channel. The contributions of DOS for the half metalicity is in the order of $Mn_d > Fe_d > V_d$.

The electronic properties of FeMnVAl compound were also examined using mBJ and GGA+U techniques. Under the mBJ method and GGA+U method, the Fermi energy level seems more enhance and clear. The mBJ method revealed a clear energy gap around the Fermi level in the spin-up channel(0.605 eV), indicating semiconducting behavior, while the spin-down channel showed metallic characteristics (Fig. 4 a, b) . Similarly, the GGA+U method also demonstrated half-metallic behavior with 0.314 eV gap at spin up channel (Fig 5 a, b). Additionally, analysis of the density of states (DOS) plots corroborated these findings, showing nearly semiconducting behavior in the spin-up channel and metallic behavior in the spin-down channel under both the mBJ and GGA+U methods. Overall, FeMnVAl exhibits true half-metallic nature, as confirmed by multiple computational methods and electronic structure analyses. There is no change in the ratio of the contributions observed from projected DOS while moving from GGA to mBJ and GGA+U.

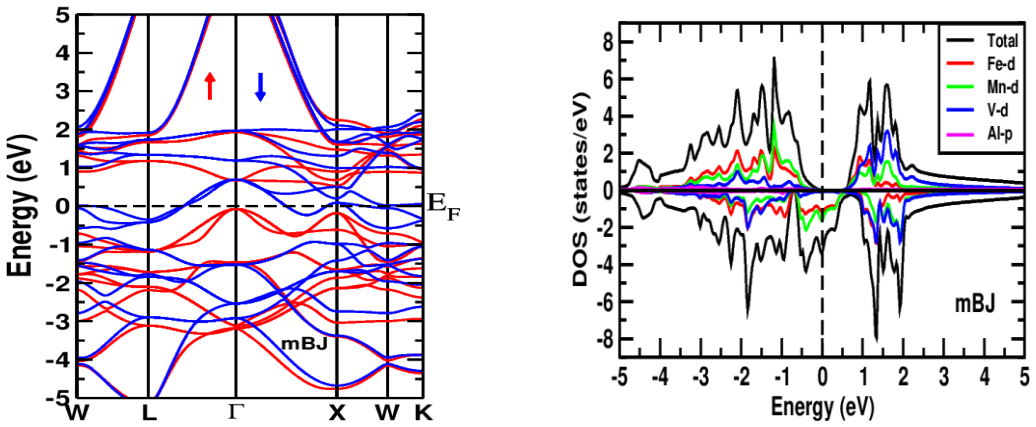

FIG. 4. (Color online) The band structure of FeMnVAl for spin-up (red) and spin-down (blue) channels under the mBJ technique.

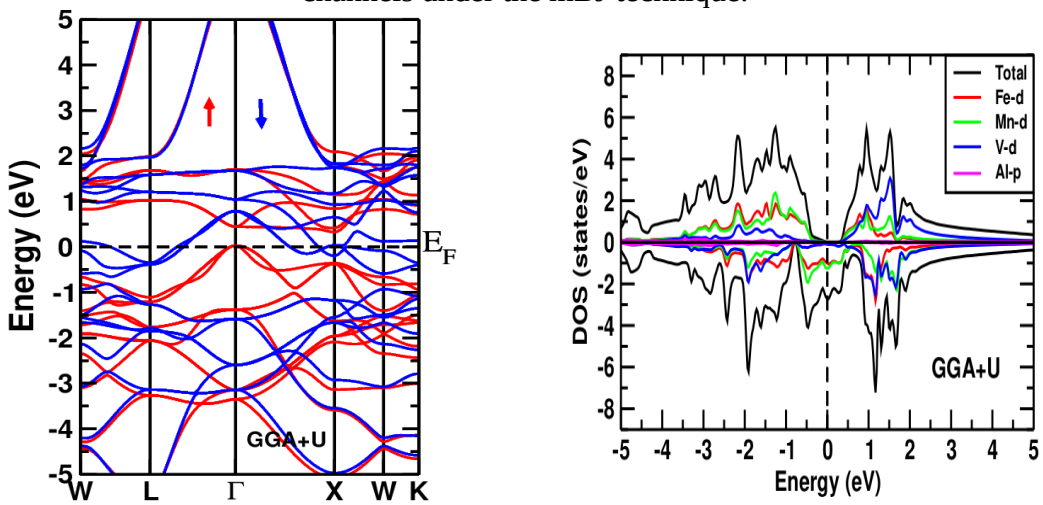

FIG. 5. (Color online) The band structure of FeMnVAl for spin-up (red) and spin-down (blue) channels under the GGA+U technique.

C: Magnetic properties

The study on FeMnVAl compound reveals its magnetic nature through asymmetrical density of states (DOS) for up and down spin channels. Total spin magnetic moments, calculated using under GGA, mBJ and GGA+U techniques which shows almost an integer value 1.00 μ_B in all techniques (Table IV), which meet with the Slater-Pauling rule $M_t = Z_t - 24$, where M_t and Z_t represents total magnetic moment and total number of valence electrons of the compound [53,54]. The positive magnetic moments in Fe and Mn dominate suggesting ferromagnetic behavior of compound.

TABLE III: Total magnetic moments $\mu_{total}(\mu_B/f.u.)$ and atomic magnetic moments $\mu_{atomic}(\mu_B/f.u.)$ of FeMnVAl under the GGA, mBJ and GGA+U techniques.

Alloy	μ_{total}	μ_{Fe}	μ_{Mn}	μ_V	μ_{Al}	**VBM**	**CBM**	E_{bg}
$FeMnVAl^{GGA}$	0.991	0.608	0.914	-0.457	-0.011	0.087	0.344	0.257
$FeMnVAl^{mBJ}$	0.999	0.654	1.006	-0.557	-0.019	-0.081	0.524	0.605
$FeMnVAl^{GGA+U}$	0.999	0.671	1.173	-0.705	-0.023	0.010	0.324	0.314

The spin polarization (P) will be analyzed using DOS of up spin and down spin electrons at the Fermi level using a relation:

$$P = \frac{n\uparrow(E_F) - n\downarrow(E_F)}{n\uparrow(E_F) + n\downarrow(E_F)} \qquad (11)$$

where $n\uparrow(E_F)$ and $n\downarrow(E_F)$ represents the DOS at the Fermi level for the majority (spin up) and minority (spin down) states respectively. The electrons are fully polarized, when $n\uparrow(E_F)$ or $n\downarrow(E_F)$ is equal to zero. The results of spin polarization indicates that FeMnVAl is 100 % spin polarized.

IV. CONCLUSIONS

We investigated the structural, mechanical, electronic, and magnetic properties of FeMnVAl alloys using GGA, mBJ, and GGA+U techniques. Structural optimization identified the stable type I structure with a ferromagnetic (FM) state. Negative values for formation and cohesive energies confirm the compound's chemical stability. The equilibrium lattice constant of FeMnVAl was found to be 5.757 Å. Mechanical stability was confirmed by Born-Huang conditions, while mechanical parameters indicate ductile behavior. Electronic structure analysis revealed nearly half-metallic (HM) behavior under GGA and true HM nature under mBJ and GGA+U techniques. The computed magnetic moment of FeMnVAl, close to 1.00 μB/f.u., adheres to the Slater-Pauling rule ($M_t = Z_t - 24$), where where M_t and Z_t represents total magnetic moment and total number of valence electrons of the compound. Such properties of the compounds are suitable for optoelectronic aswell as spintronics device applications.

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