ABSTRACT

In this work, the electronic band structure calculations of heavy rare earth nitrides (REN, RE=Tb, Dy, Ho, Er, Tm, Yb and Lu), Fe doped zirconium nitride (Zr\(_{1-x}\)Fe\(_x\)N), transition metal doped cadmium nitride (Cd\(_{1-x}\)M\(_x\)N, M=Fe, Mn) and transition metal doped zinc nitride (Zn\(_{1-x}\)M\(_x\)N, M=Cr, V) were carried out using the Full Potential Linearized Augmented Plane Wave (FP-LAPW) method. The electronic and magnetic properties were investigated for all the selected compounds. In addition, the thermal and mechanical properties have been determined for the heavy Rare Earth Nitrides (REN) and Fe-doped zirconium nitride. Half metallic ferromagnetism has been predicted for Fe, Mn, Cr and V doped cadmium and zinc nitrides.

The Full Potential Linearized Augmented Plane Wave (FP-LAPW) method has been used to study the electronic, magnetic, elastic, thermal and bonding properties of heavy rare earth nitrides REN(RE=Tb-Lu). The plots of band structure and Density Of States (DOS) have been obtained for these compounds and the results are compared. The magnetic moments for the heavy rare earth compounds have been calculated. Among the REN (TbN - LuN), TbN exhibits a high magnetic moment of 6.03 \(\mu_B\) while LuN shows a low magnetic moment value of 0.003 \(\mu_B\) indicating a decreasing trend in magnetic moments from TbN to LuN. The calculated values of elastic constant are in reasonable agreement with the elastic constant values reported in previous works.
It has been found that the values of Young's modulus increase with the decrease in lattice constants from TbN to LuN. The calculated Poisson's ratio for these compounds show that there is possibility of ionic nature in chemical bonding between RE and nitrogen ions. For the compound to exhibit ionic nature, the Poisson's ratio is equal to 0.25. But, for YbN and LuN, the Poisson's ratio is less than 0.25 and hence a decrease in ionicity (brittleness) is predicted. The charge density contours for RE nitrides were plotted and these plots were used to understand the trend in the obtained elastic constants. The ionic nature in these compounds is also substantiated by the appearance of spherical symmetry in the charge density plots of these compounds.

Full Potential- Linear Augmented Plane Wave (FP-LAPW) method has been employed to study the electronic, magnetic, elastic and thermal properties of Iron-doped Zirconium nitride. In this work, Fe-atoms were doped into the super cell of ZrN in doping concentrations of 12.5%, 25% and 37.5% to replace Zr atoms. The electronic and magnetic properties were studied for Fe doped ZrN compounds. The band structure and DOS of Fe-doped compounds were obtained. The charge density contours of the doped compounds have been plotted in this work. The charge density contours indicate the ionic nature for all the compounds. The obtained magnetic moments of the doped compounds were found to increase with increase in doping concentration of Fe. The elastic constants of doped ZrN have been calculated for various concentrations of Fe. After doping Fe in different concentrations, the hardness and elastic strength decrease for ZrN with increase in Fe concentration. It is found that brittleness of the compound increases with increase in doping concentration. The calculated Poisson’s ratio determined for the doped compounds also suggest the brittle nature of these compounds. ZrN has high Debye temperature which on doping, decreases significantly. Molar heat capacity has been calculated for these
compounds which is found to increase with increase in doping concentration of Fe.

The investigations on the half metallic ferromagnetic property for Fe(Mn) doped CdN and ZnN have been reported in this work. Fe and Mn atoms are substituted in CdN and ZnN replacing Cd and Zn atoms. The doping concentration of Fe(Mn) is 37.5% in the host compound. The volume and structural optimizations were achieved for the Fe and Mn doped CdN and ZnN compounds. The Fe doped compounds Cd\(_{0.625}\)Fe\(_{0.375}\)N and Zn\(_{0.625}\)Fe\(_{0.375}\)N exhibit energy gap in the spin up direction and in the spin down direction metallic nature is indicated. The Mn doped compound Cd\(_{0.625}\)Mn\(_{0.375}\)N does not exhibit any significant band gap in both the spins but Zn\(_{0.625}\)Mn\(_{0.375}\)N shows a small energy gap (0.3 eV) in spin down direction. The compounds, Cd\(_{0.625}\)Fe\(_{0.375}\)N and Cd\(_{0.625}\)Mn\(_{0.375}\)N produced spin polarization of 71.4% and 87%, respectively while Zn\(_{0.625}\)Fe\(_{0.375}\)N and Zn\(_{0.625}\)Mn\(_{0.375}\)N yielded 89% and 100%, respectively. The Fe and Mn doped CdN and ZnN compounds are found to exhibit magnetic ordering. The magnetic properties of doped compounds can be understood from the induced magnetic moments due to Fe and Mn doping. Thus, in this work, the compounds Cd\(_{0.625}\)Fe\(_{0.375}\)N, Zn\(_{0.625}\)Fe\(_{0.375}\)N and Zn\(_{0.625}\)Mn\(_{0.375}\)N are predicted to exhibit half metallic ferromagnetism.

Similarly, the half metallic ferromagnetic property of Cr, V doped CdN and ZnN have been investigated. In this work, the half metallic ferromagnetism is predicted in transition metal doped CdN and ZnN. Electronic structures were plotted for the doped compounds. The volume optimization was done for all the doped compounds Cd\(_{0.625}\)Cr\(_{0.375}\)N, Cd\(_{0.625}\)V\(_{0.375}\)N, Zn\(_{0.625}\)Cr\(_{0.375}\)N and Zn\(_{0.625}\)V\(_{0.375}\)N. The calculated total energies were fitted to Birch-Murnaghan equation of state to obtain the equilibrium lattice constants. The doped compounds exhibit magnetic
ordering. Band structure diagrams and density of states (DOS) have been plotted in GGA and GGA+U methods for the Cr-doped compounds and compared. The plots showed that Cr-doped compounds Cd$_{0.625}$Cr$_{0.375}$N and Zn$_{0.625}$Cr$_{0.375}$N exhibit band gap in down spin at a Hubbard potential (U = 6.0 eV). These two compounds also showed significant amount of spin polarization also. Vanadium doped compounds do not favour much for the half metallic ferromagnetism. Magnetic properties such as number of magnetic moments in terms of Bohr magneton are evaluated and found to increase with increasing values of U.