

Supporting Information

for

Ferroelectricity and magnetism in metal-formate frameworks of

$[\text{NH}_4][\text{M}(\text{HCOO})_3]$ (M=Sc to Zn) : A first-principles study

Yingjie Sun,^a Zhiwen Zhuo^b and Xiaojun Wu^c

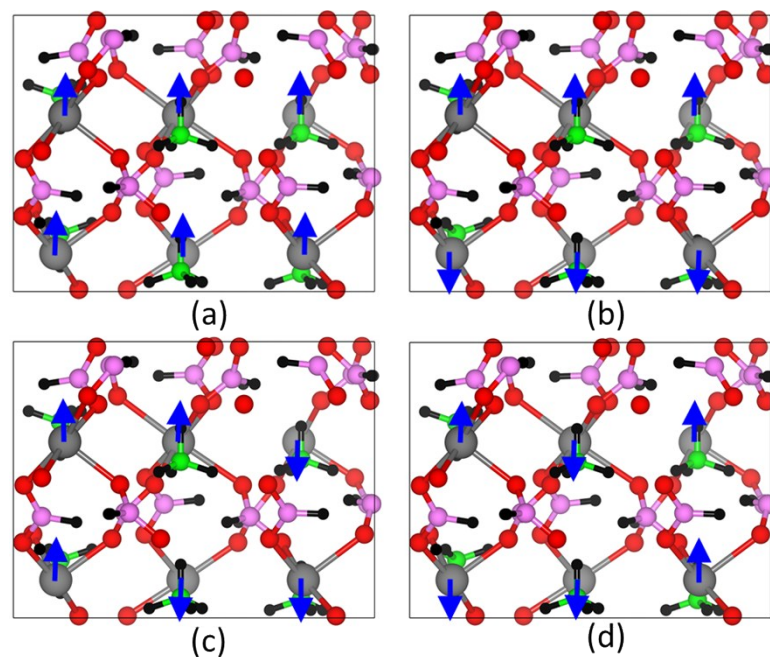


Fig. S1. Magnetic orders in metal-MFFs. (a) Ferromagnetic (FM). (b)-(c) Different antiferromagnetic magnetic orders. (b) AF1, (c) AF2, (d) AF3. Atom scheme: H, black; C, pink; O, red; Zn, gray; N, green.

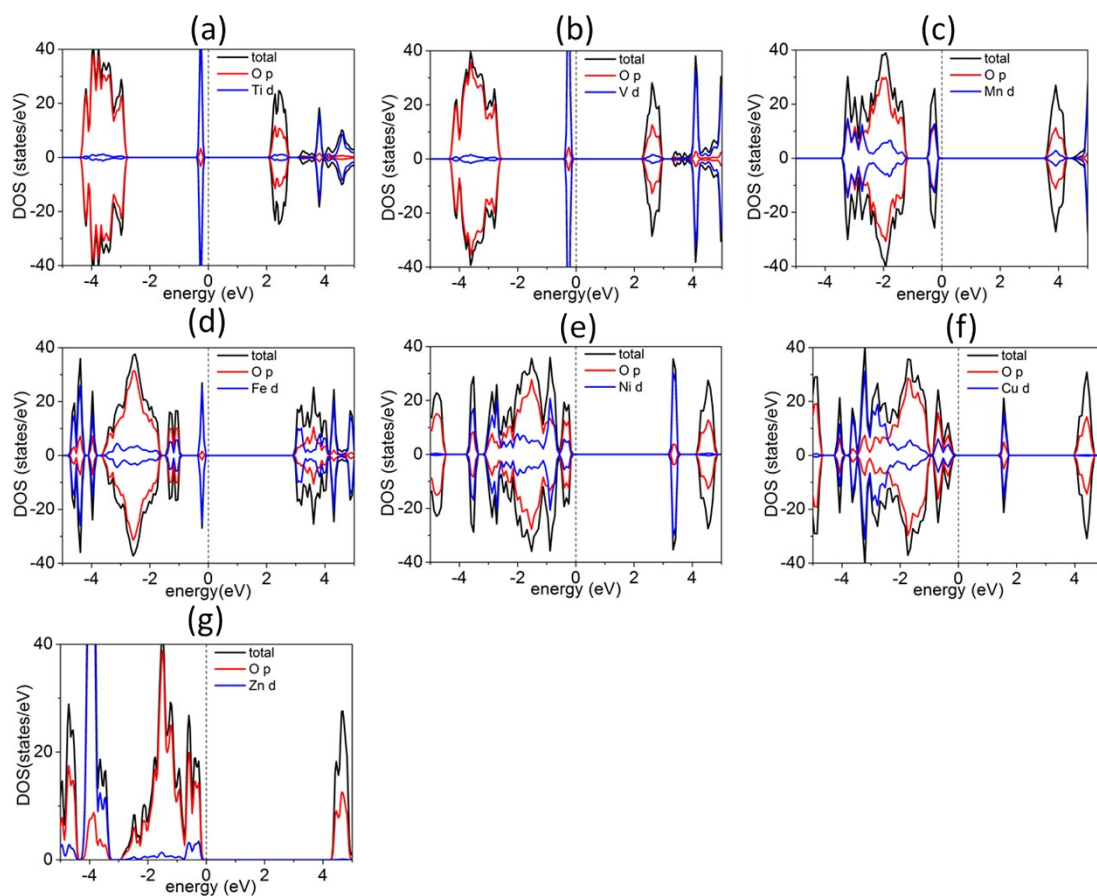


Fig.S2 (a)-(g) Spin-polarized partial density of states (PDOS) for Ti, V, Mn, Fe, Ni, Cu and Zn MFF from top to bottom, respectively.

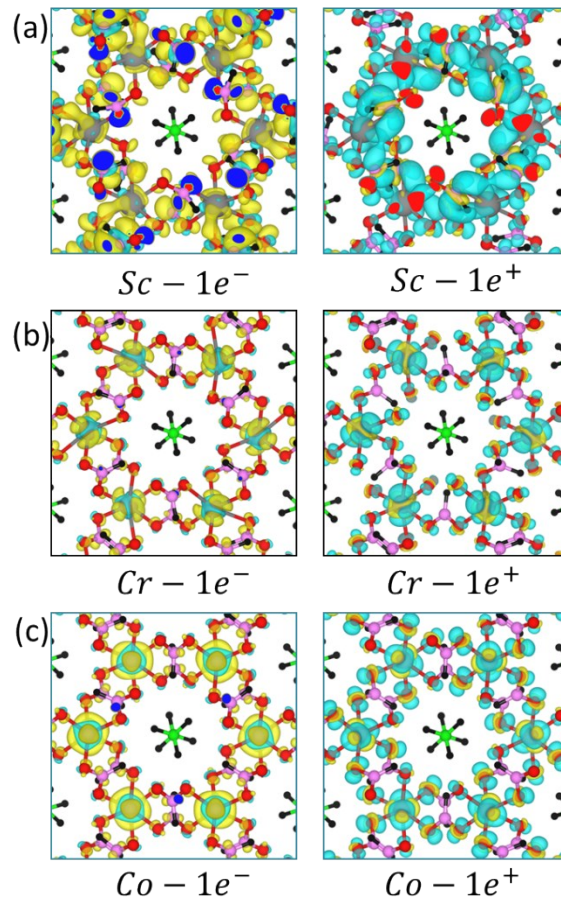


Fig. S3 Deformation density maps of carrier doping Sc-MFF, Cr-MFF and Co-MFF. One electron ($1e^-$) charged(left) and one hole ($1e^+$) charged(right). (a) Isosurface level is $0.0005 e/\text{\AA}^3$. (b) and (c) Isosurface level is $0.001 e/\text{\AA}^3$. The yellow and green parts correspond to electron density increase and decrease, respectively.