Electronic Supplementary Material (ESI) for Nanoscale.

Supporting Information for

Metal-organic Frameworks: Possible New Two-Dimensional Magnetic and Topological materials

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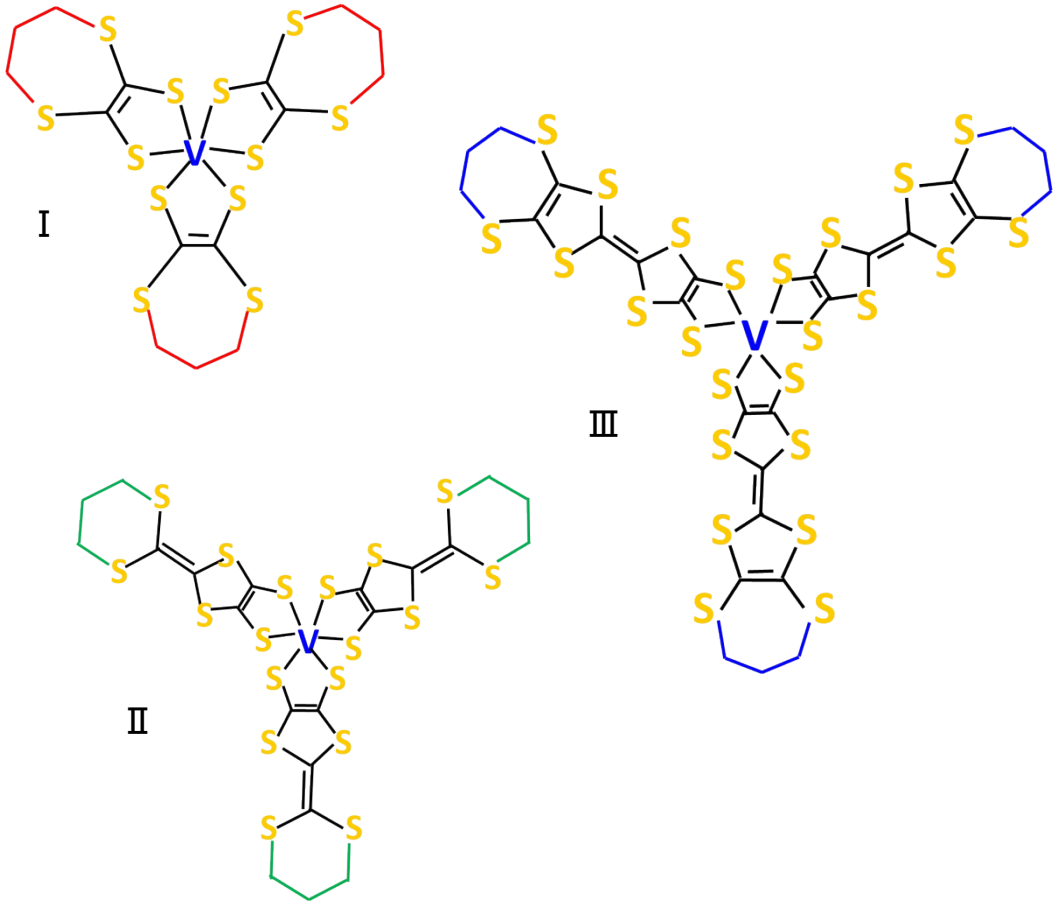

Fig. S1. Crystal structures of complexes of Ⅰ-Ⅲ.

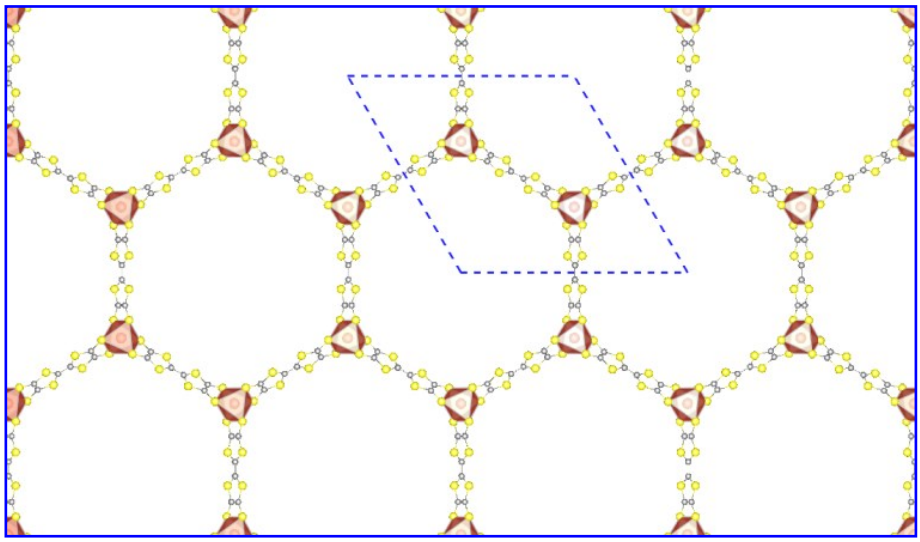

Fig. S2. The schematic structure of the predicted 2D M-Hex-Ⅱ.

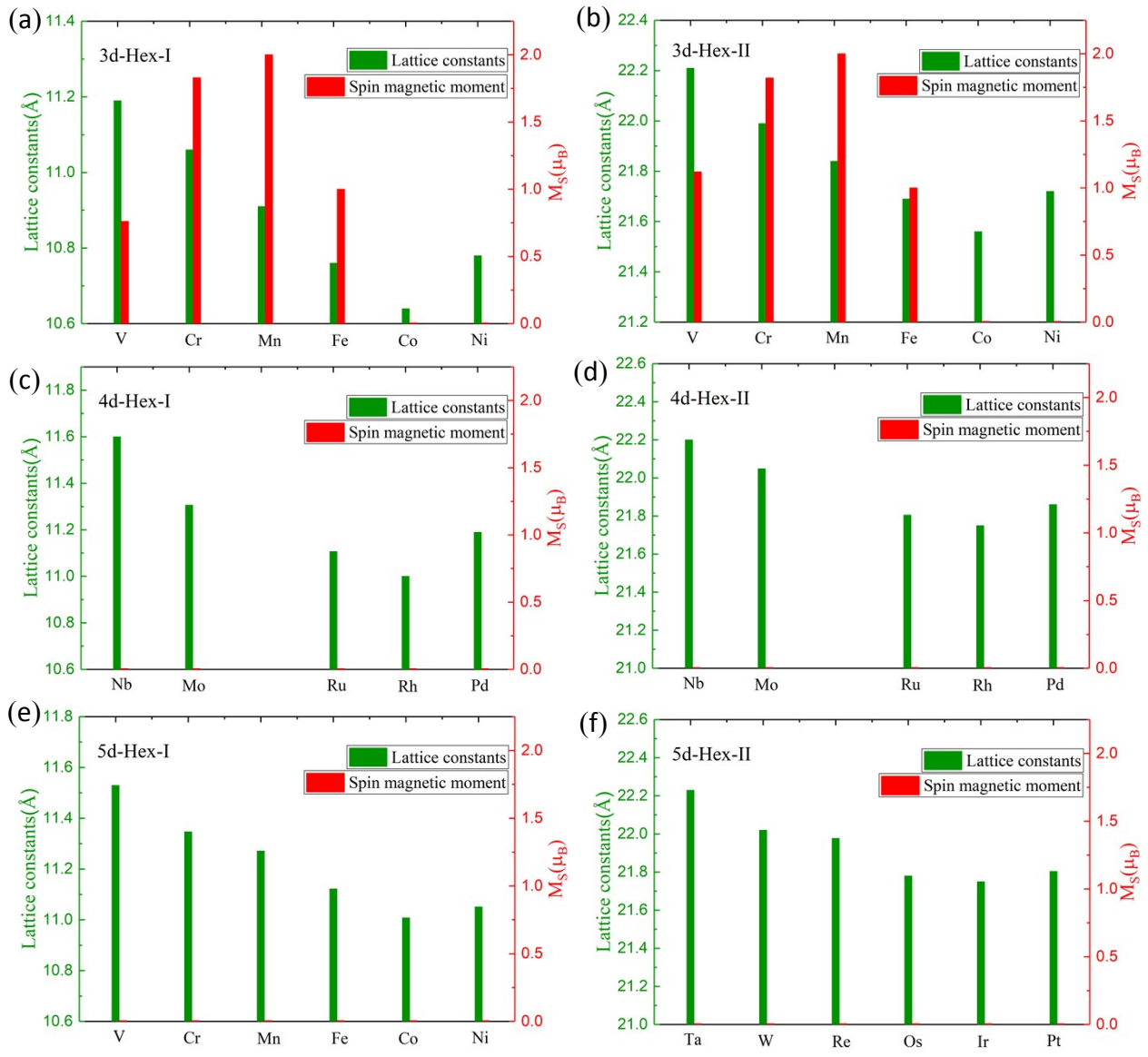

Fig. S3. The lattice constants and spin magnetic moments of different TM-Hex-Ⅰ/Ⅱ lattices.

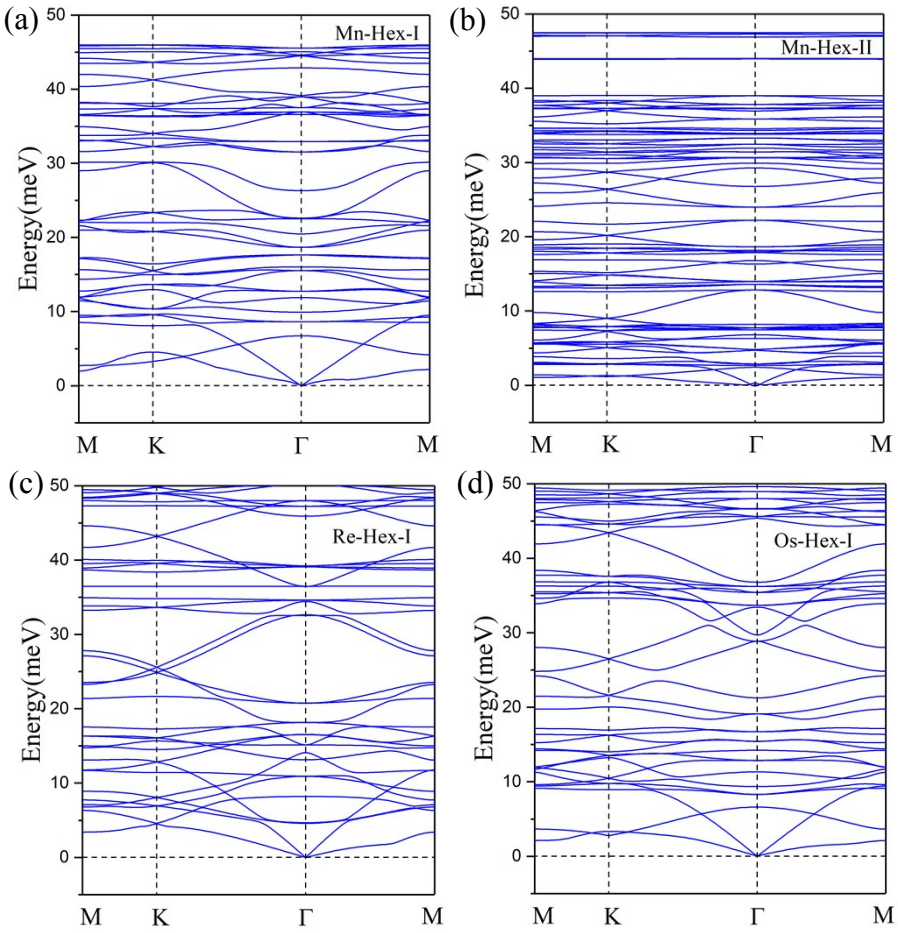

Fig. S4. (a)-(d) The phonon spectrum of Mn-Hex-I, Mn-Hex-Ⅱ, Re-Hex-I and Os-Hex-I, respectively.

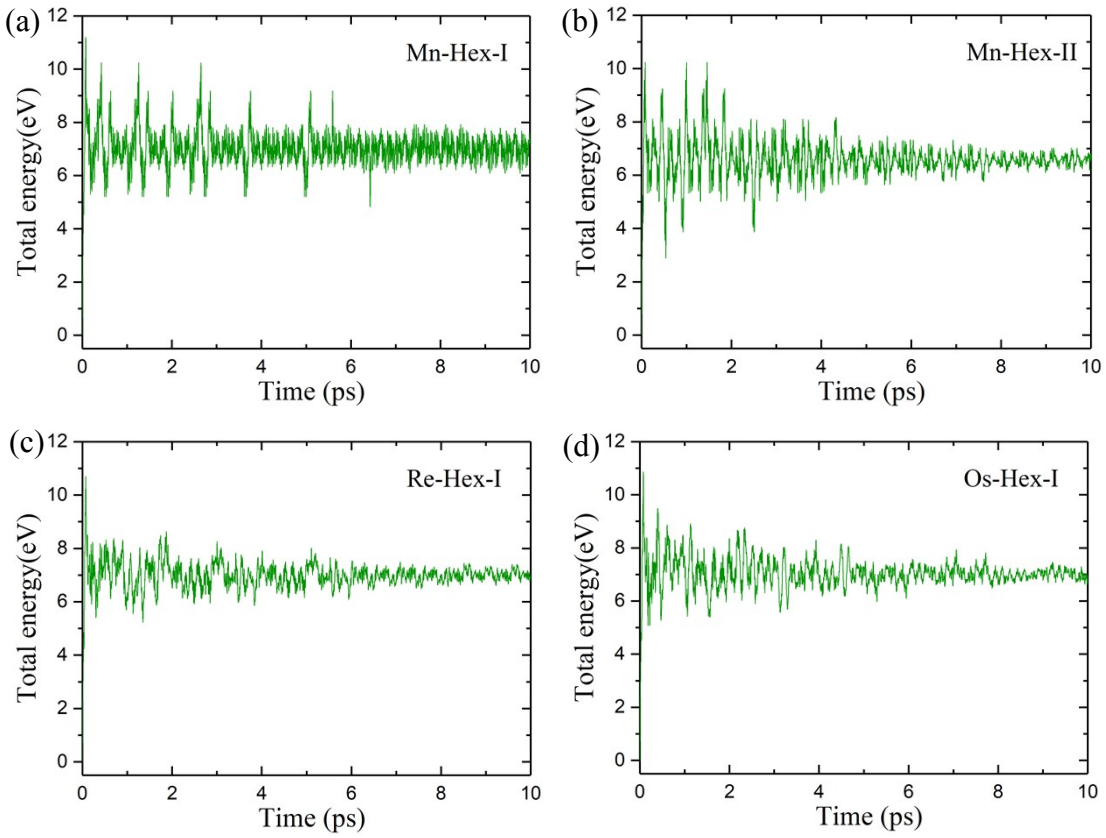

Fig. S5. (a)-(d) The relative total energy as function of time for Mn-Hex-I, Mn-Hex-Ⅱ, Re-Hex-I and Os-Hex-I, respectively.

	V-Hex-I	Mn-Hex-I	Fe-Hex-I	V-Hex-II	Mn-Hex-II	Fe-Hex-II
ΔE_{AFM-FM} (meV)	65.1	398.1	116.9	13.4	126.6	43.5
MAE(meV)	0.01	0.75	-0.23	0.006	0.86	-0.21
J_1	37.08	60.60	55.72	8.87	22.08	18.35
J_2	2.42	5.34	6.76	0.64	1.3	1.4

Table SI. The exchange energy, magnetocrystalline anisotropy energy and exchange parameters, J_i, of V(Mn, Fe)-Hex-I(II).

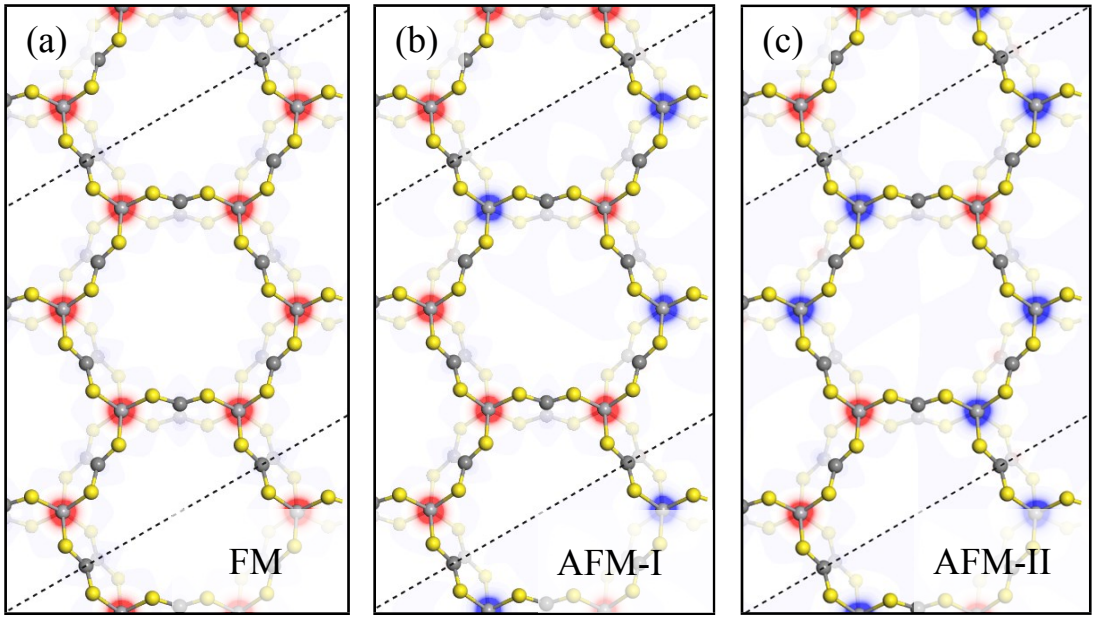

Fig. S6. (a)-(c) The schematic diagram of three different magnetic ordering (FM, AFM-I and AFM-II), respectively. Red and blue color represent spin up and spin down, respectively.

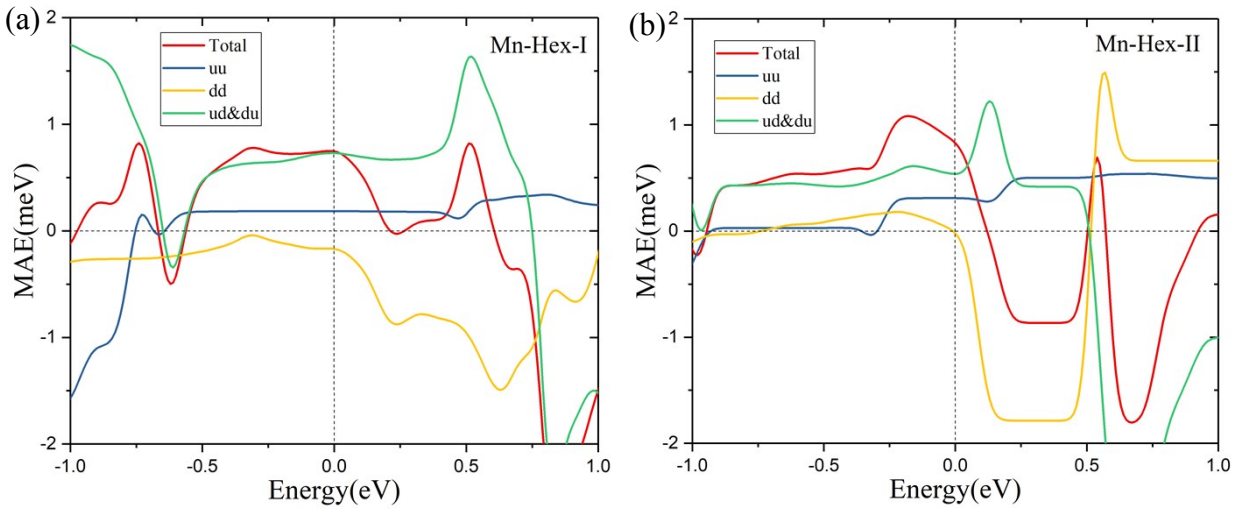

Fig. S7. (a) (b) The Fermi level dependent total and spin channel decomposed MAEs of Mn-Hex-I(II) from the rigid band model analyses.

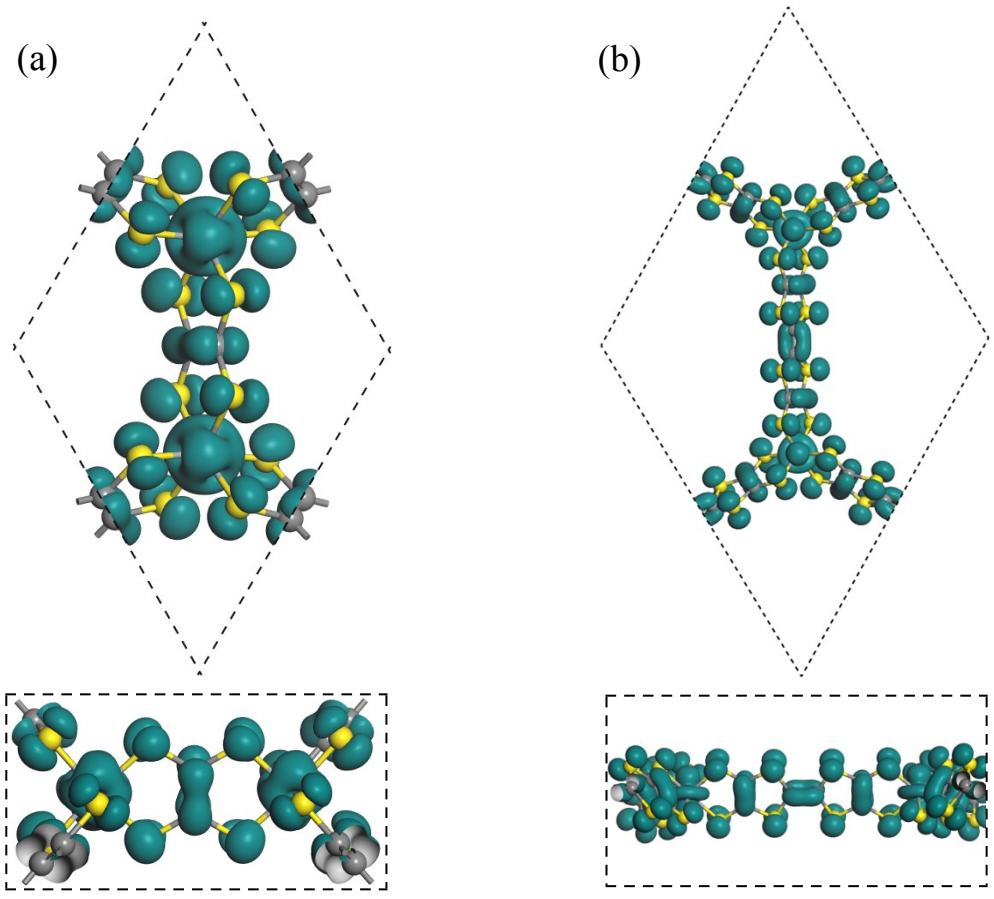

Fig. S8. (a) (b)Top and side view of the partial charge density distribution around the Fermi level (-0.2-0.2eV, l= 0.0005e/Å^3) of Mn-Hex-I (II), respectively.

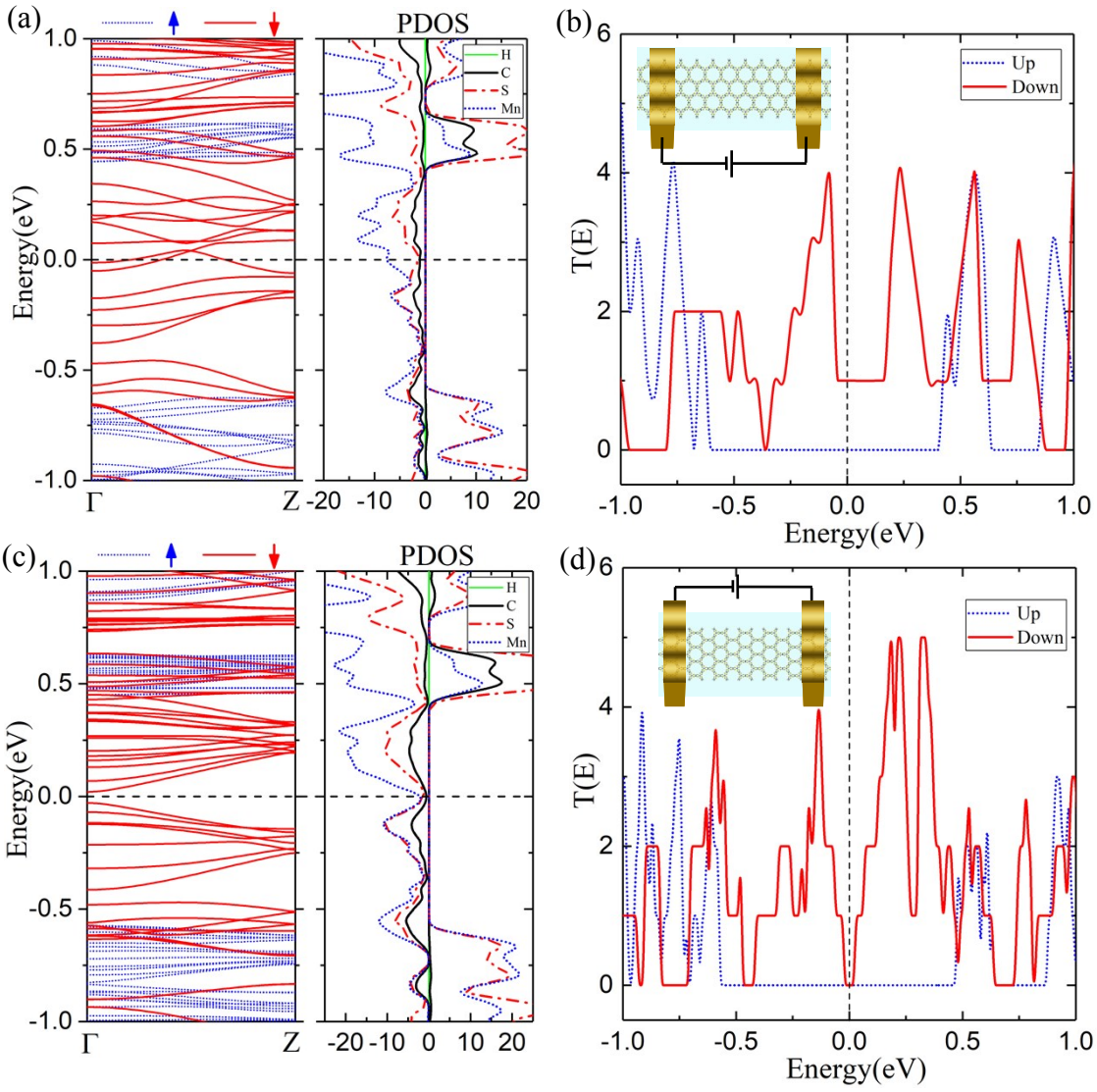

Fig. S9. (a) and (c)The band structure and PDOS of zigzag and armchair Mn-Hex-I nanoribbon, respectively. (b) and (d) The corresponding transmission spectra at zero bias. The transmission coefficients under zero bias can be calculated from $T(E,V) = Tr[\Gamma_L(E)G^R(E)\Gamma_R(E)G^A(E)$, with

$\Gamma_{L(R)} = i(\sum_{L(R)}^{R} - \sum_{L(R)}^{A})$; $G^A(E)$ and $G^R(E)$ are the advanced and retarded Green's functions of the scattering region; and $\sum_{L(R)}^{R(A)}$ *are electrodes' self energies* .

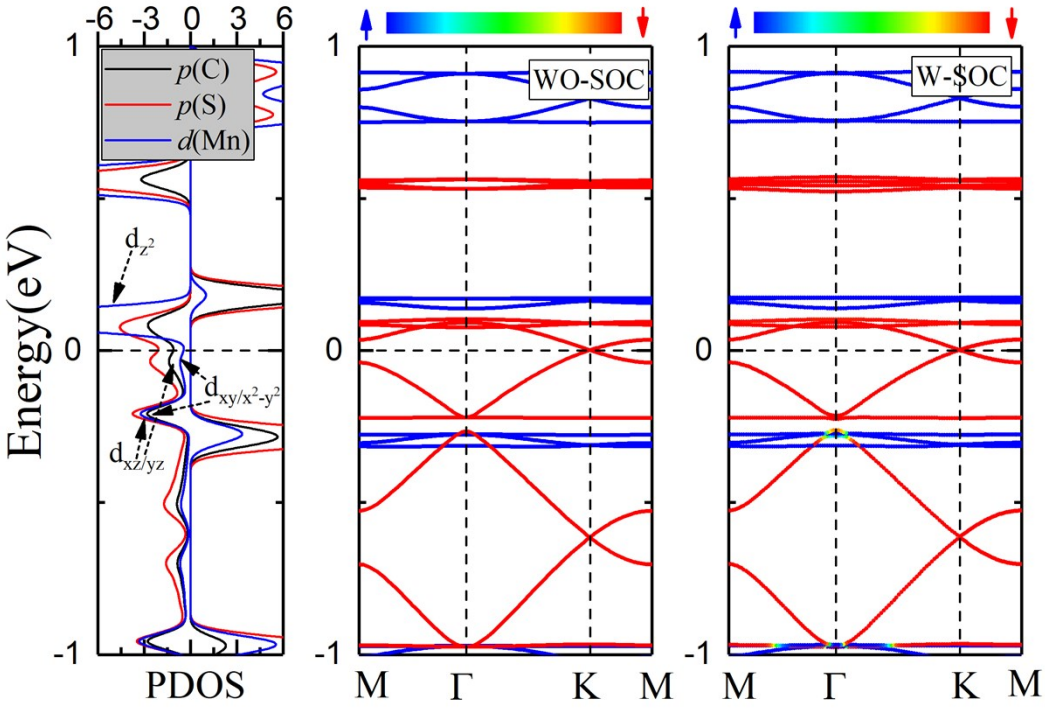

Fig. S10. (Left) The PDOS of Mn-Hex-II. (Middle and Right) The band structures of Mn-Hex-II without and with SOC, respectively.

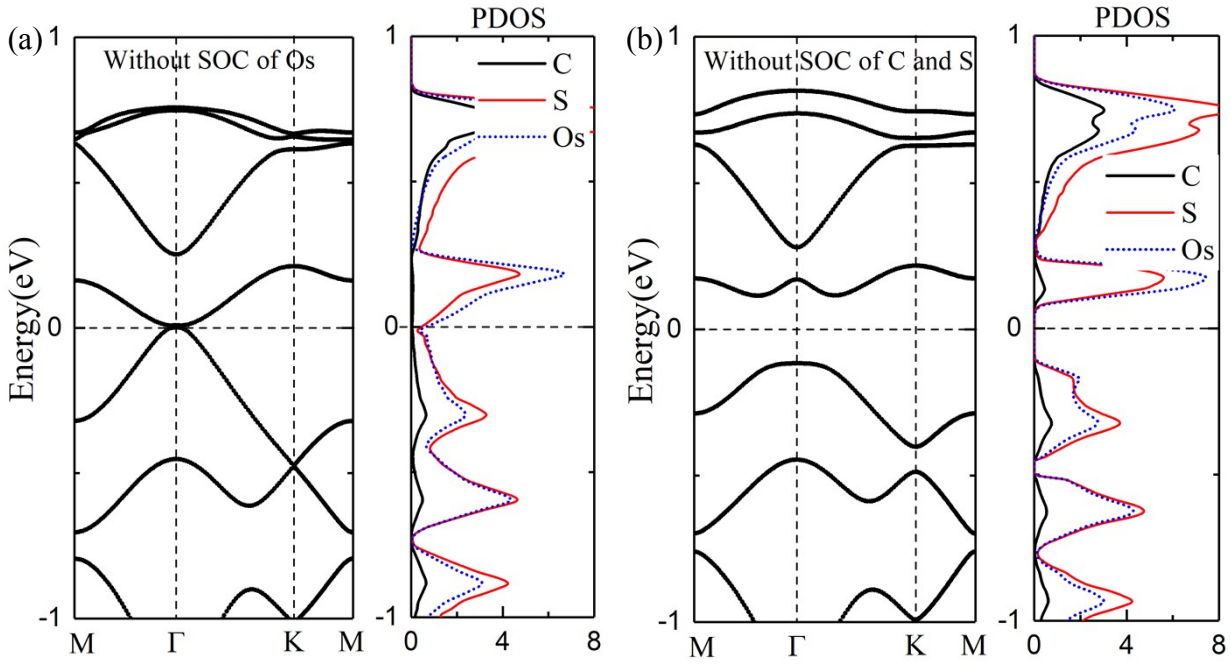

Fig. S11. (a) (b) The band structure and PDOS of Os-Hex-I without SOC of Os atoms and without SOC of C and S atoms, respectively.

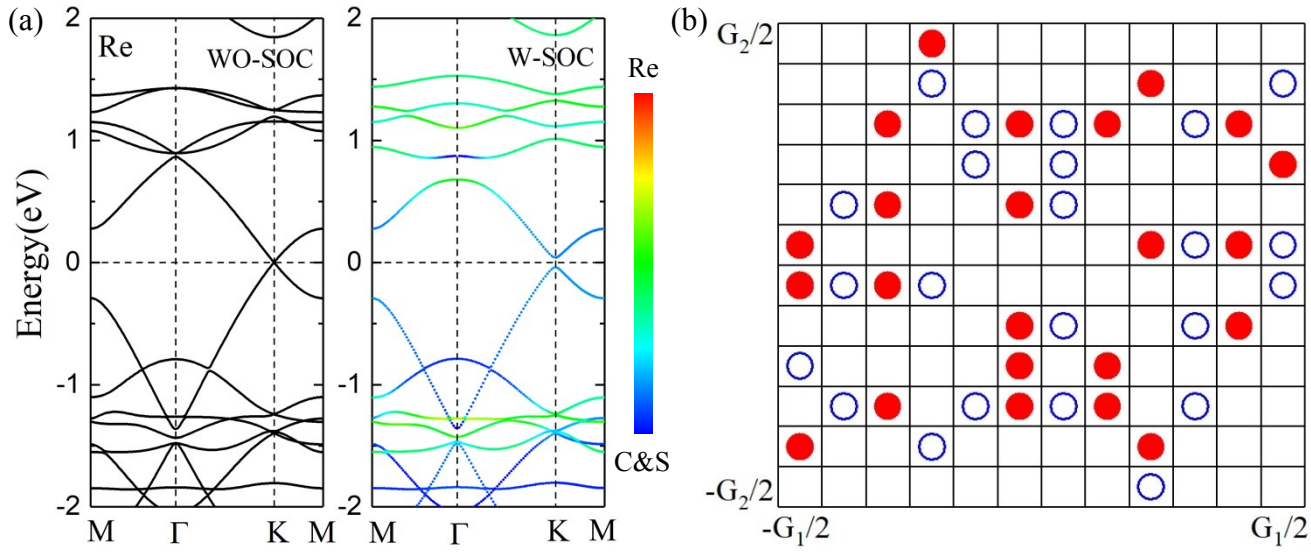

Fig. S12. (a) (b) The band structure (without and with SOC) and corresponding n-field configuration of Re-Hex-I, respectively.

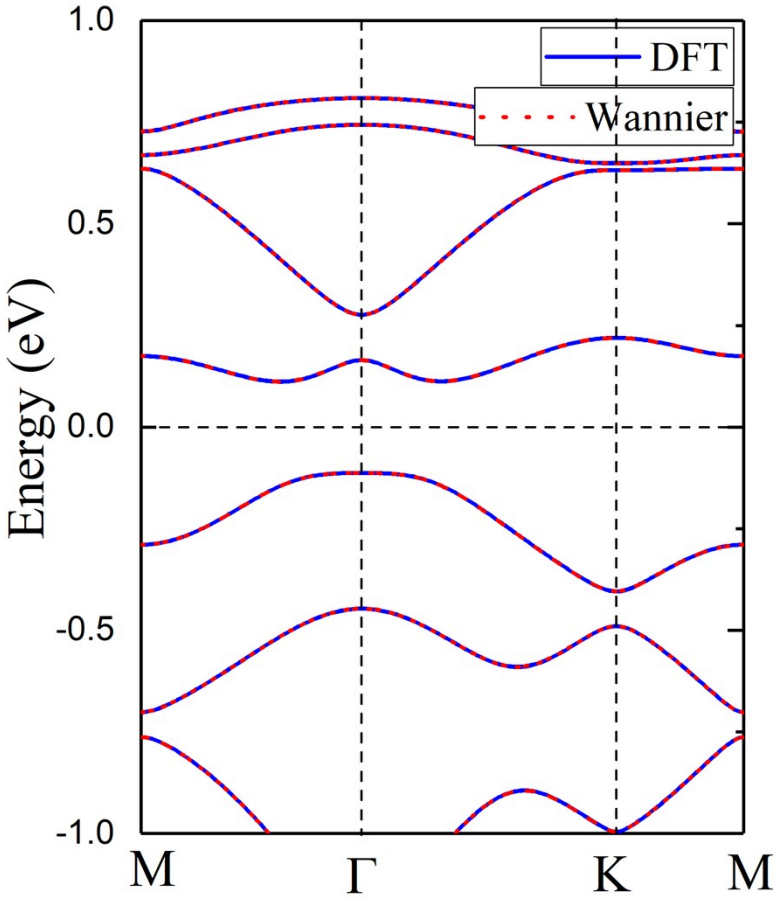

Fig. S13. The band structure of Os-Hex-I from DFT and the maximally localized Wannier functions calculations, respectively.