materials*, *406*, pp.48-59.

[43] Sawatzky, G.A. and Allen, J.W., 1984. Magnitude and origin of the band gap in NiO. *Physical Review Letters*, *53*(24), p.2339.