Supplementary Information

Effect of transition metal substitution doping on the structure and magnetic properties of biphenylene†

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Table S1: Convergence test results for different k-point meshes, showing the calculated total energy and relative energy change (ΔE) between successive meshes. The total energy stabilizes as the k-point mesh increases, with a minimal relative change ($\Delta E < 0.001$ eV) achieved at the 6×6×1 and 7×7×1 meshes, indicating that these are sufficiently dense for convergence.

k-Point Mesh	Total Energy (eV)	Relative Energy Change (ΔE, eV)
3×3×1	-.20699136E+03	-
4×4×1	-.20696635E+03	0.0250
5×5×1	-.20695882E+03	0.0075
6×6×1	-.20695365E+03	0.0052
7×7×1	-.20695437E+03	0.0007

Table S2: Convergence test results for the energy cutoff values, showing the total energy and relative energy change (ΔE) between consecutive cutoff values. Between 500 eV and 550 eV, ΔE reduces to 0.005 eV, suggesting that this range achieves energy convergence. However, as the cutoff values increase to 600 eV and 650 eV, the total energy displays slight fluctuations, indicating minor instability. Thus, a cutoff range of 500-550 eV is recommended to balance convergence accuracy and computational efficiency.

Energy Cutoff (eV)	Total Energy (eV)	Relative Energy Change (ΔE, eV)
450	-.20700295E+03	-
500	-.20695437E+03	0.049
550	-.20695945E+03	0.005
600	-.20699985E+03	0.040
650	-.20705003E+03	0.050

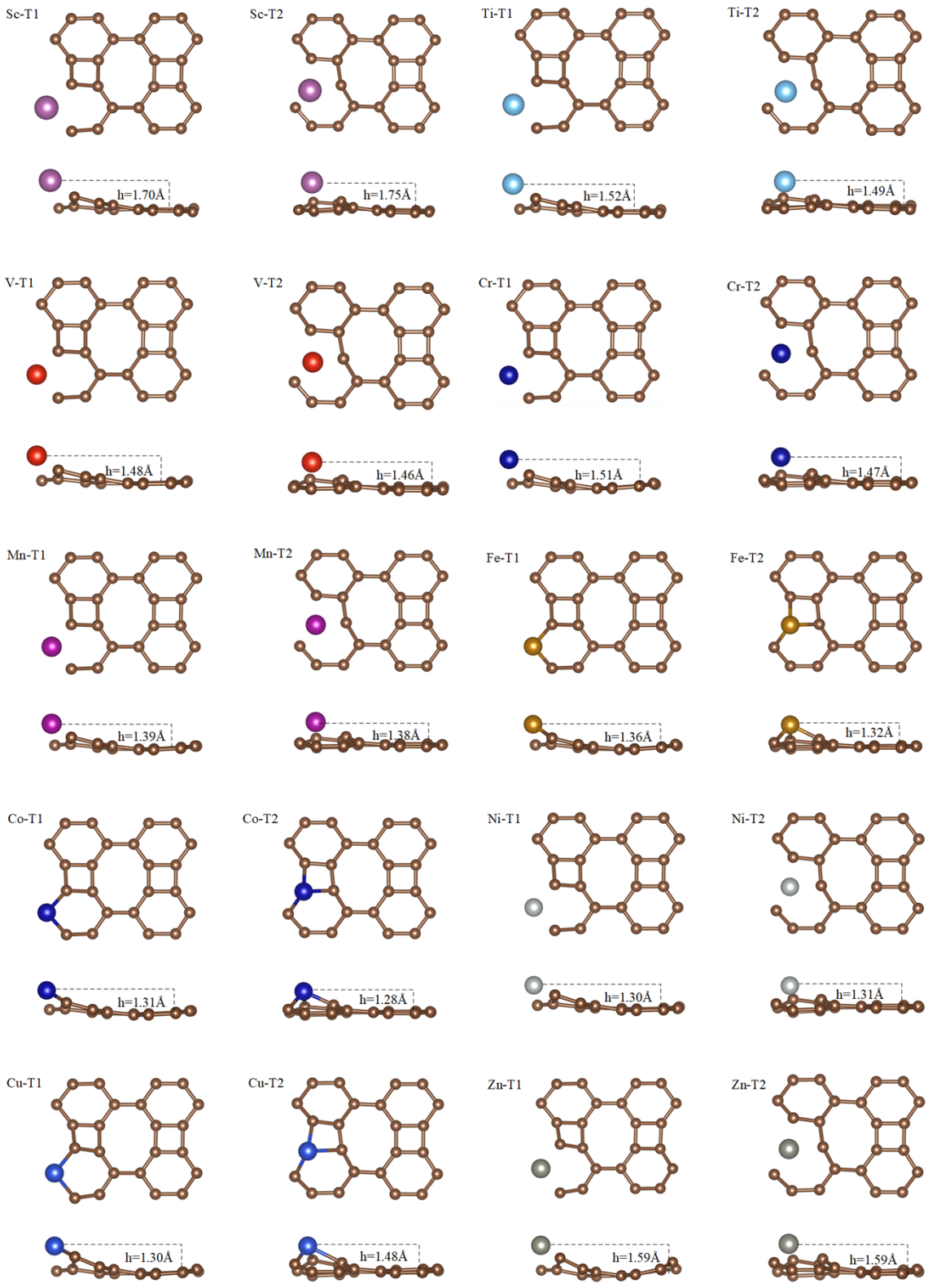

Figure S1: Diagrams of 10 types of TM-BPN structures.

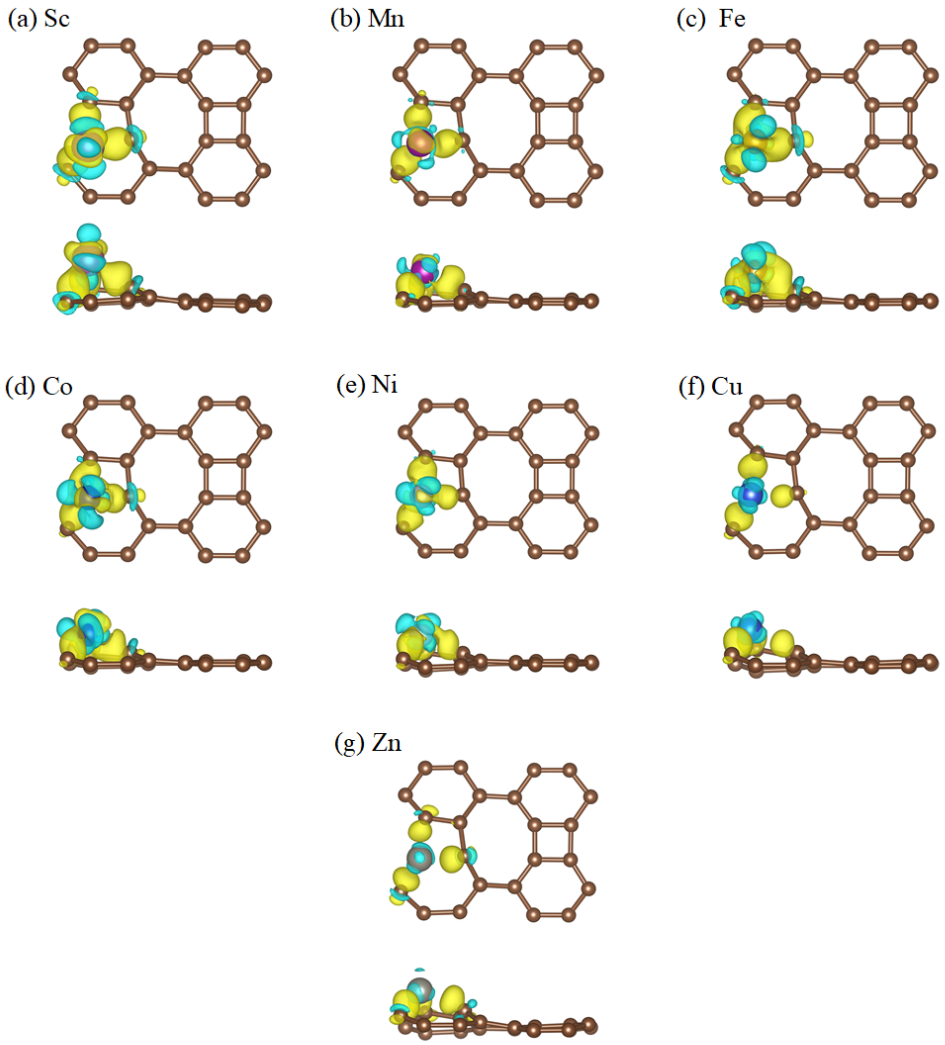

Figure S2: Charge difference diagrams of 8 types of TM-T2 doped systems. Yellow represents charge accumulation, and blue represents charge depletion.

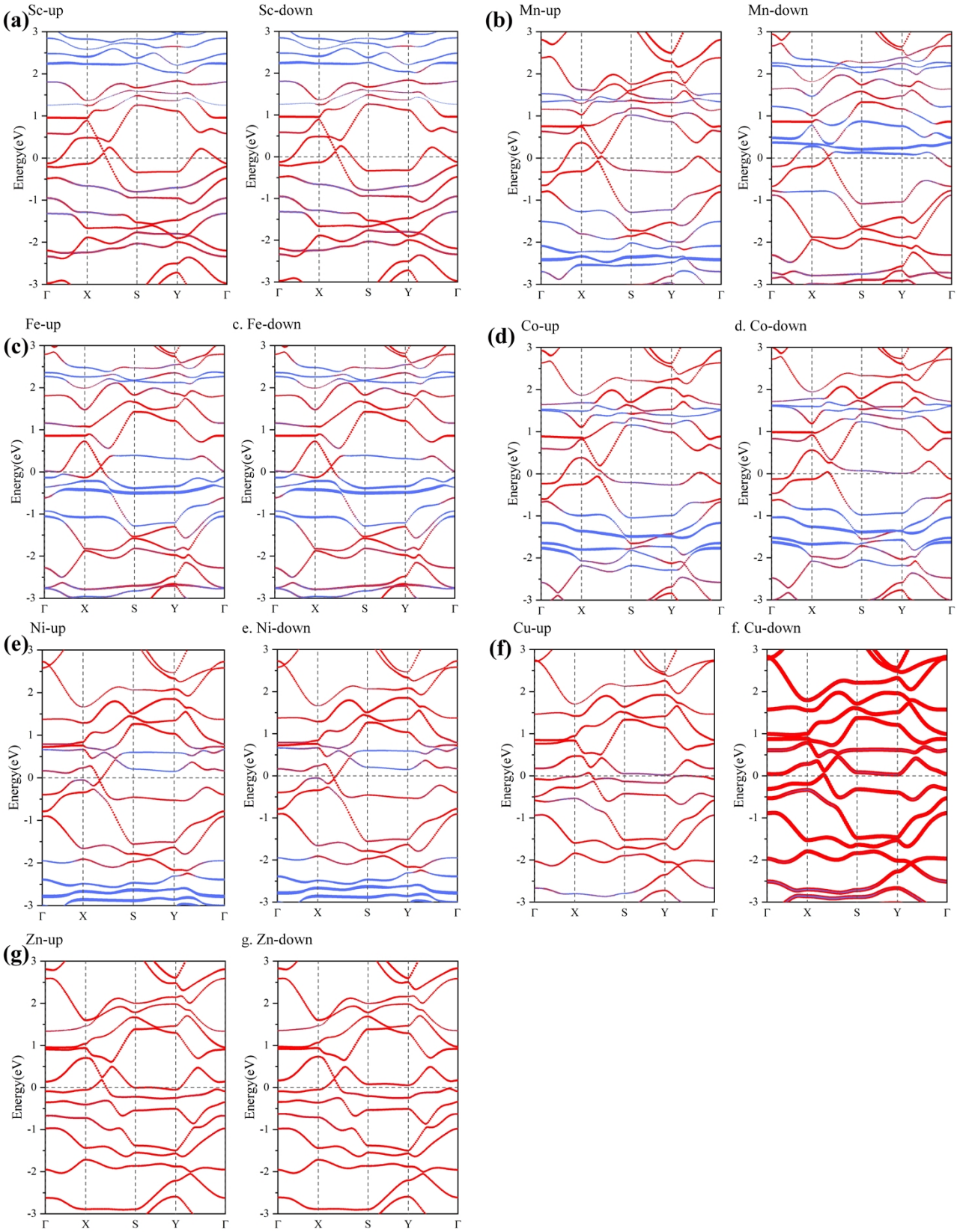

Figure S3: Projected band structures of 8 types of TM-T2 structures, with red representing carbon elements and blue representing transition metal elements.

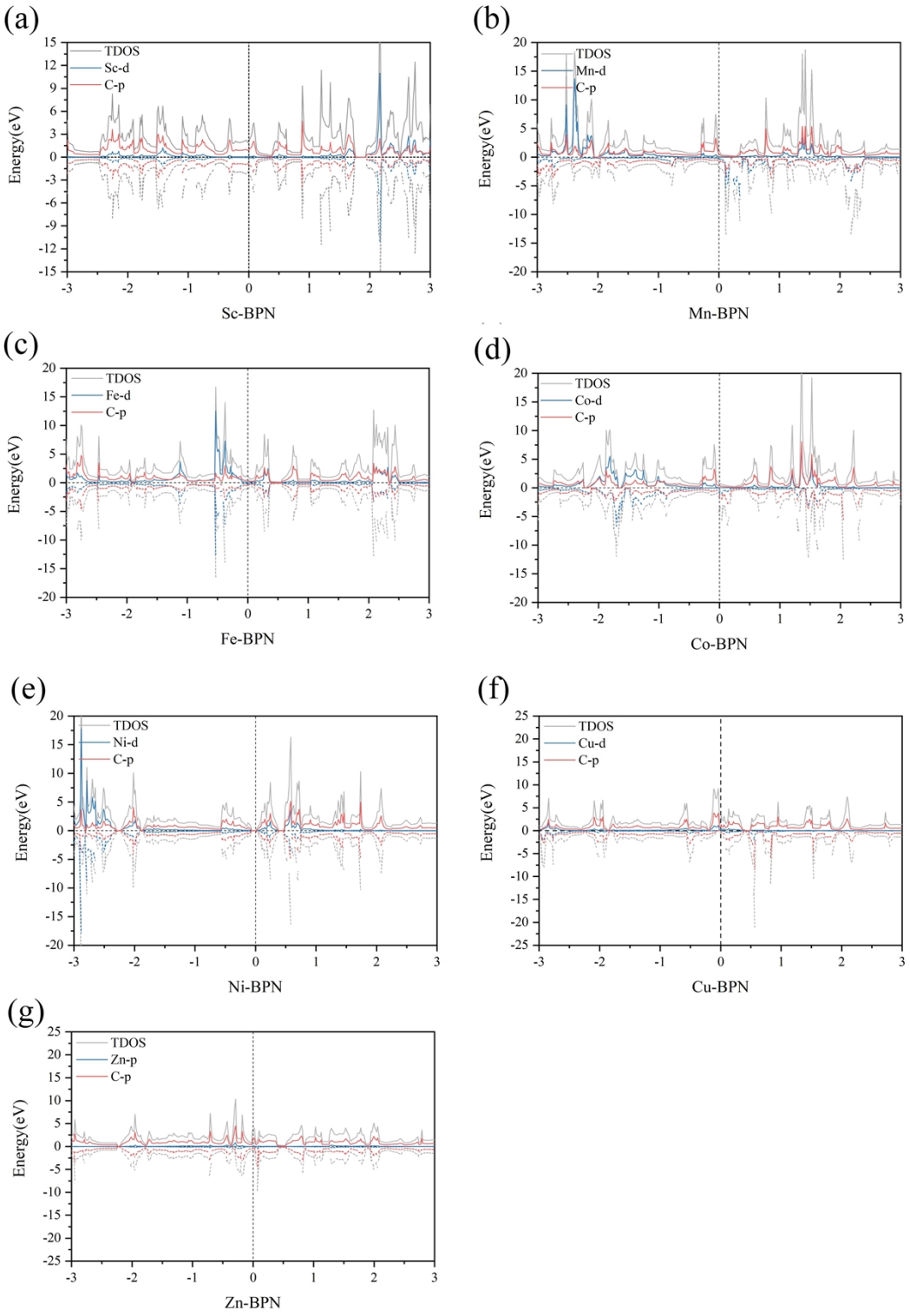

Figure S4: Density of states of 7 types of TM-T2 systems.

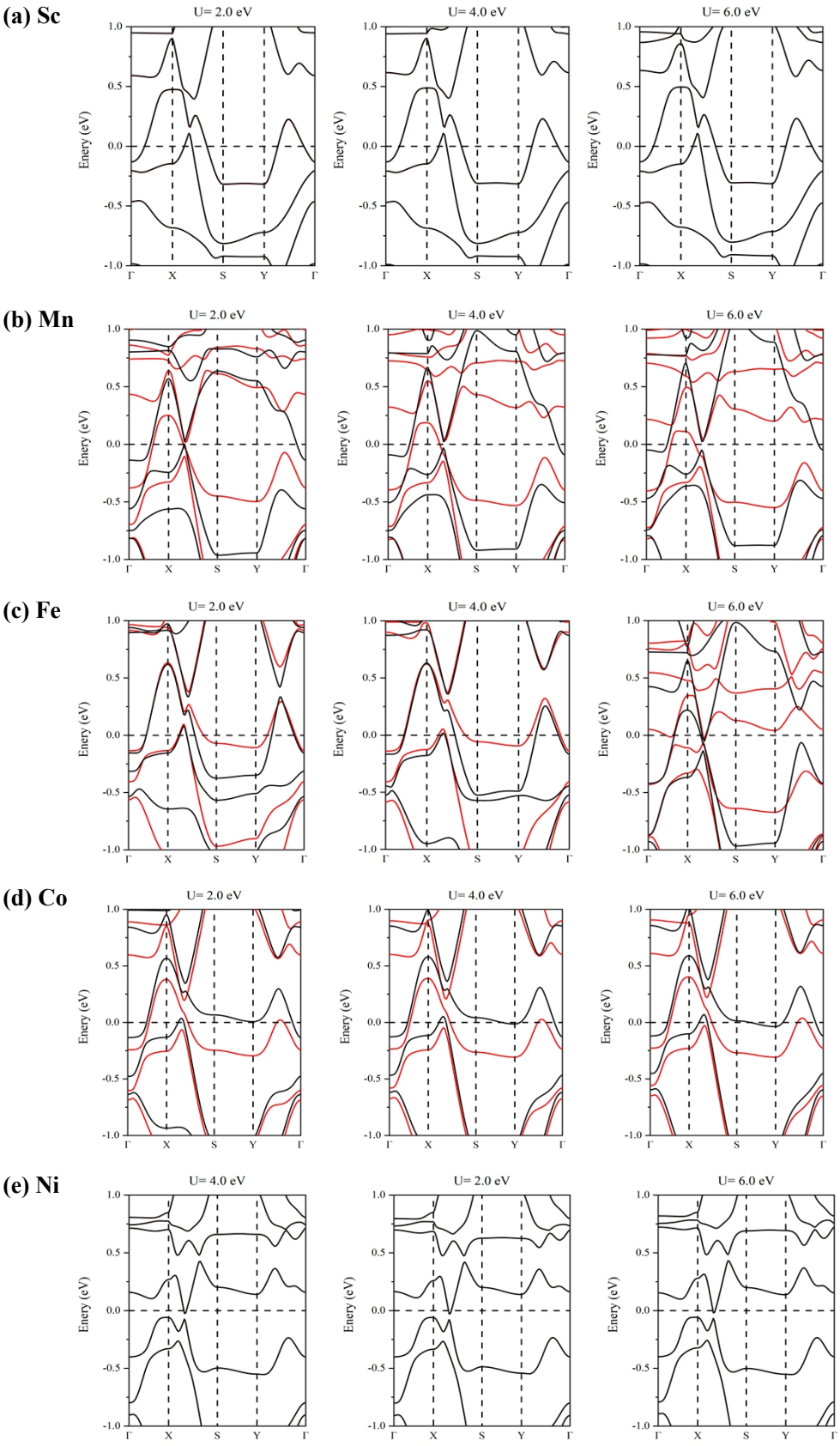

Figure S5: Band structure diagrams for Sc-, Mn-, Fe-, Co-, and Ni-doped systems at U = 2, 4 and 6 eV. The red lines denote spin-up states, while the black lines represent spin-down states.