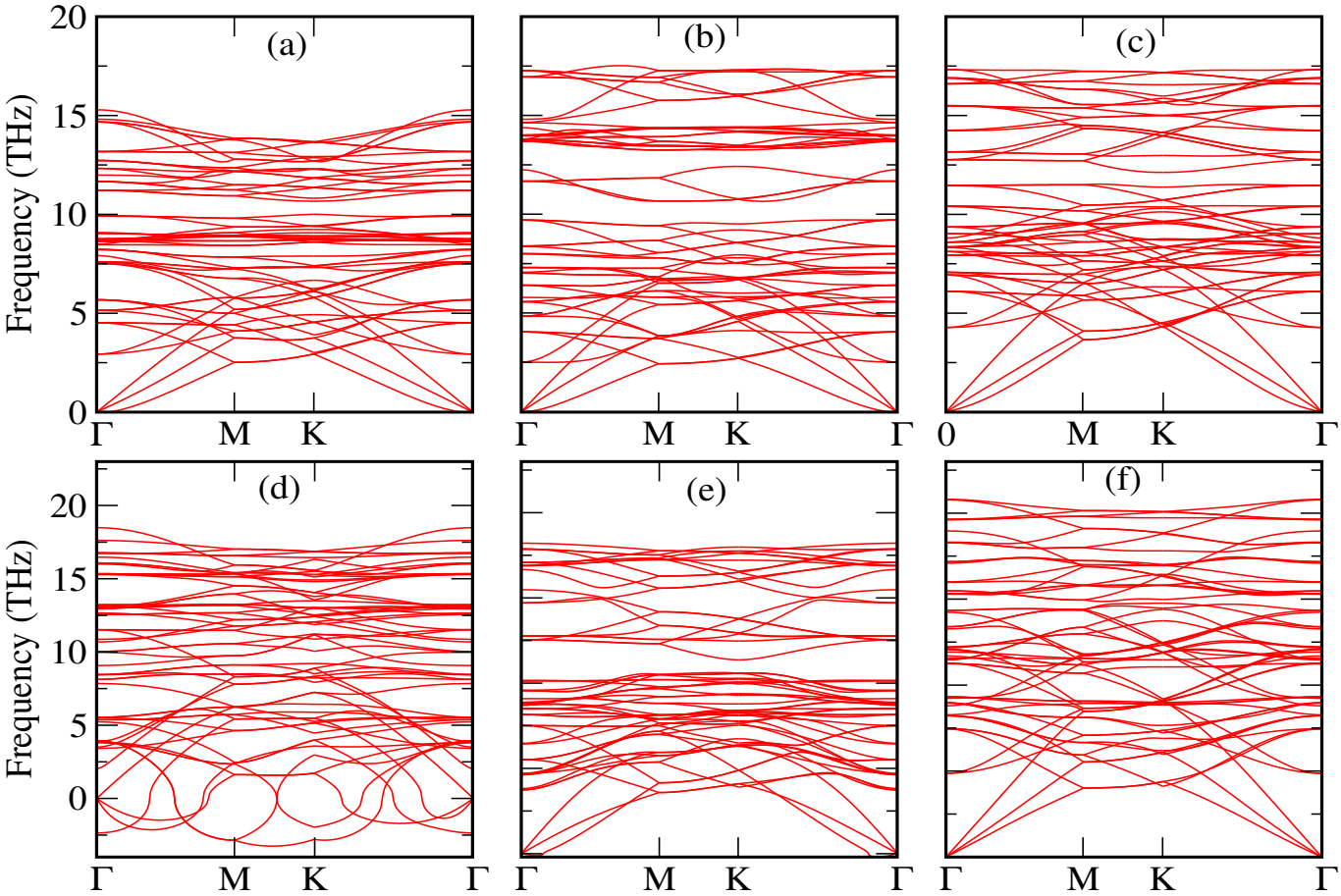
Supplementary Information for

Tunable magnetism in Nitride MXenes:consequences of atomic layer stacking

Himangshu Sekhar Sarmah and Subhradip Ghosh*
Department of Physics, Indian Institute of Technology Guwahati, Guwahati-781039, Assam, India.

I. PHONON DISPERSION RELATIONS OF THE MXENES CONSIDERED

The dynamical stability of the MXenes are obtained from the phonon dispersion curves. Figure S1 shows the phonon dispersion relations for all 10 MXenes considered in this work in ABA stacking. MXenes with positive phonon frequency are dynamically stable whereas the ones with negative frequency are dynamically unstable. Among the MXenes considered, Ti_2NO_2 and Mn_2NO_2 are found to be dynamically unstable.



* subhra@iitg.ac.in

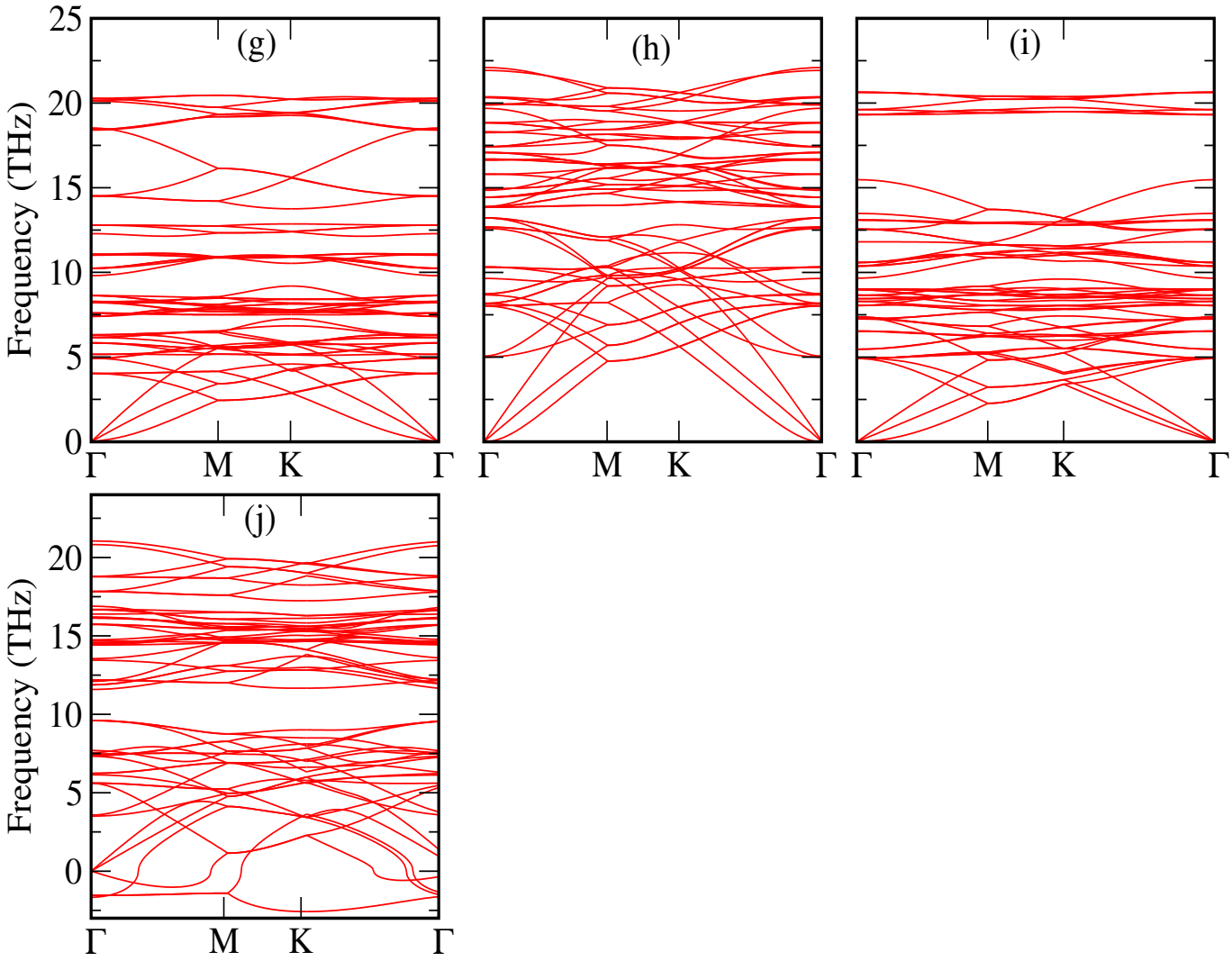


Fig S 1: Phonon spectra of (a)Sc_2NF_2 (b) Sc_2NO_2 (c) Ti_2NF_2 (d) Ti_2NO_2 (e) V_2NF_2 (f) V_2NO_2 (g) Cr_2NF_2 (h) Cr_2NO_2 (i) Mn_2NF_2 (j) Mn_2NO_2

II. ATOM RESOLVED DENSITIES OF STATES

The atom resolved spin polarised Densities of States for both ABA and ABC stacked MXenes are provided in this section .

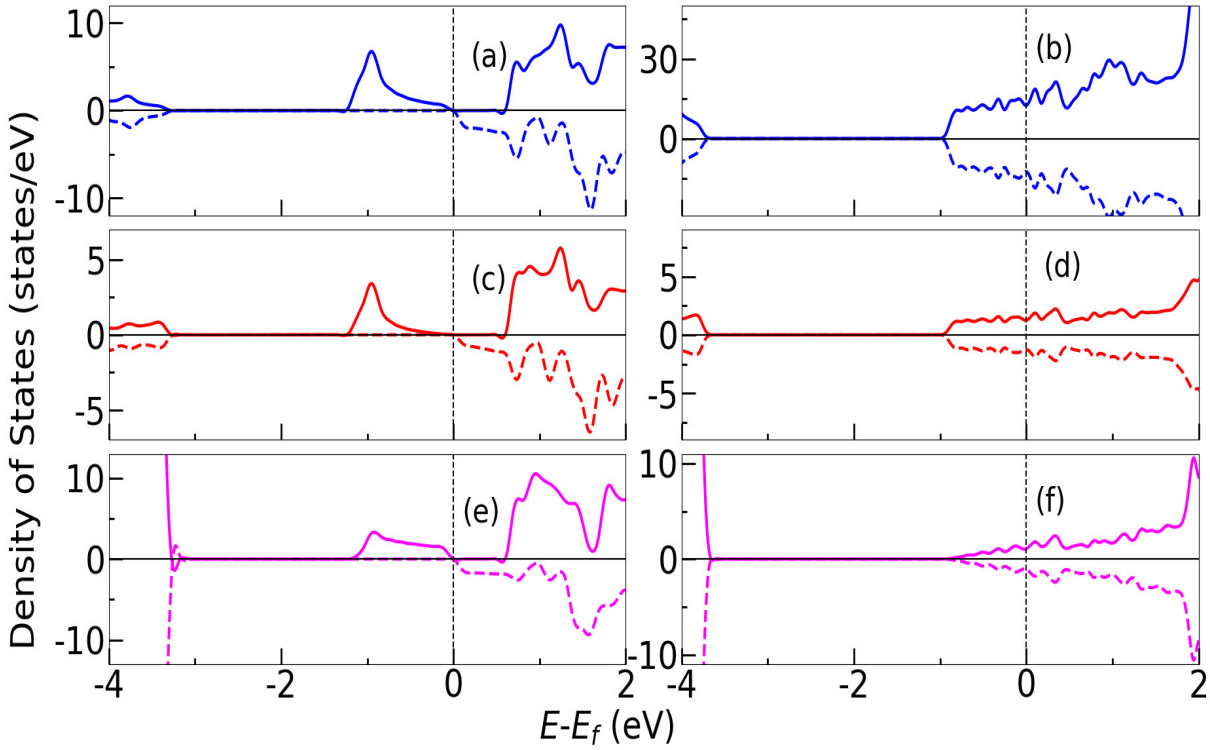


Fig S 2: Atom resolved spin polarised densities of states of ABA stacked (left panel) and ABC stacked (right panel) Sc_2NF_2 .(a,b), (c,d) and (e,f) are the densities of states of Sc, F and N, respectively.

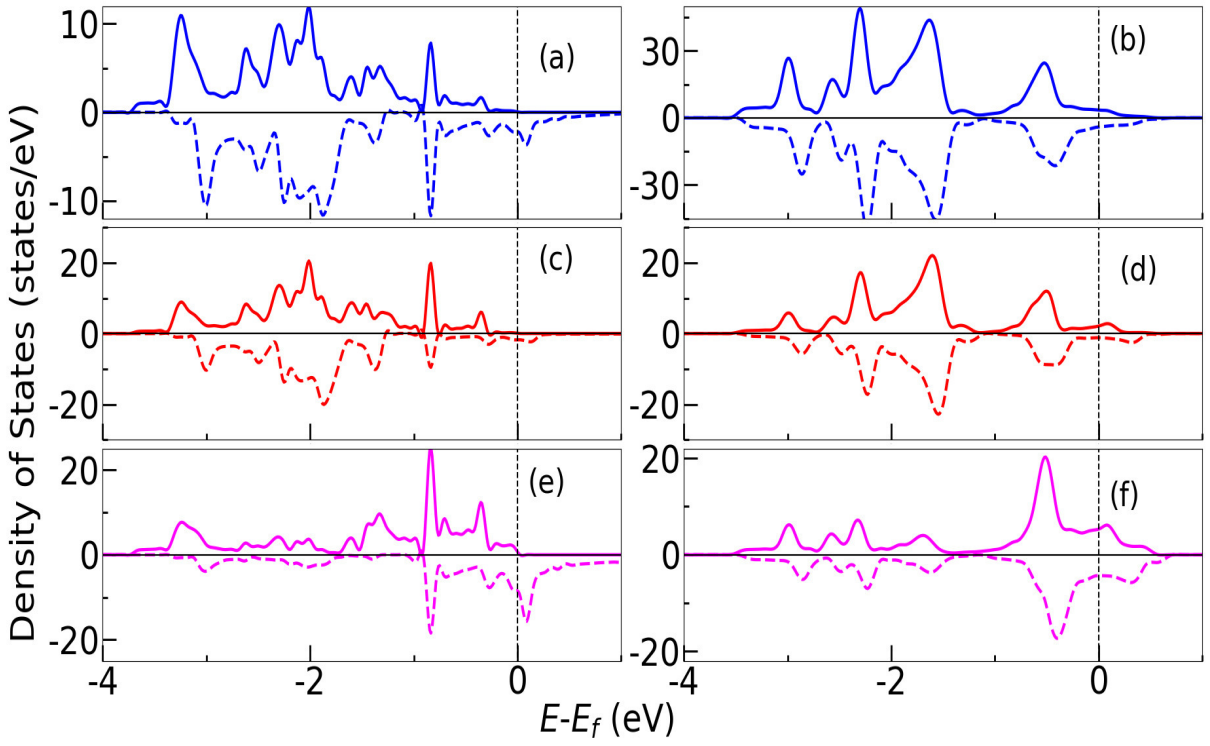


Fig S 3: Atom resolved spin polarised densities of states of ABA stacked (left panel) and ABC stacked (right panel) Sc_2NO_2.a,b), (c,d) and (e,f) are the densities of states of Sc, O and N, respectively.

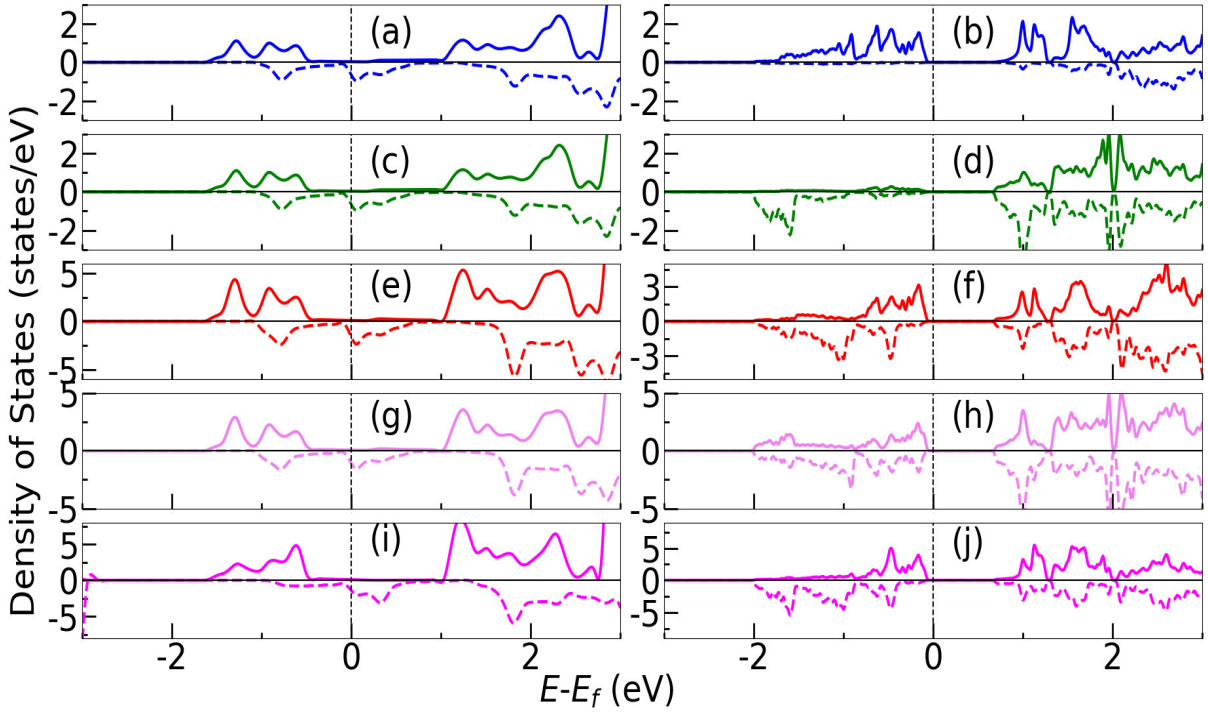


Fig S 4: Atom resolved densities of states of ABA stacked (left panel) and ABC stacked (right panel) Ti_2NF_2. (a and b), (c and d), (e and f), (g and h) and (i and j) are the densities of states of Ti^{I}, Ti^{II},F^{I},F^{II} and N, respectively. F^{I} and F^{II} are fluorene atoms associated with Ti^{I} and Ti^{II}

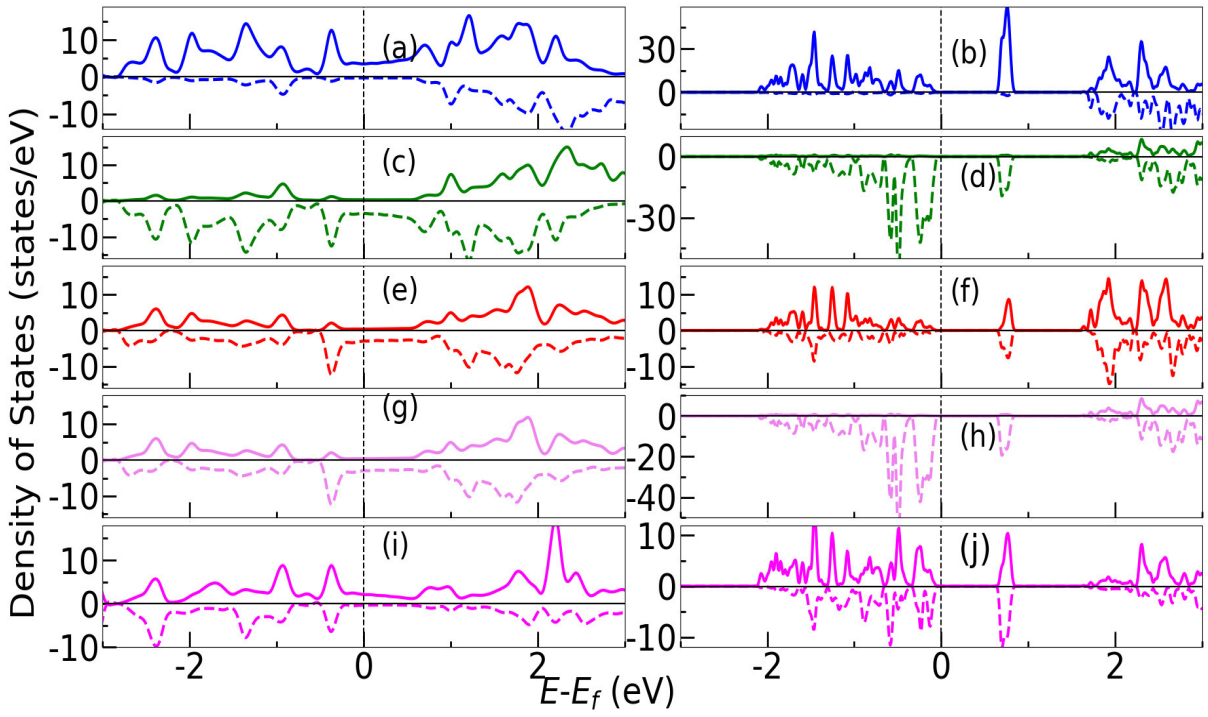


Fig S 5: Atom resolved densities of states of ABA stacked (left panel) and ABC stacked (right panel) V_2NF_2.a and b), (c and d), (e and f), (g and h) and (i and j) are the densities of states of V^{I}, V^{II},F^{I},F^{II} and N, respectively. F^{I} and F^{II} are fluorene atoms associated with V^{I} and V^{II}

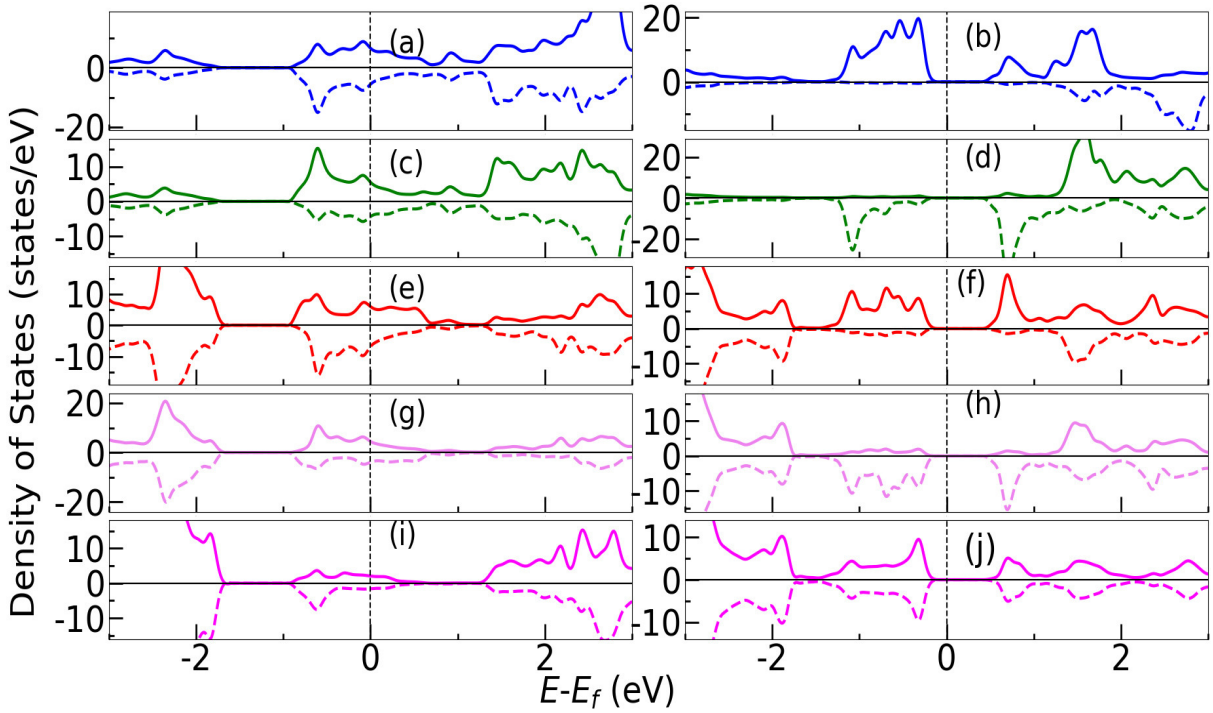


Fig S 6: Atom resolved densities of states of ABA stacked (left panel) and ABC stacked (right panel) V_2NO_2.a and b), (c and d), (e and f), (g and h) and (i and j) are the densities of states of V^{I}, V^{II},O^{I},O^{II} and N, respectively. O^{I} and O^{II} are fluorene atoms associated with V^{I} and V^{II}

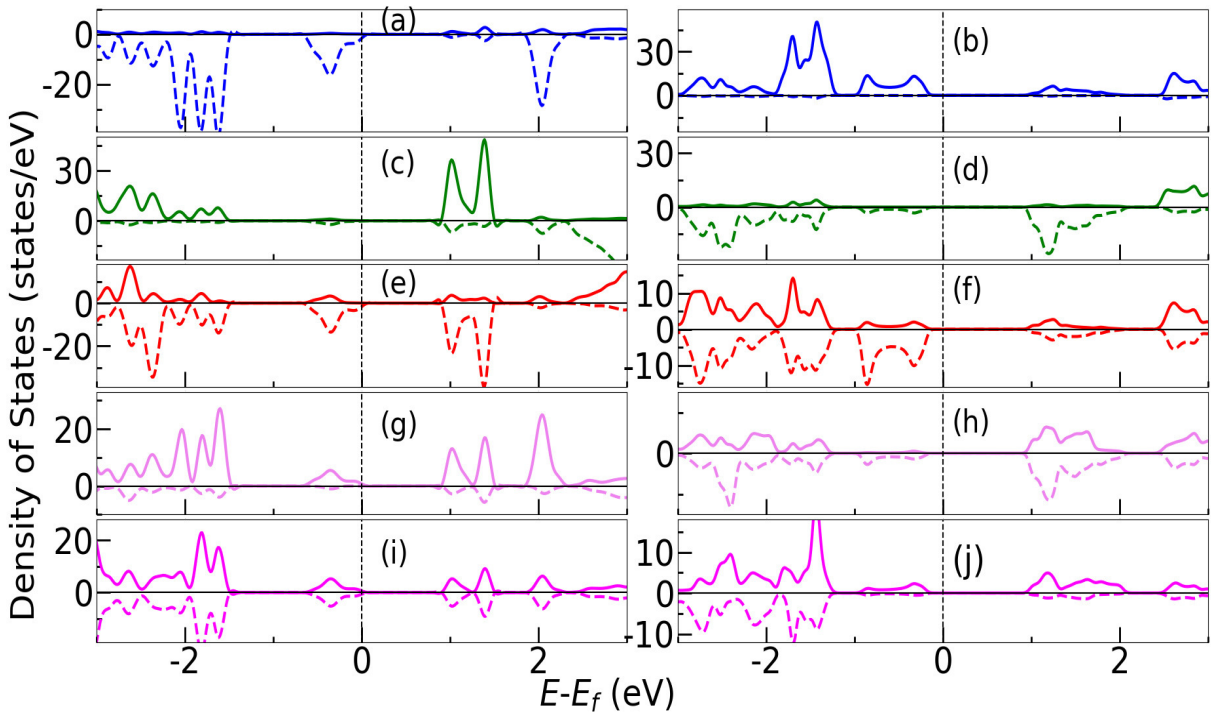


Fig S 7: Atom resolved densities of states of ABA stacked (left panel) and ABC stacked (right panel) Cr_2NF_2.a and b), (c and d), (e and f), (g and h) and (i and j) are the densities of states of Cr^{I}, Cr^{II},F^{I},F^{II} and N, respectively. F^{I} and F^{II} are fluorene atoms associated with Cr^{I} and Cr^{II}

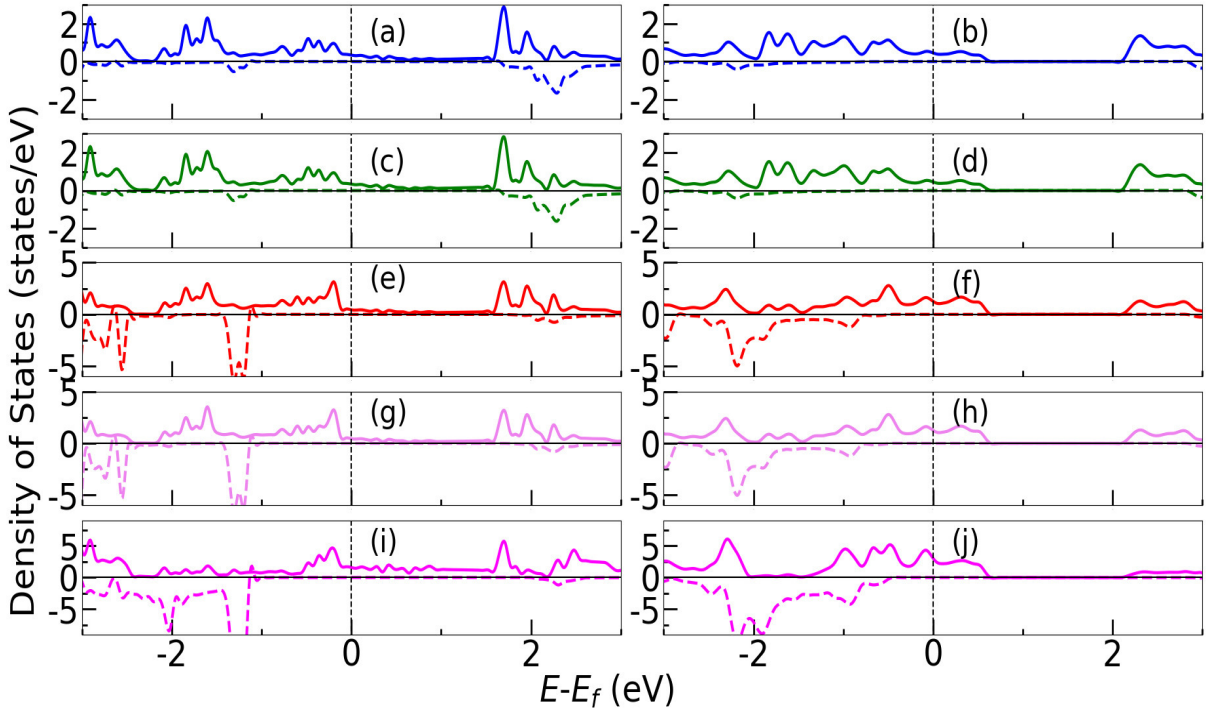


Fig S 8: Atom resolved densities of states of ABA stacked (left panel) and ABC stacked (right panel) Cr_2NO_2.a and b), (c and d), (e and f), (g and h) and (i and j) are the densities of states of Cr^{I}, Cr^{II},O^{I},O^{II} and N, respectively. O^{I} and O^{II} are fluorene atoms associated with Cr^{I} and Cr^{II}

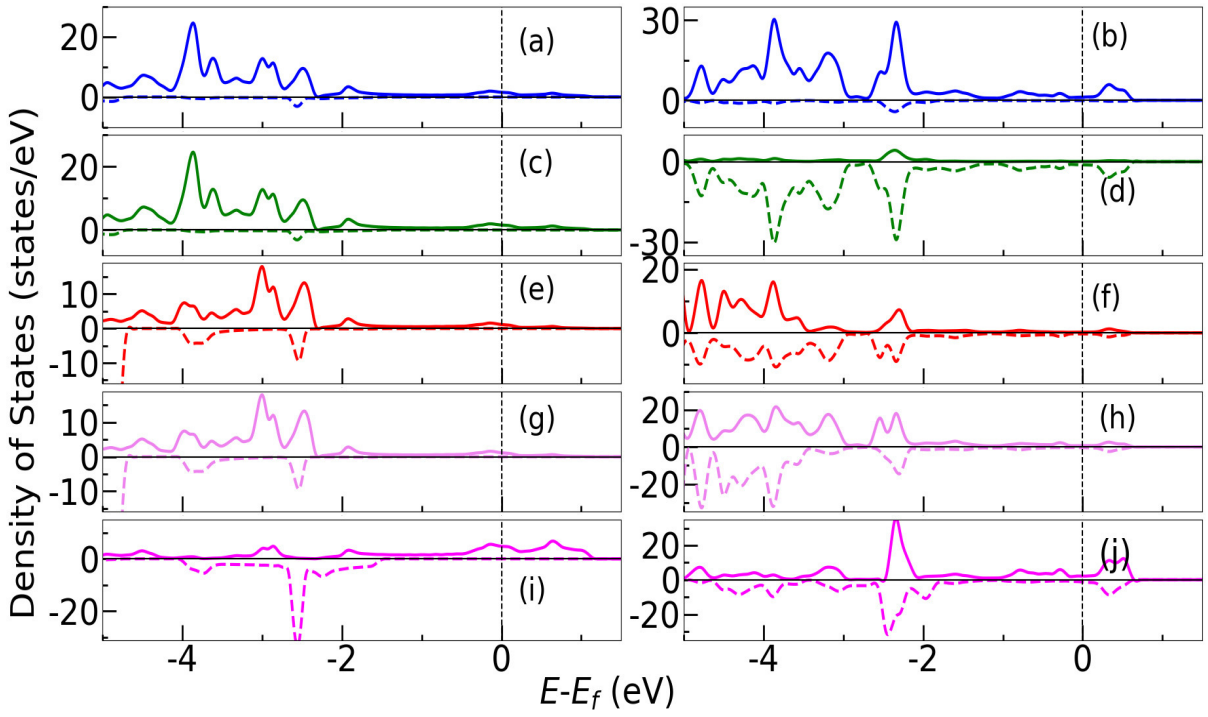


Fig S 9: Atom resolved densities of states of ABA stacked (left panel) and ABC stacked (right panel) Mn_2NF_2.a and b), (c and d), (e and f), (g and h) and (i and j) are the densities of states of Mn^{I}, Mn^{II},F^{I},F^{II} and N, respectively. F^{I} and F^{II} are fluorene atoms associated with Mn^{I} and Mn^{II}

III. ORBITAL RESOLVED DENSITY OF STATES

The *d*-orbital resolved densities of states for both ABA and ABC stacked MXenes are given in this section.

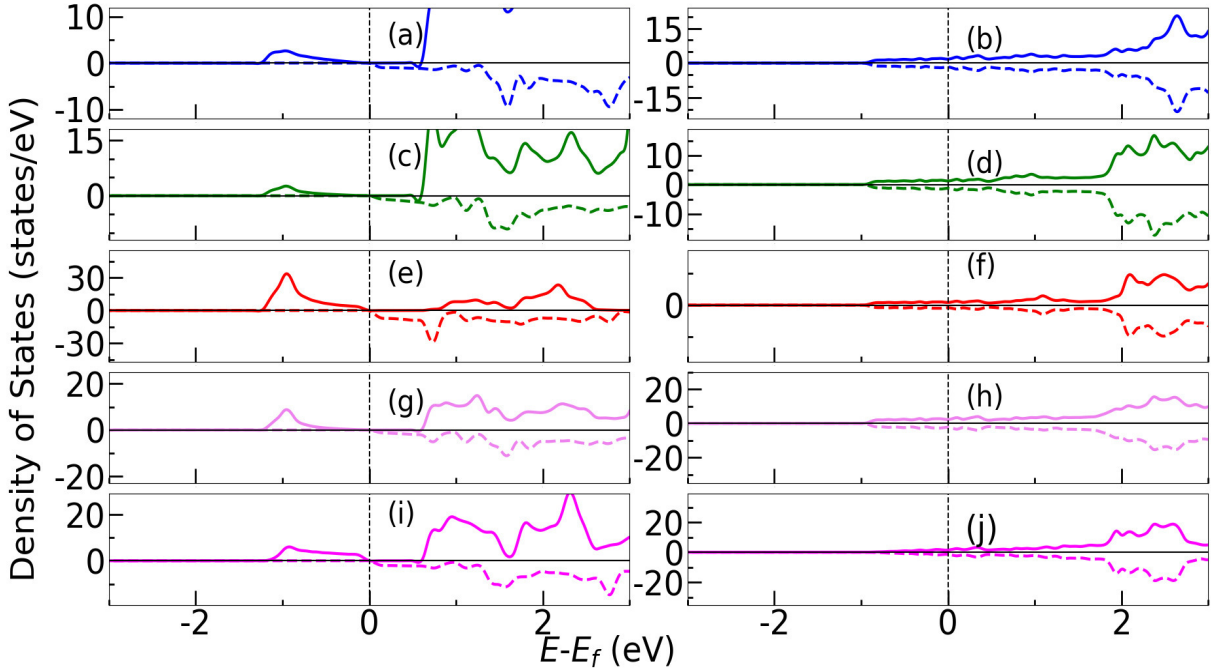


Fig S 10: Densities of states of e_2 (a and b), e_1(c and d), a_1 (e and f) orbitals of Sc along with F (g and h) and N (i and j) of Sc_2NF_2.The left panel is for ABA and right panel is for ABC.

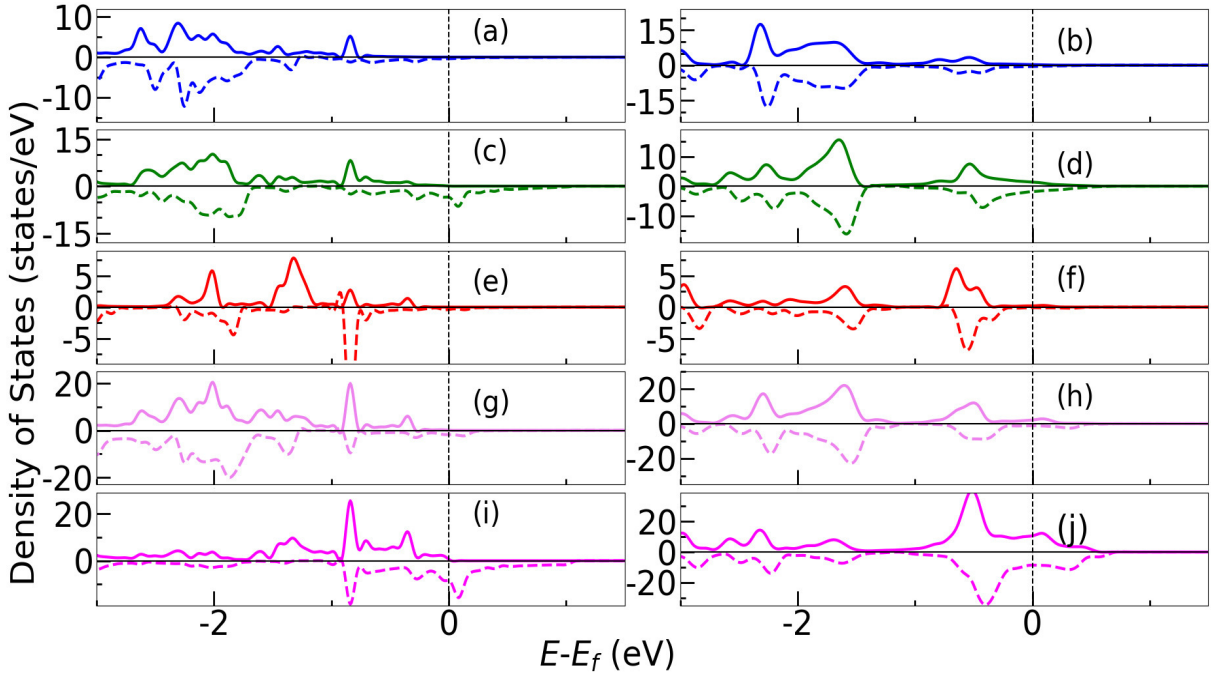


Fig S 11: Densities of states of e_2 (a and b), e_1(c and d), a_1 (e and f) orbitals of Sc along with O (g and h) and N (i and j) of Sc_2NO_2.The left panel is for ABA and right panel is for ABC.

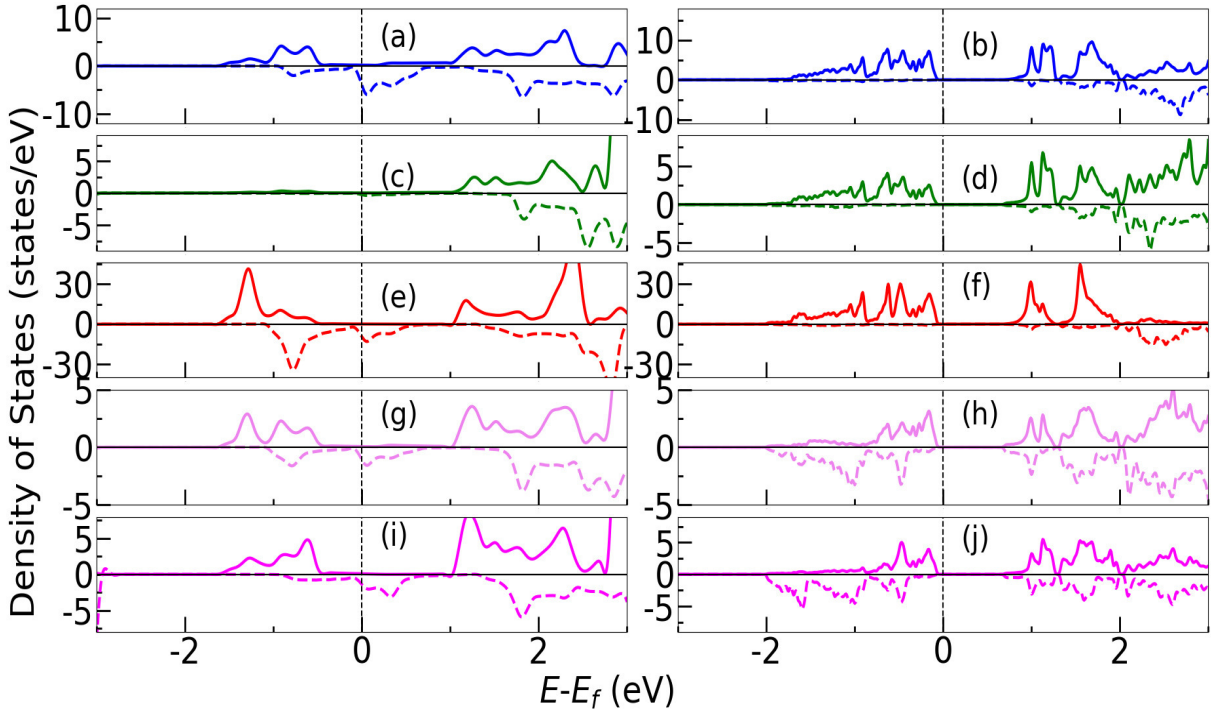


Fig S 12: Densities of states of e_2 (a and b), e_1(c and d), a_1 (e and f) orbitals of Ti^{I} along with F (g and h) and N (i and j) of Ti_2NF_2.The left panel is for ABA and right panel is for ABC.

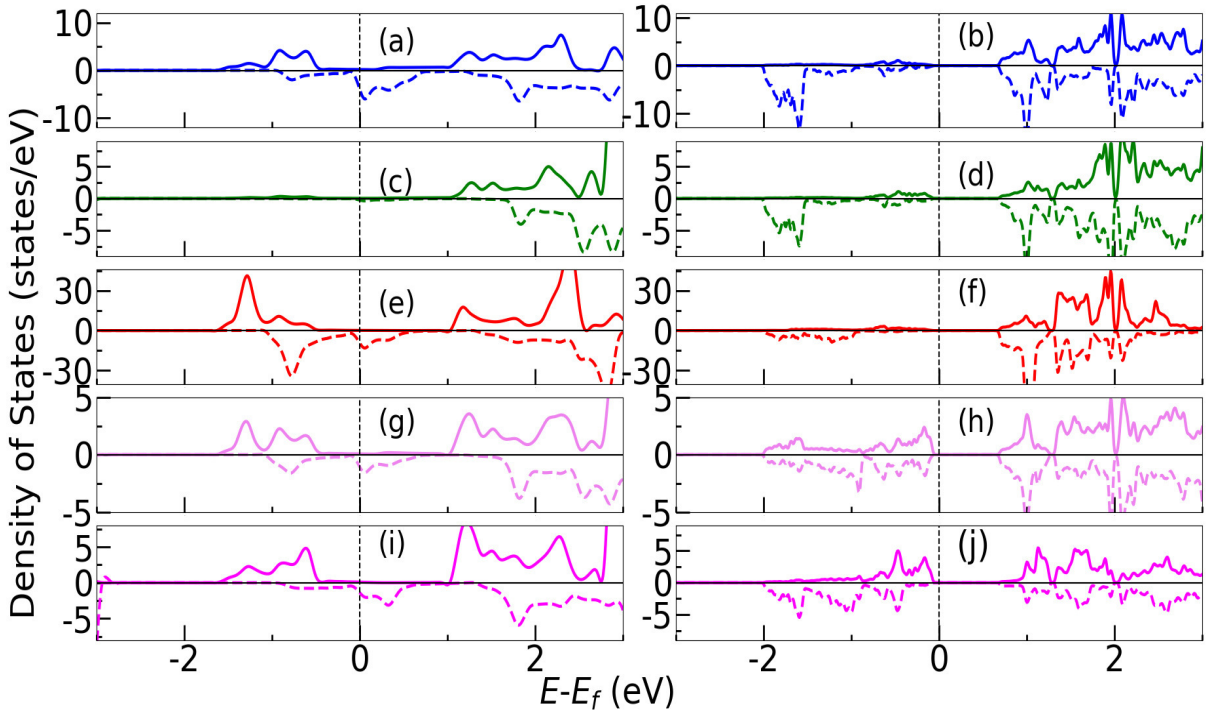


Fig S 13: Densities of states of e_2 (a and b), e_1(c and d), a_1 (e and f) orbitals of Ti^{II} along with F (g and h) and N (i and j) of Ti_2NF_2.The left panel is for ABA and right panel is for ABC.

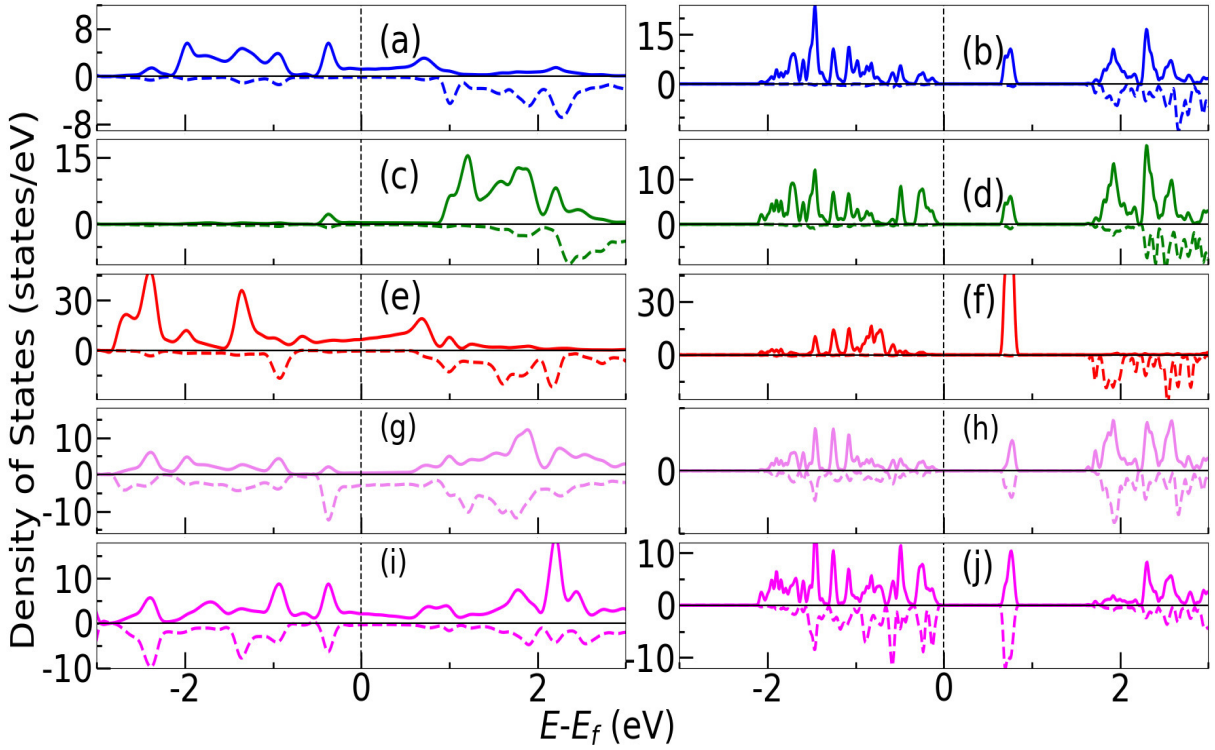


Fig S 14: Densities of states of e_2 (a and b), e_1(c and d), a_1 (e and f) orbitals of V^I along with F (g and h) and N (i and j) of V_2NF_2.The left panel is for ABA and right panel is for ABC.

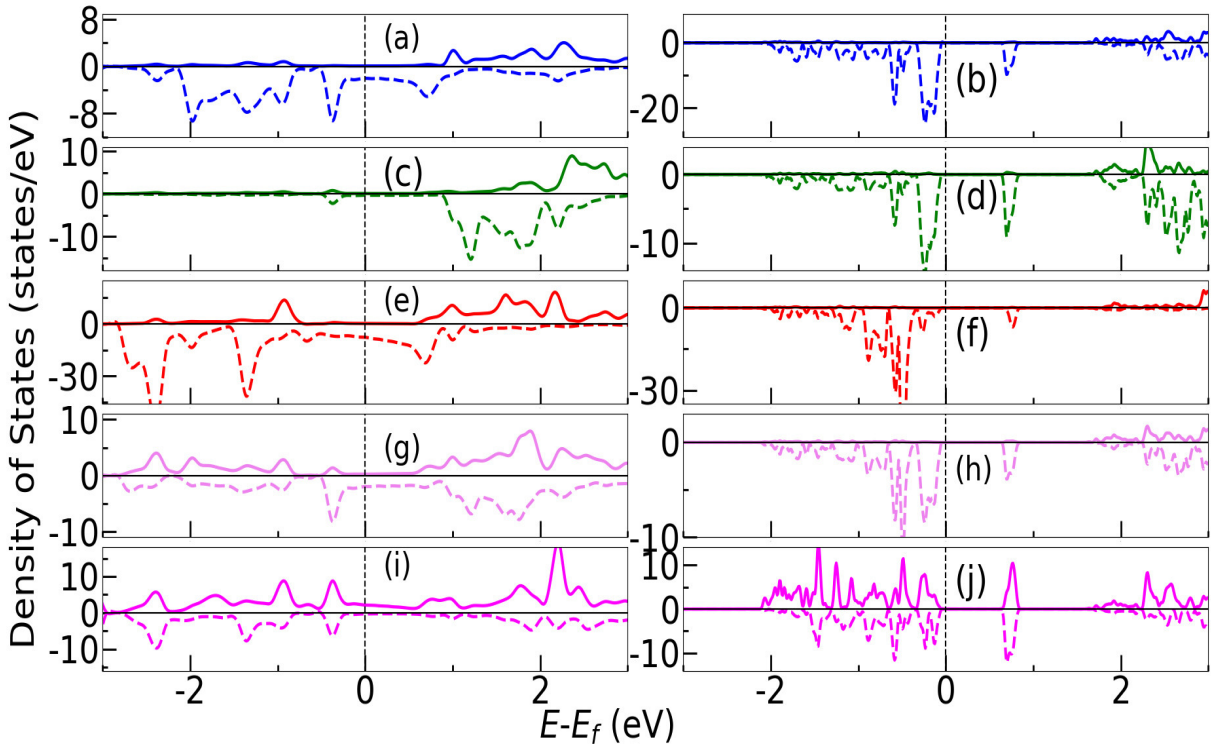


Fig S 15: Densities of states of e_2 (a and b), e_1(c and d), a_1 (e and f) orbitals of V^{II} along with F (g and h) and N (i and j) of V_2NF_2.The left panel is for ABA and right panel is for ABC.

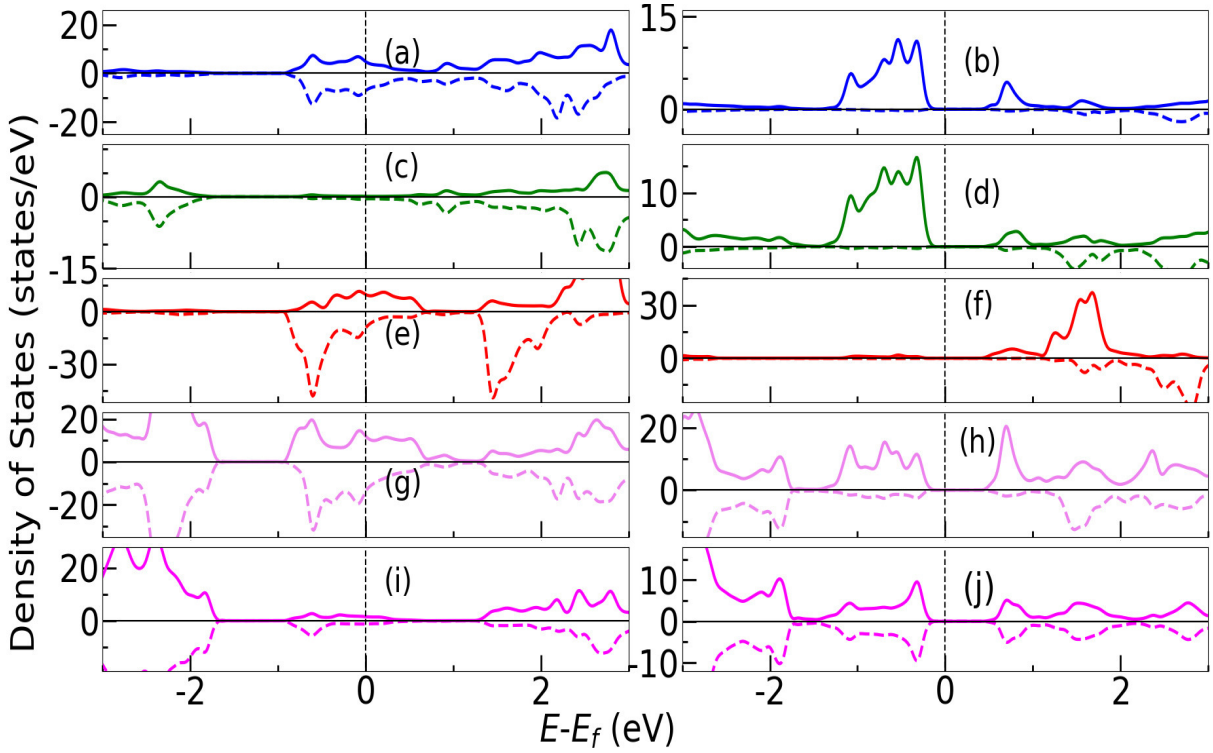


Fig S 16: Densities of states of e_2 (a and b), e_1(c and d), a_1 (e and f) orbitals of V^{I} along with O (g and h) and N (i and j) of V_2NO_2.The left panel is for ABA and right panel is for ABC.

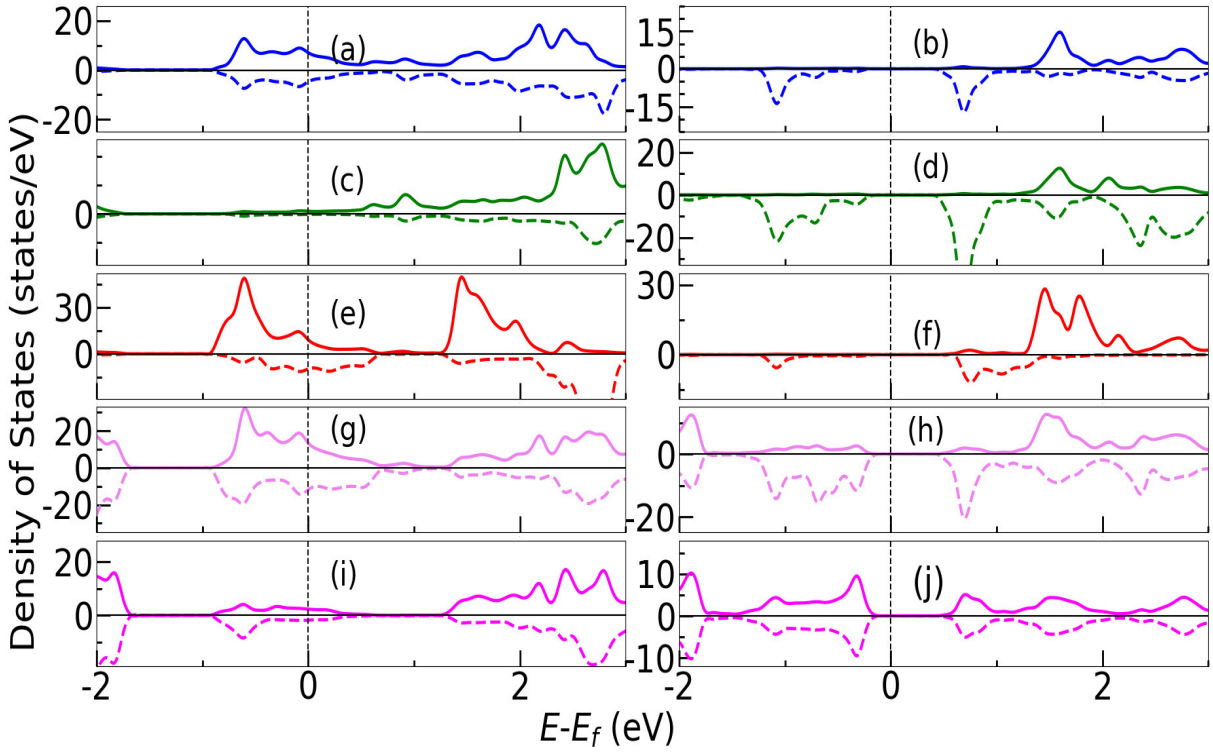


Fig S 17: Densities of states of e_2 (a and b), e_1(c and d), a_1 (e and f) orbitals of V^{II} along with O (g and h) and N (i and j) of V_2NO_2.The left panel is for ABA and right panel is for ABC.

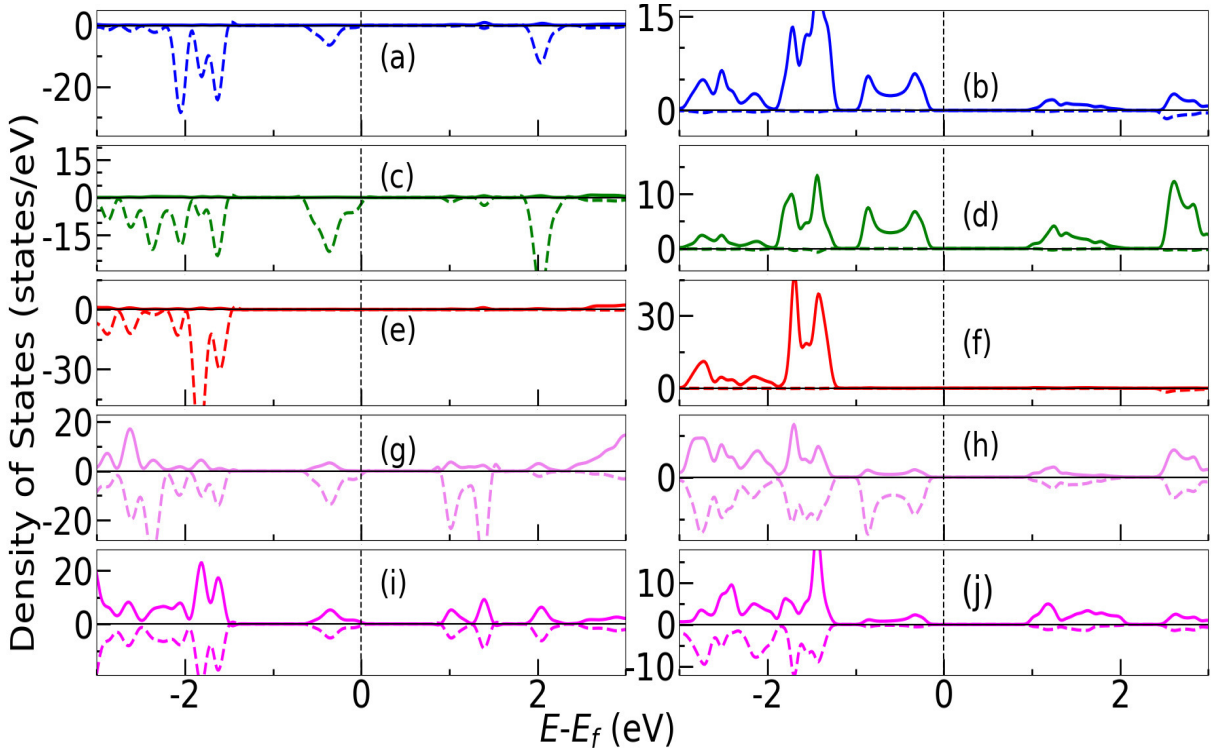


Fig S 18: Densities of states of e_2 (a and b), e_1(c and d), a_1 (e and f) orbitals of Cr^I along with F (g and h) and N (i and j) of Cr_2NF_2.The left panel is for ABA and right panel is for ABC.

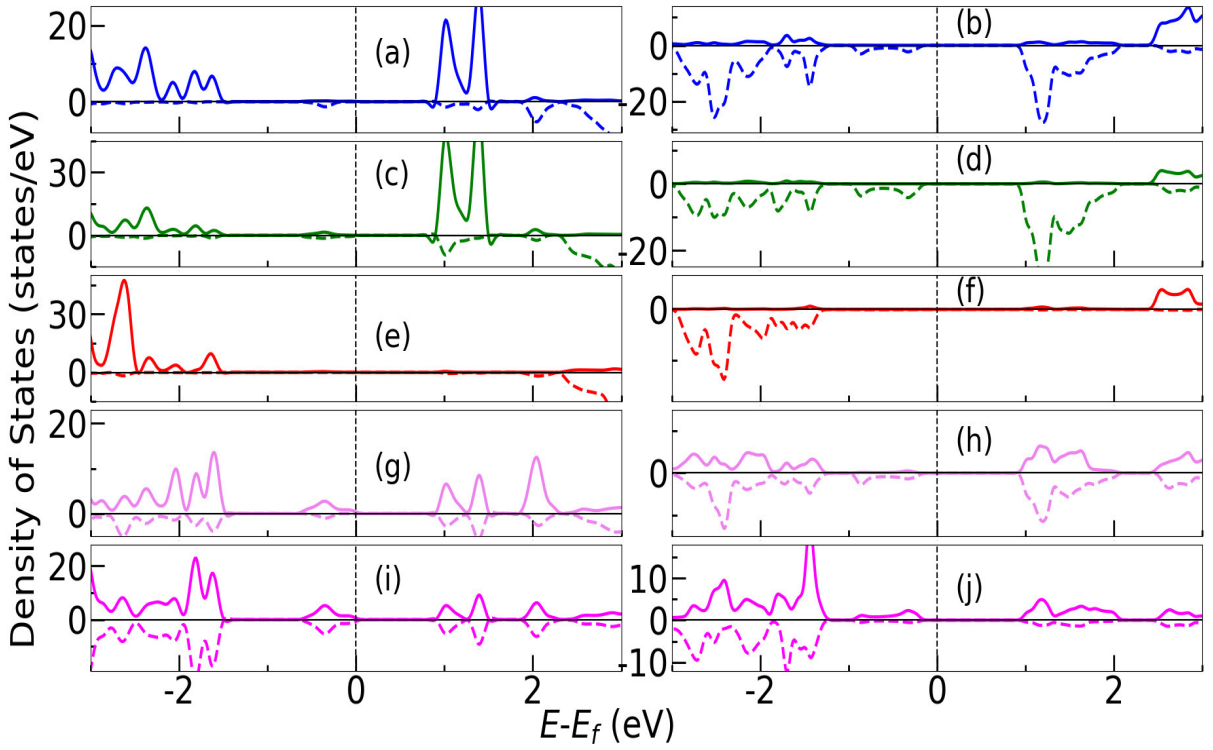


Fig S 19: Densities of states of e_2 (a and b), e_1(c and d), a_1 (e and f) orbitals of Cr^{II} along with F (g and h) and N (i and j) of Cr_2NF_2.The left panel is for ABA and right panel is for ABC.

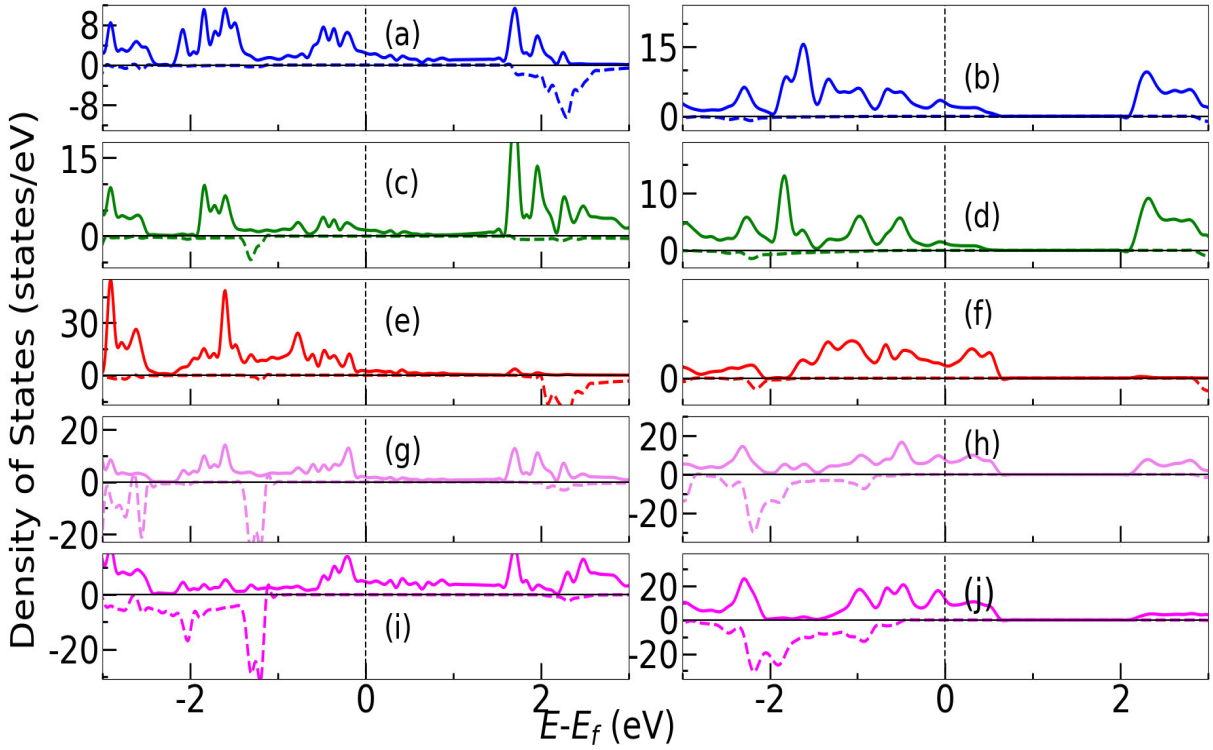


Fig S 20: Densities of states of e_2 (a and b), e_1(c and d), a_1 (e and f) orbitals of Cr along with O (g and h) and N (i and j) of Cr_2NO_2.The left panel is for ABA and right panel is for ABC.

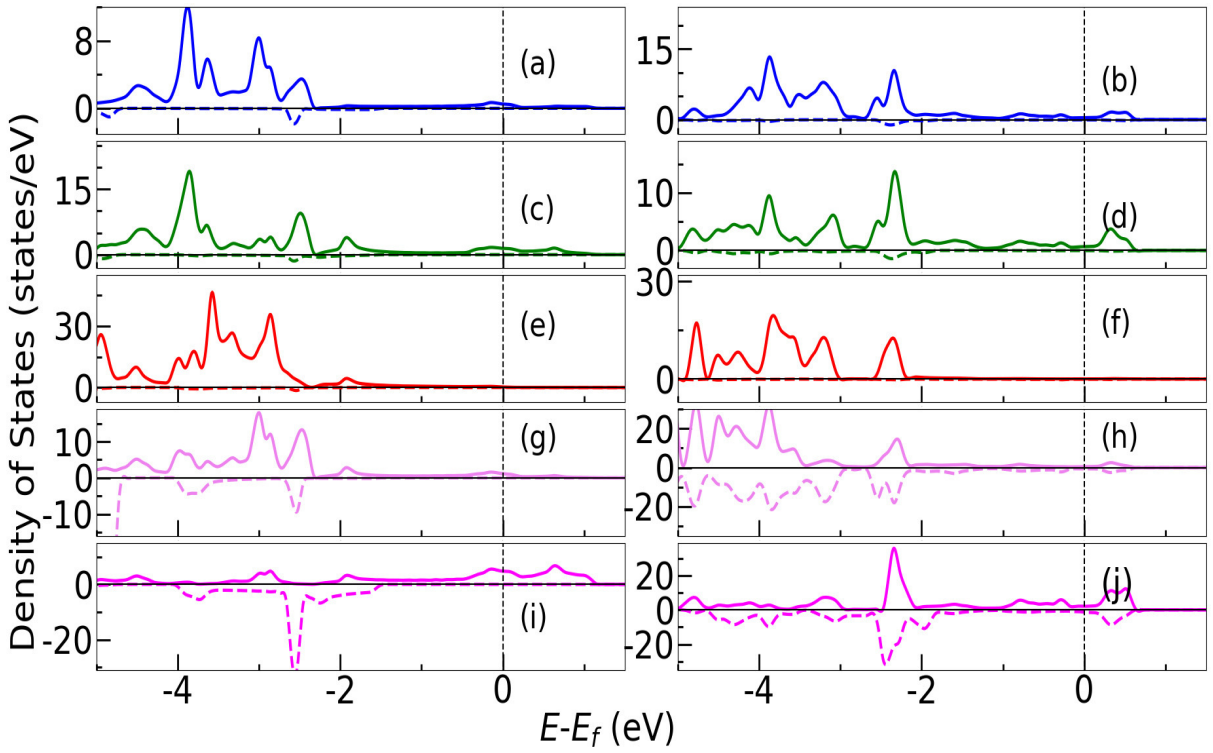


Fig S 21: Densities of states of e_2 (a and b), e_1(c and d), a_1 (e and f) orbitals of Mn along with F (g and h) and N (i and j) of Mn_2NF_2.The left panel is for ABA and right panel is for ABC.

IV. MAGNETIC EXCHANGE PARAMETERS

The interatomic exchange parameters for ABA and ABC stacked MXenes are plotted in Figure S22 and S23 . The magnetic ground states can be understood by interpreting these exchange parameters.

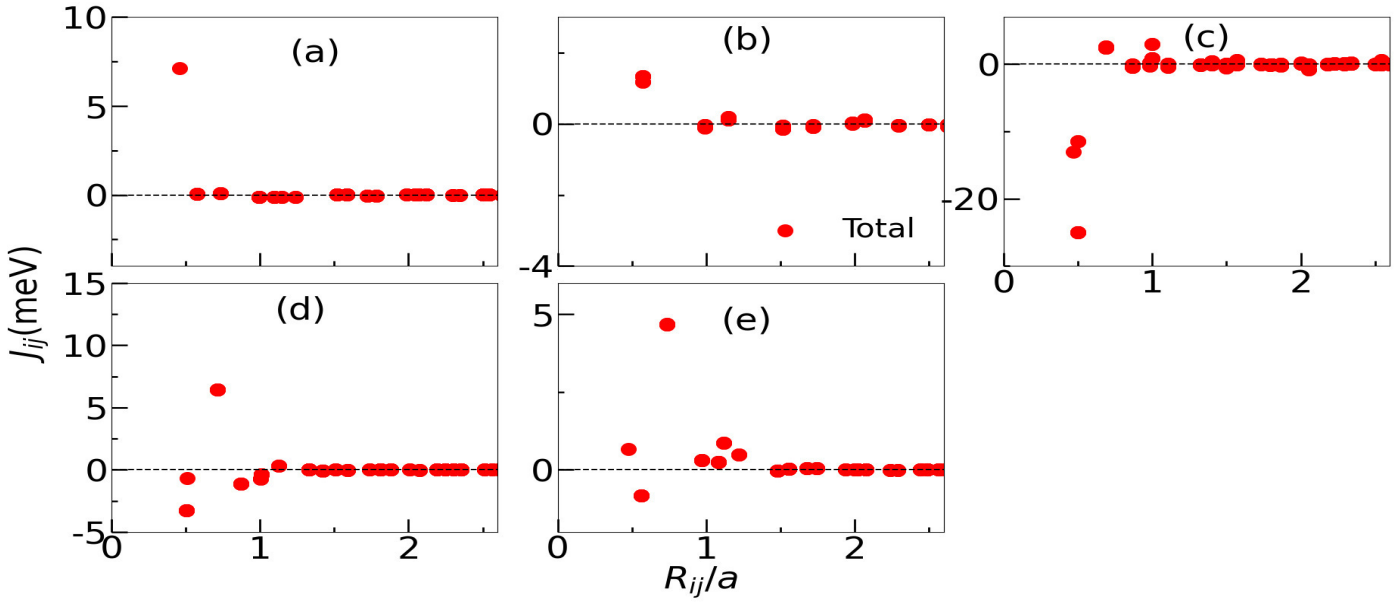


Fig S 22: Interatomic exchange parameter as a function of interatomic distance in ABA stacked (a)Sc_2NF_2 (b) Sc_2NO_2 (c) V_2NF_2(d) Cr_2NO_2 (e) Mn_2NF_2

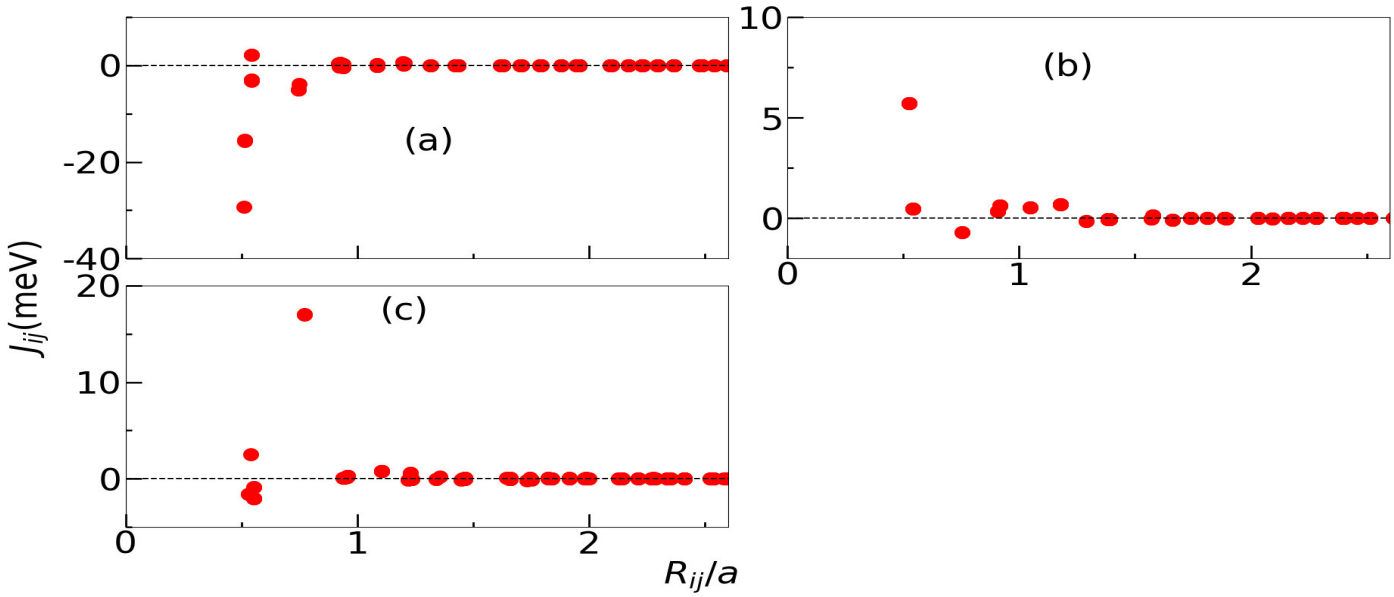


Fig S 23: Interatomic exchange parameter as a function of interatomic distance in ABC stacked (a)V_2NF_2 (b) Cr_2NO_2 (c) Mn_2NF_2

V. ORBITAL RESOLVED MAGNETIC ANISOTROPY ENERGIES

The orbital resolved MAE for both ABA and ABC stacked MXenes are provided in Figure S24 and S25 respectively
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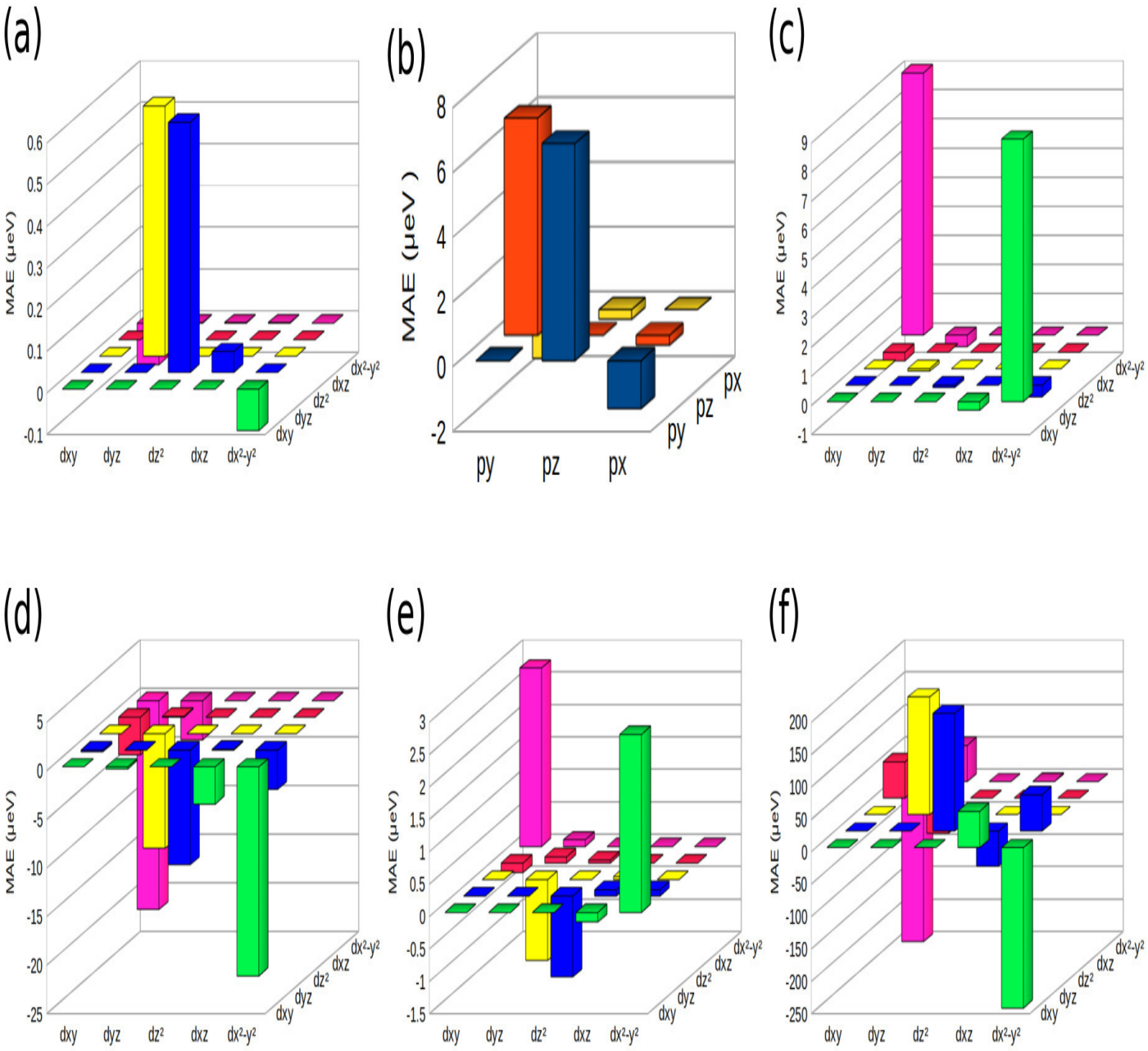

Fig S 24: Orbital decomposed magnetic anisotropy energy of ABA stacked (a)Sc_2NF_2 (b) Sc_2NO_2 (c) Ti_2NF_2(d) V_2NF_2 (e) V_2NO_2 (f) Mn_2NF_2.

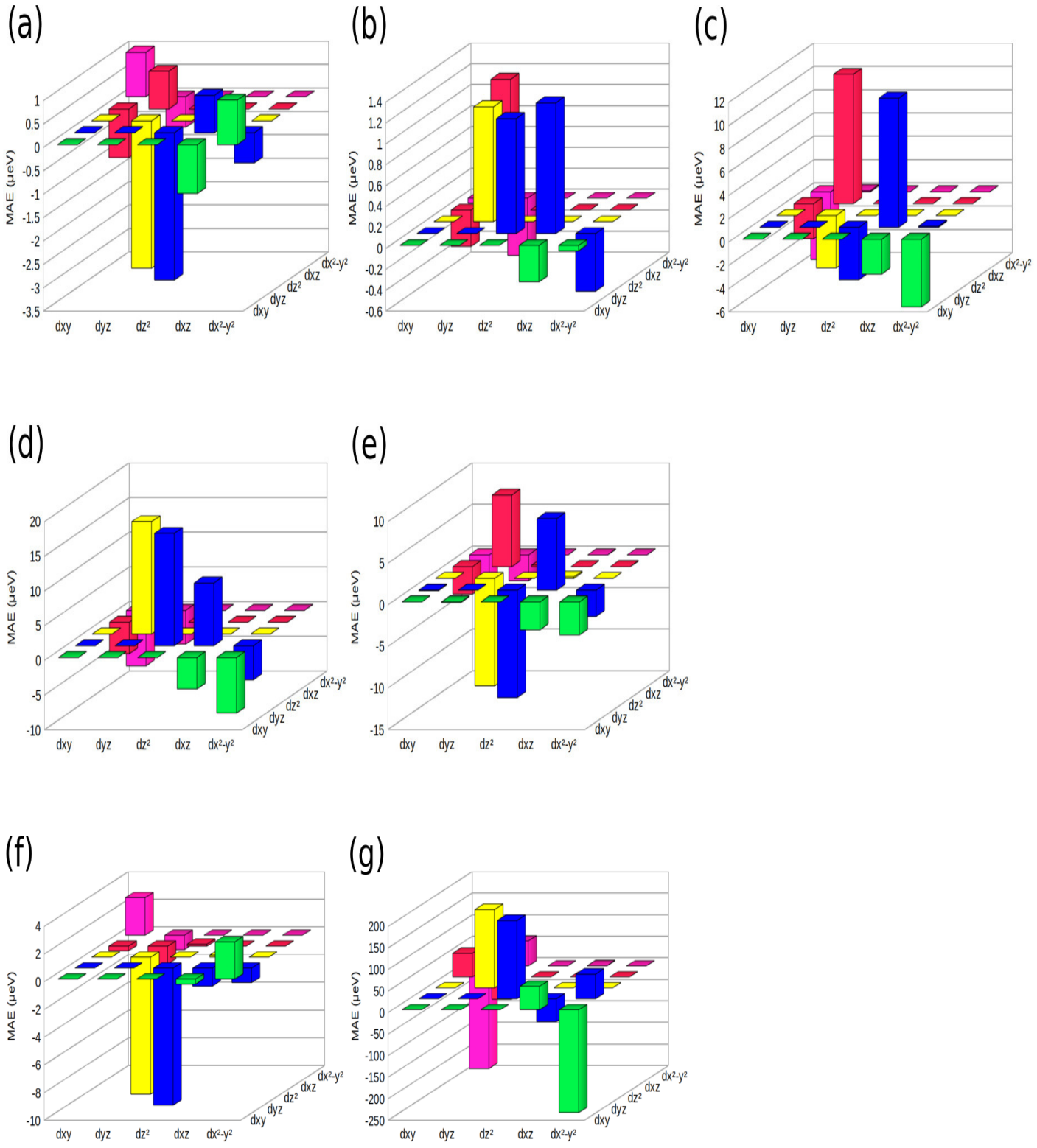

Fig S 25: Orbital decomposed magnetic anisotropy energy of ABC stacked (a)Ti^I of Ti_2NF_2 (b) Ti^{II} of Ti_2NF_2 (c) V^I of V_2NF_2(d) V^{II} of V_2NF_2 (e) V^I of V_2NO_2(f) V^{II} of V_2 NO_2 (g) Mn_2NF_2