Supplementary Information File

Tuning the Electronic, Magnetic and Sensing Properties of Single Atom Embedded C_3N_6 Monolayer Towards XO_2 (X=C,N,S) Gases

Swapnil S. Deshpande[a], Mrinalini D. Deshpande[a,*], Rajeev Ahuja[b,c], Tanveer Hussain[d,e,**]

[a] Department of Physics, H. P. T. Arts and R. Y. K. Science College, Nasik - 422005, Maharashtra, India.
[b] Department of Physics, Indian Institute of Technology, Ropar, Rupnagar 140001, Punjab, India.
[c] Condensed Matter Theory Group, Materials Theory Division, Department of Physics and Astronomy, Uppsala University, Box 516, SE-75120, Uppsala, Sweden.
[d] School of Chemical Engineering, The University of Queensland, St Lucia, Brisbane 4072. Australia.
[e] School of Science and Technology, University of New England, Armidale, New South Wales 2351, Australia.

Corresponding author
Email addresses: * d_mrinal@yahoo.com (Mrinalini D. Deshpande),
** tanveer.hussain@une.edu.au (Tanveer Hussain).

Electronic band structure and Total and projected density of states of C_3N_6 monolayer :
The electronic band structure, total and projected density of states analysis (TDOS and PDOS) are shown in Figure S1 (a) and (b), respectively. The band gap of C_3N_6 analyzed by ultra-violet visible spectroscopy is 3.05 eV reported in the recent study.[S1] The ML is observed to be semiconducting with direct band gap of 0.87 eV. As expected, PBE/GGA predictions underestimate the band gap value. It is seen that the both valence band and conduction bands are flat in electronic band structures. Furthermore, spin-up and spin-down TDOS and PDOS of C and N are symmetrical, which indicate that pristine C_3N_6 ML possess the characteristics of a non-magnetic ground state. In addition, we can also see from PDOS (Figure S1 (b), that the valence band edge is mainly composed of the strong hybridization of p_x and p_y orbitals of C and N atoms, while the conduction band edge mostly consists of the p_z orbitals of C and N atoms, which is consistent with the earlier study.[S2]

References
(S1) I. Y. Kim, S. Kim, S. Premkumar, J. H. Yang, S. Umapathy, and A. Vinu, Small, (2019) 1903572-1903578.
(S2) B. Mortazavi, F. Shojaei, M. Shahrokhi, M. Azizi, T. Rabczuk, A. V. Shapeev, X. Zhuang, Carbon, 167 (2020) 40-50.

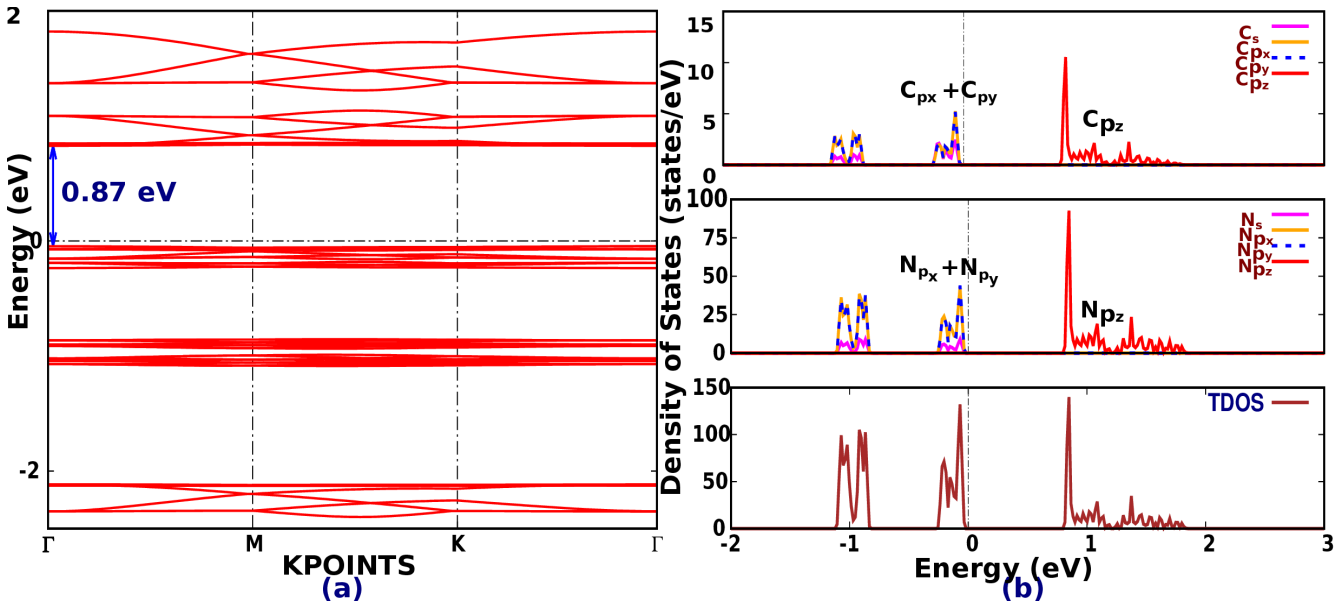

Figure S1. (a) Electronic band structure, and (b) Total and projected density of states of C_3N_6 monolayer, respectively at GGA-PBE level. Fermi energy level is shifted to 0 eV. (A color version of this figure can be viewed online.)

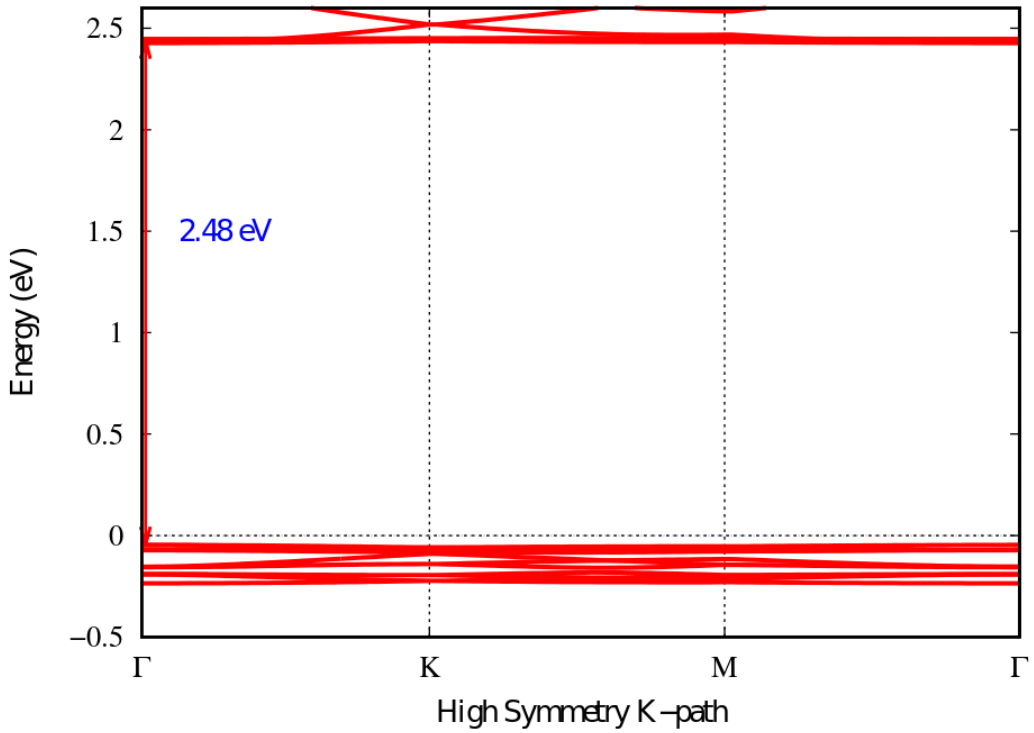

Figure S2: Electronic band structure of pristine C_3N_6 monolayer using HSE06 method.

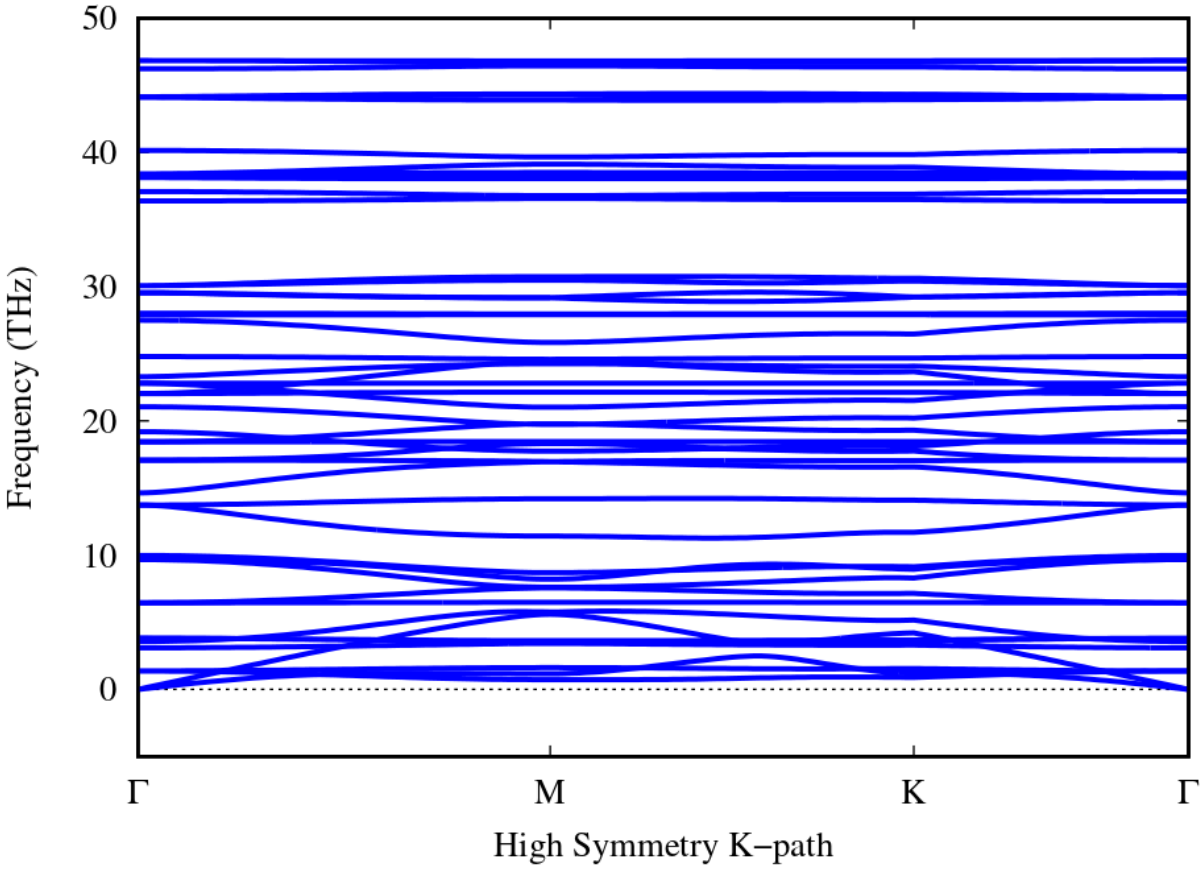

Figure S3: Phonon dispersion of pristine C_3N_6 monolayer.

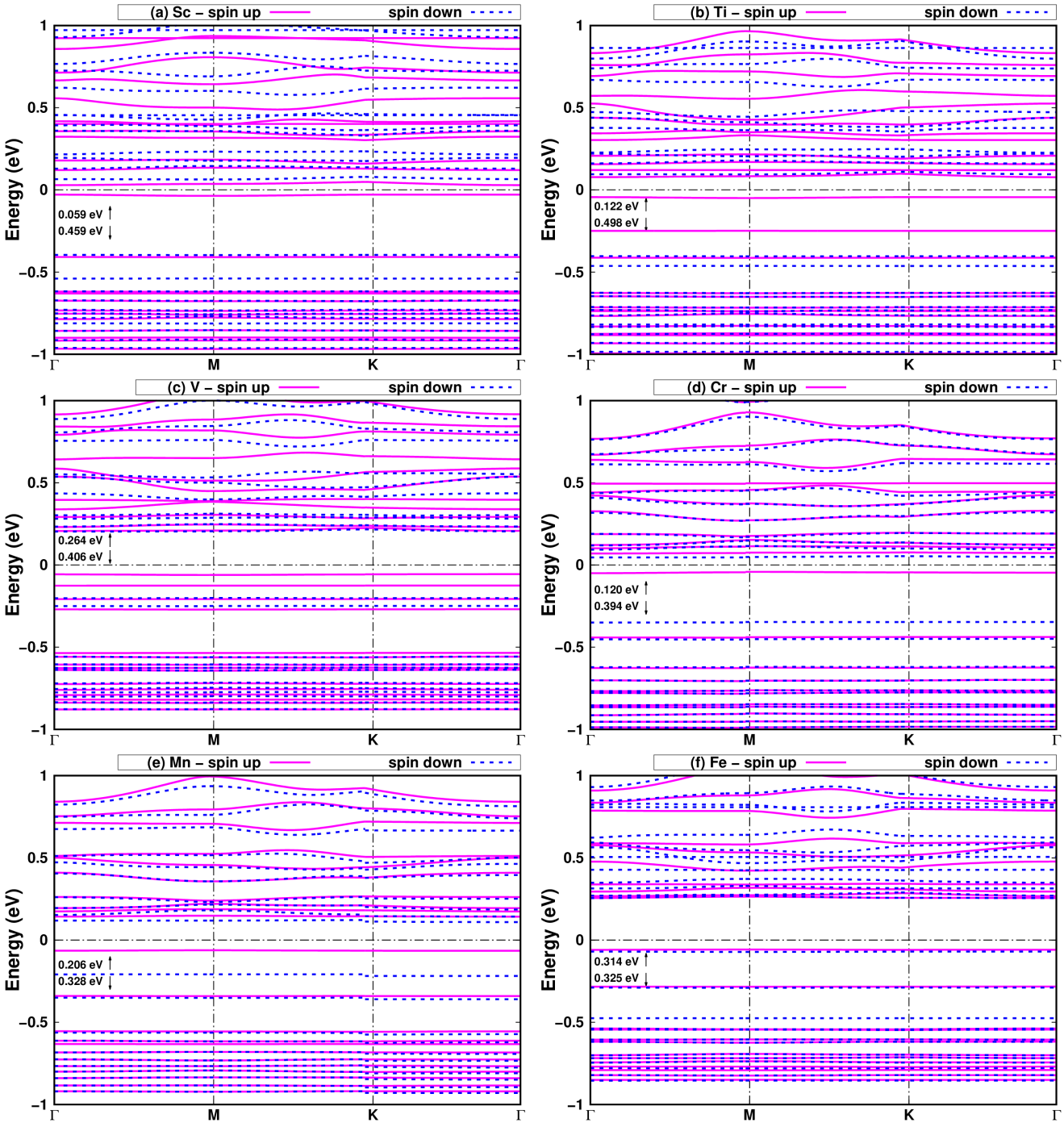

Figure S4. Electronic band structure of (a) Sc, (b) Ti, (c) V, (d) Cr, (e) Mn,and (f) Fe atom embedded C_3N_6 monolayer, respectively. Fermi energy levelis shifted to 0 eV. Spin up (↑) and spin down (↓) states are shown in magenta (continuous line) and blue (dashed line) colors, respectively. (A color version of this figure can be viewed online.)

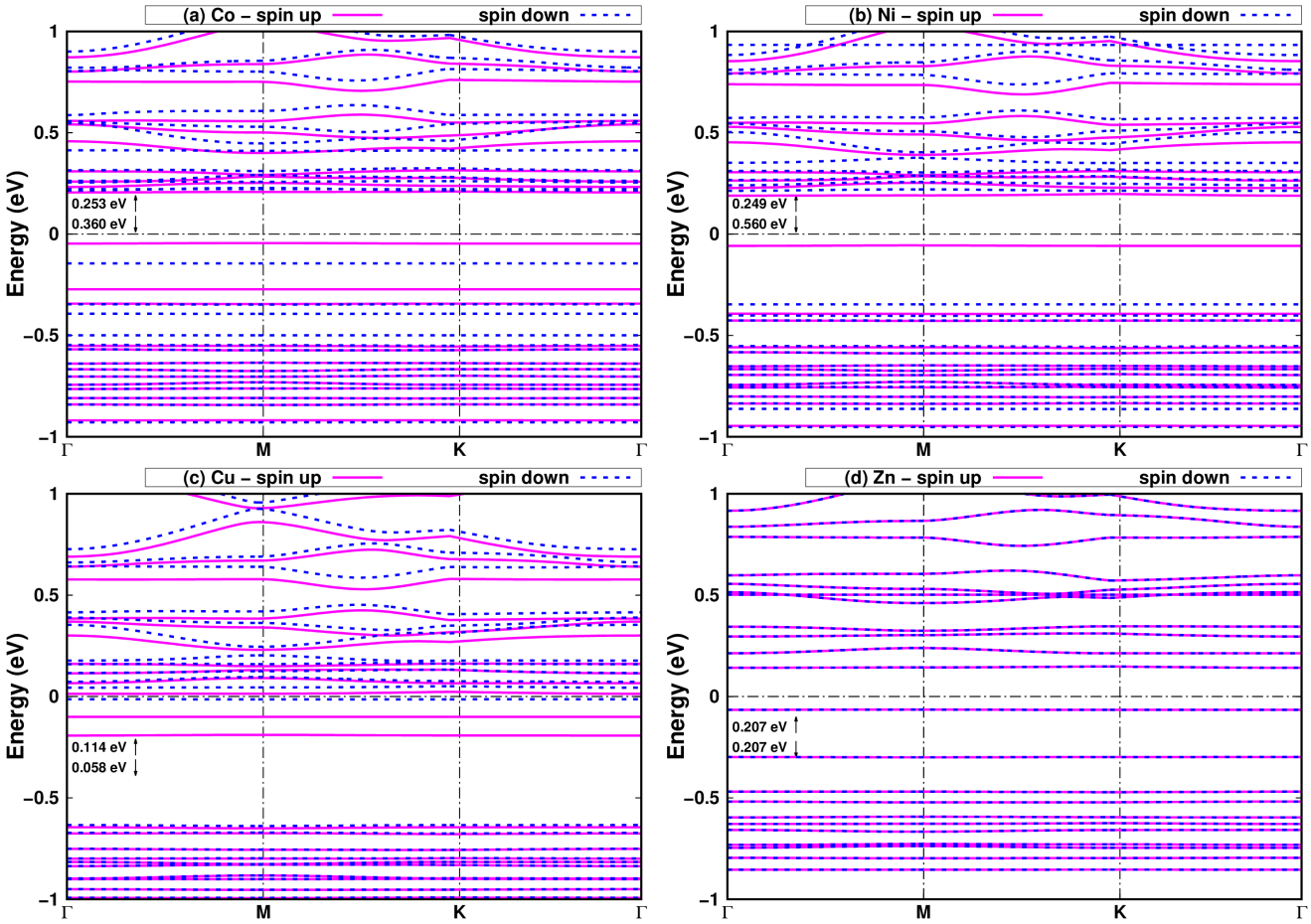

Figure S5. Electronic band structure of (a) Co, (b) Ni, (c) Cu, and (d) Zn atom embedded C_3N_6 monolayer. Fermi energy level is shifted to 0 eV. Spin up (↑) andspin down (↓) states are shown in magenta (continuous line) and blue (dashed line) colors, respectively. (A color version of this figure can be viewed online.)

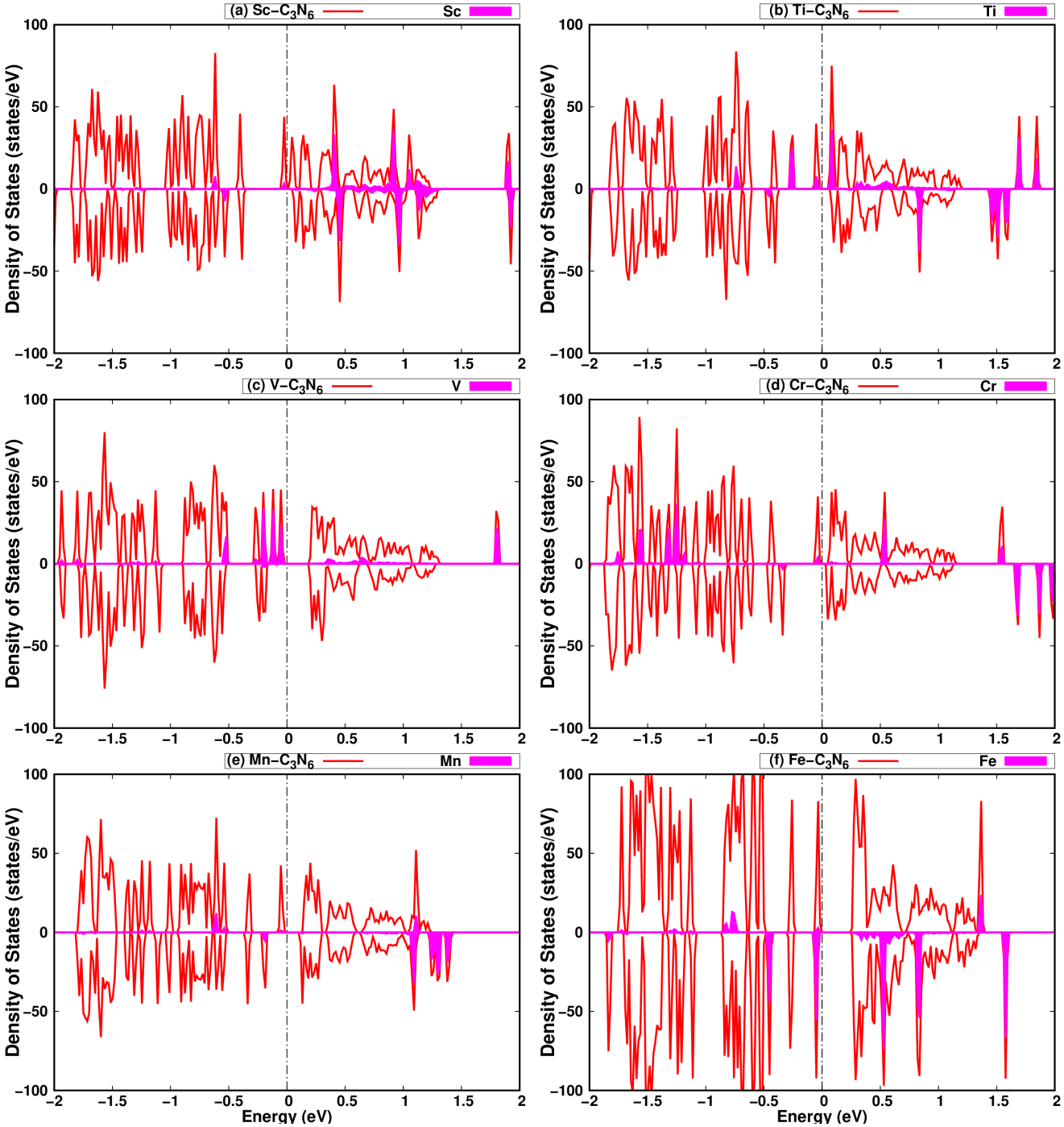

Figure S6. Total Density of States of (a) Sc, (b) Ti, (c) V, (d) Cr, (e) Mn, and (f) Fe atom embedded C_3N_6 monolayer, respectively (Shown in red color). Total contribution of embedded TM atom is shown in magenta color. Fermi energy level is shifted to 0 eV. (A color version of this figure can be viewed online.)

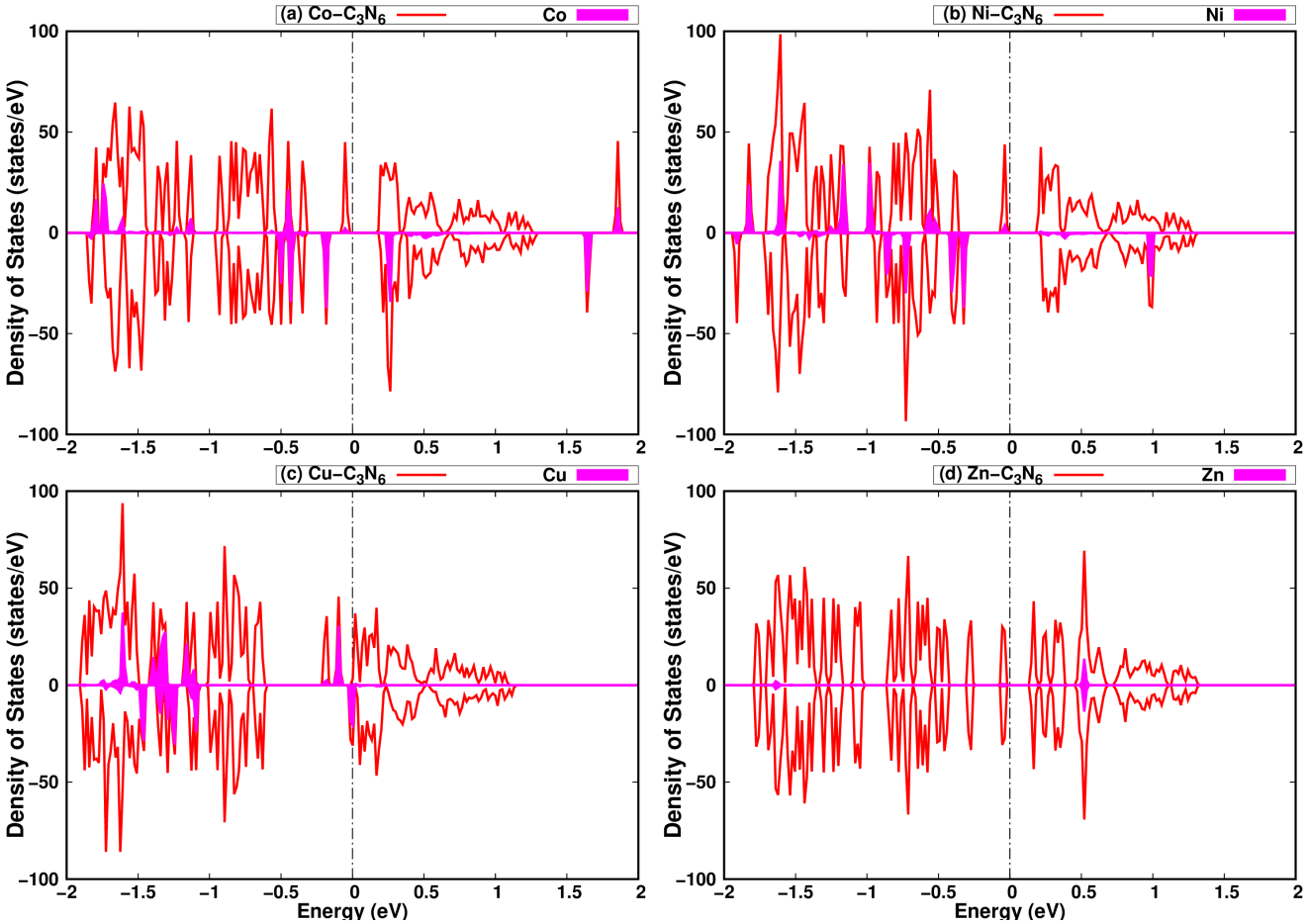

Figure S7. Total Density of States of (a) Co, (b) Ni, (c) Cu, and (d) Zn atom embedded C_3N_6 monolayer, respectively (Shown in red color). Total contribution of embedded TM atom is shown in magenta color. Fermi energy level is shifted to 0 eV. (A color version of this figure can be viewed online.)

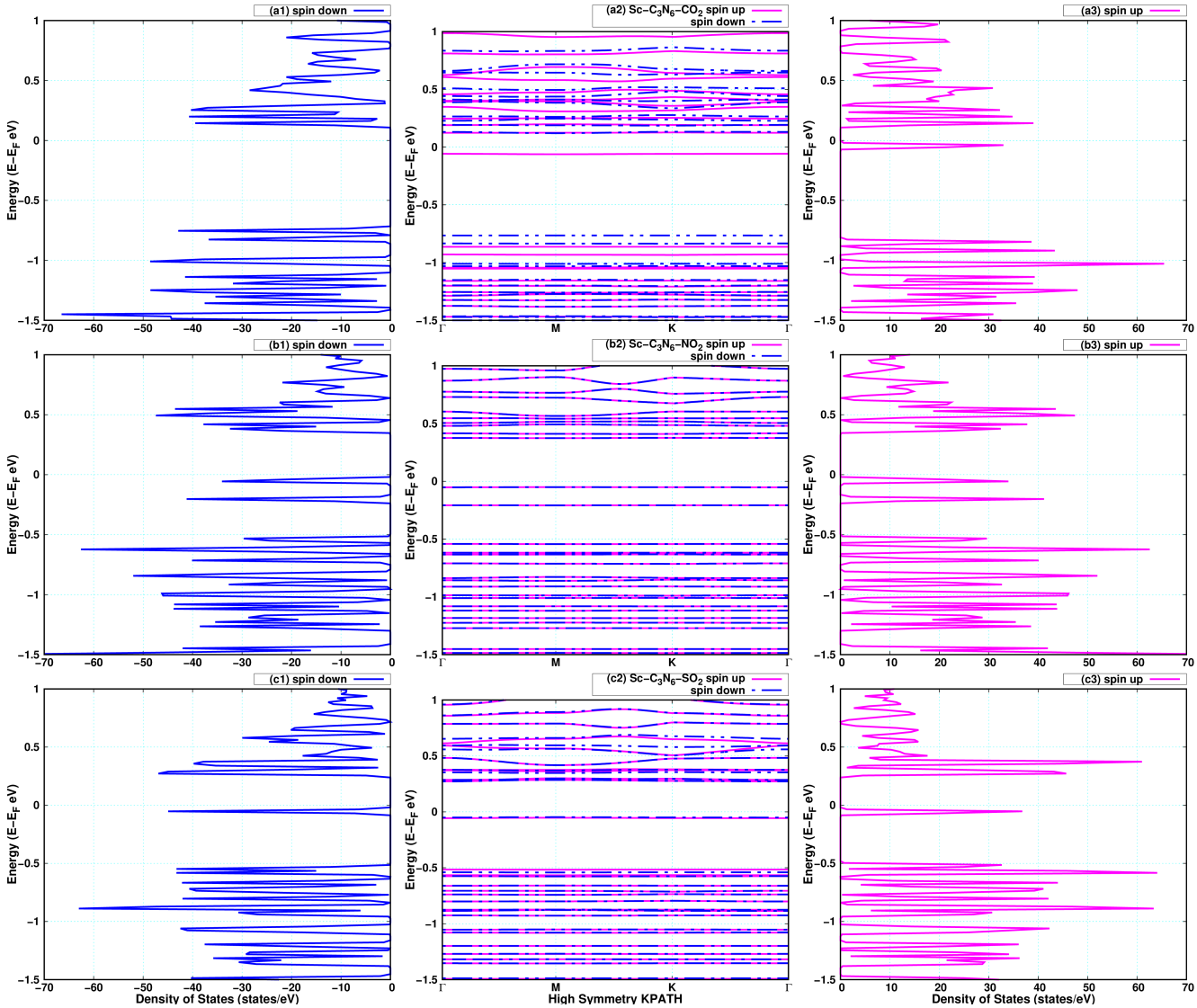

Figure S8. Total density of states and Eletronic bandstructure of Sc-C_3N_6 mono-layer towards (a1-a3) CO_2 (b1-b3) NO_2 (c1-c3) SO_2, respectively. Fermi energy level is shifted to 0 eV. (A color version of this figure can be viewed online.)

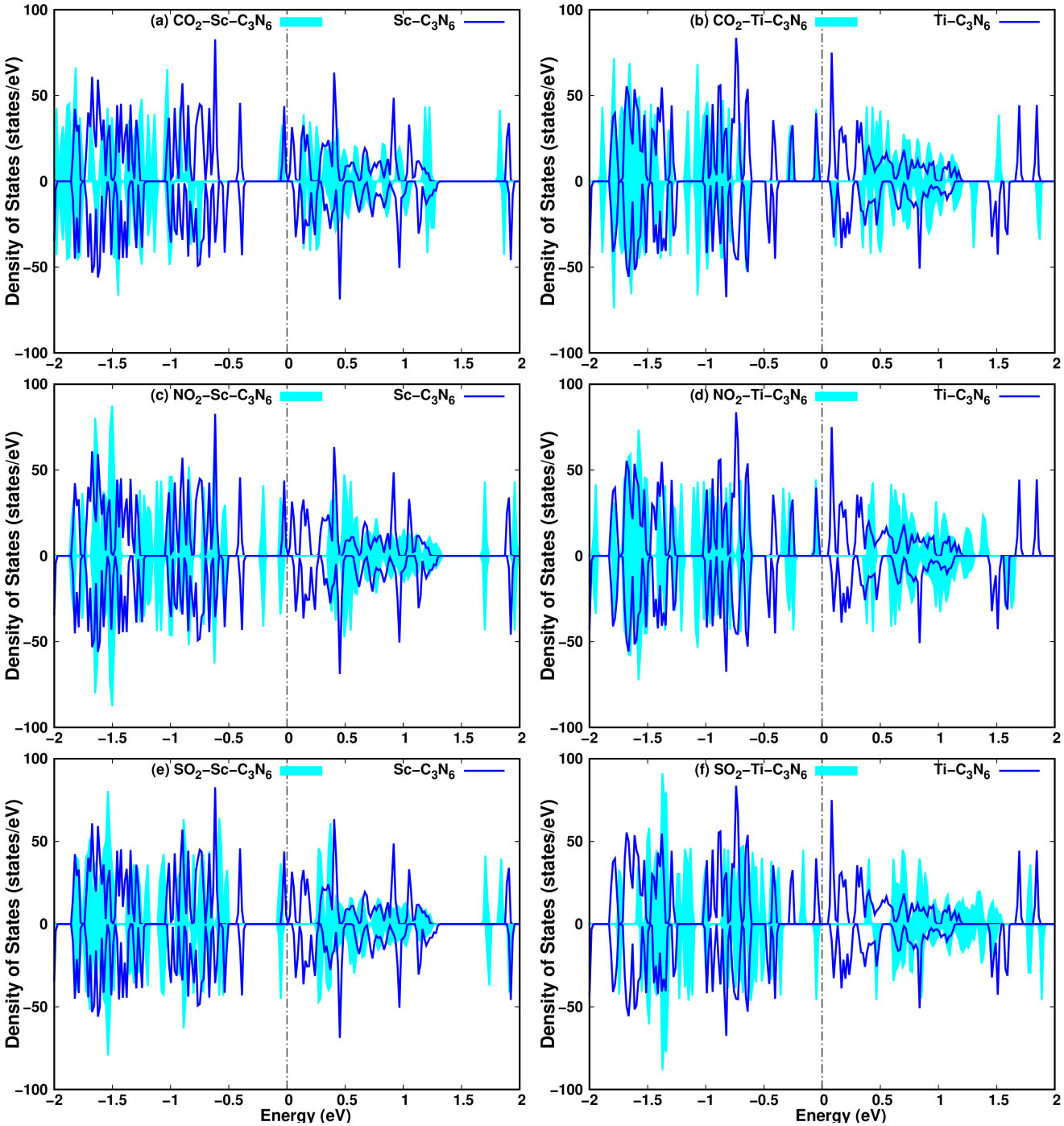

Figure S9. Total density of states of Sc-C_3N_6 monolayer compared with Sc embedded C_3N_6 monolayer towards (a) CO_2 (c) NO_2 (e) SO_2, respectively, and Ti-C_3N_6 compared with Ti embedded C_3N_6 monolayer towards (b) CO_2 (d) NO_2 (f) SO_2, respectively. (A color version of this figure can be viewed online.)