

TABLE I: The lattice constant in the c axial direction, the electronic ground state (GS), the band gap for semiconductor and half metal cases, the total supercell magnetic moment (M) per TM and valence electron distribution (VED) of $[\text{TM}_2(\text{Ant})]_\infty$ (TM= Sc, Ti, V, Cr, Mn and Fe).

meV	$c(\text{\AA})$	GS	band gap (eV)	$M(\mu_B)$	VED
Sc	7.89	$NN(\text{metal})$	0.00	0.00	$3d^1 4s^2$
Ti	7.37	$FA(\text{metal})$	0.00	0.00	$3d^2 4s^2$
V	7.01	$FF(\text{half metal})$	0.76(direct)	2.00	$3d^3 4s^2$
Cr	6.79	$FF(\text{half metal})$	1.25(direct)	0.96	$3d^4 4s^2$
Mn	6.64	$NN(\text{semicond})$	0.66(direct)	0.00	$3d^5 4s^2$
Fe	6.87	$AF(\text{metal})$	0.00	0.00	$3d^6 4s^2$