Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary material

Transition in electronic and magnetic properties of transition metal embedded semimetallic B-graphyne

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(Dated: September 19, 2023)

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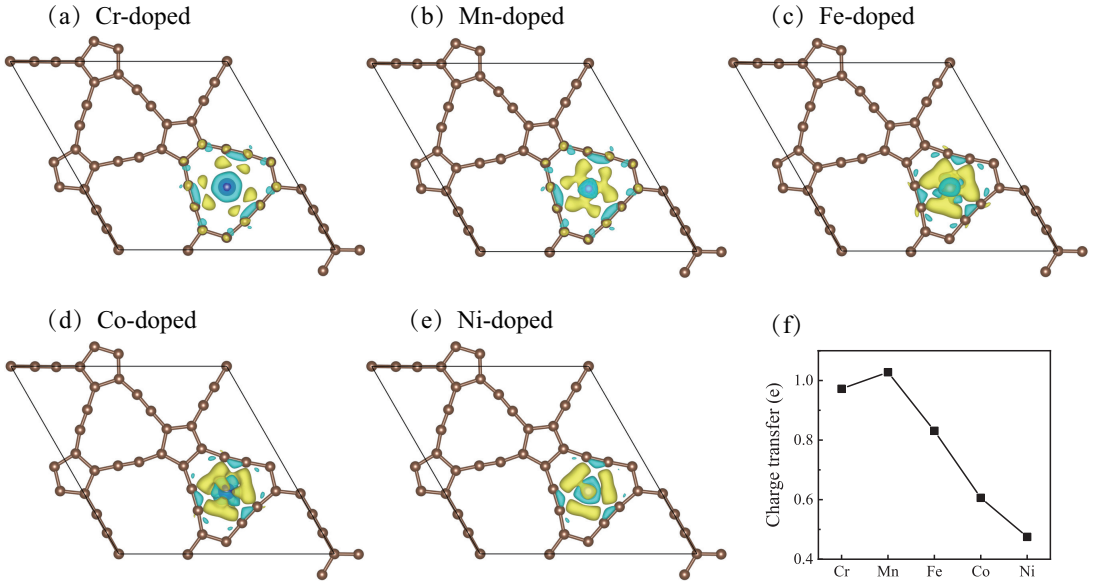

Figure S1. Differential charge density and charge transfer amount calculated using the GGA method. (a)-(e) Differential charge density of TM@B-GY with isosurface set to 0.005 e/Bohr^3. Yellow and blue indicate charge accumulation and loss, respectively. (f) Charge transfer amount of B-GY doped with different TM.

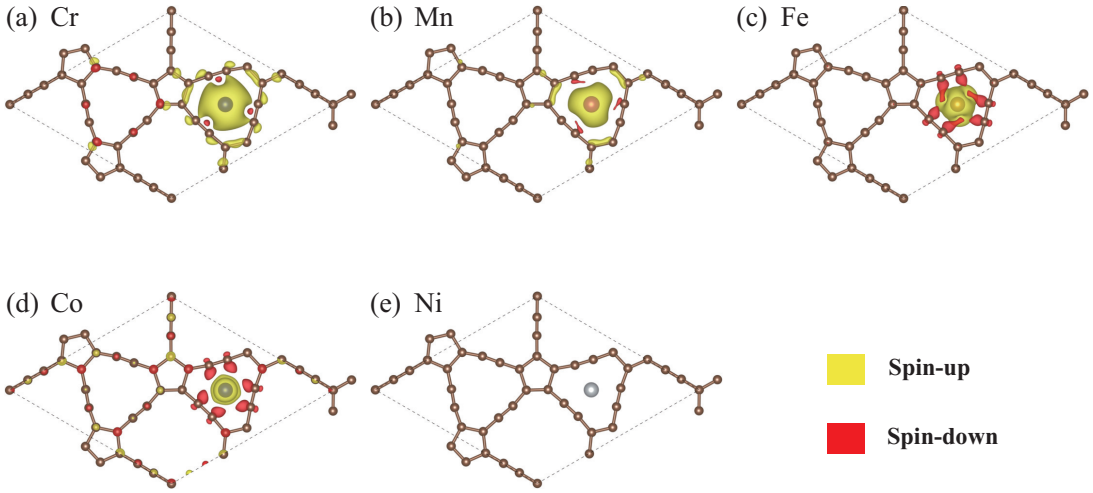

Figure S2. Spin density distribution of TM@B-GY, where yellow and red colors represent spin-up and spin-down charge densities, respectively. (a) Cr-doped, (b) Mn-doped, (c) Fe-doped, (d) Co-doped and (e) Ni-doped. The isosurface is set to 0.002 e/Bohr^3.

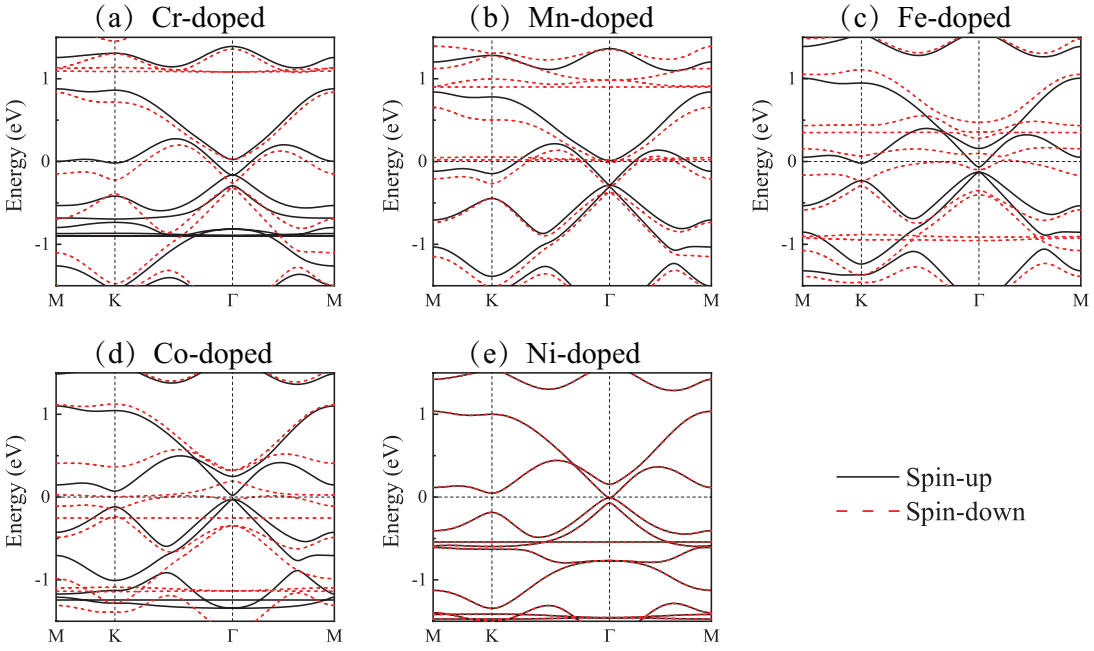

Figure S3. Band structure of TM@B-GY calculated by the GGA method. (a) Cr-doped, (b) Mn-doped, (c) Fe-doped, (d) Co-doped, (e) Ni-doped.

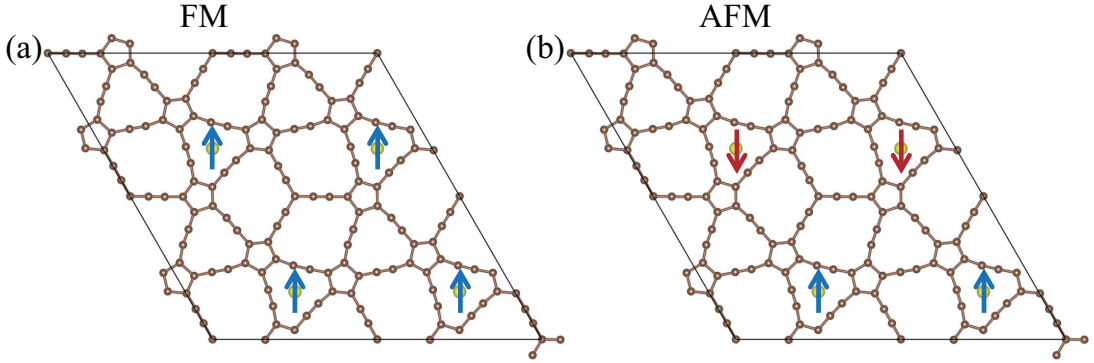

Figure S4. (a) Ferromagnetic and (b) antiferromagnetic configurations of the TM@B-GY monolayer, where brown and yellow spheres represent C and TM (Cr, Mn, Fe and Co) atoms, respectively. Arrows on TM atoms indicate different spin directions.

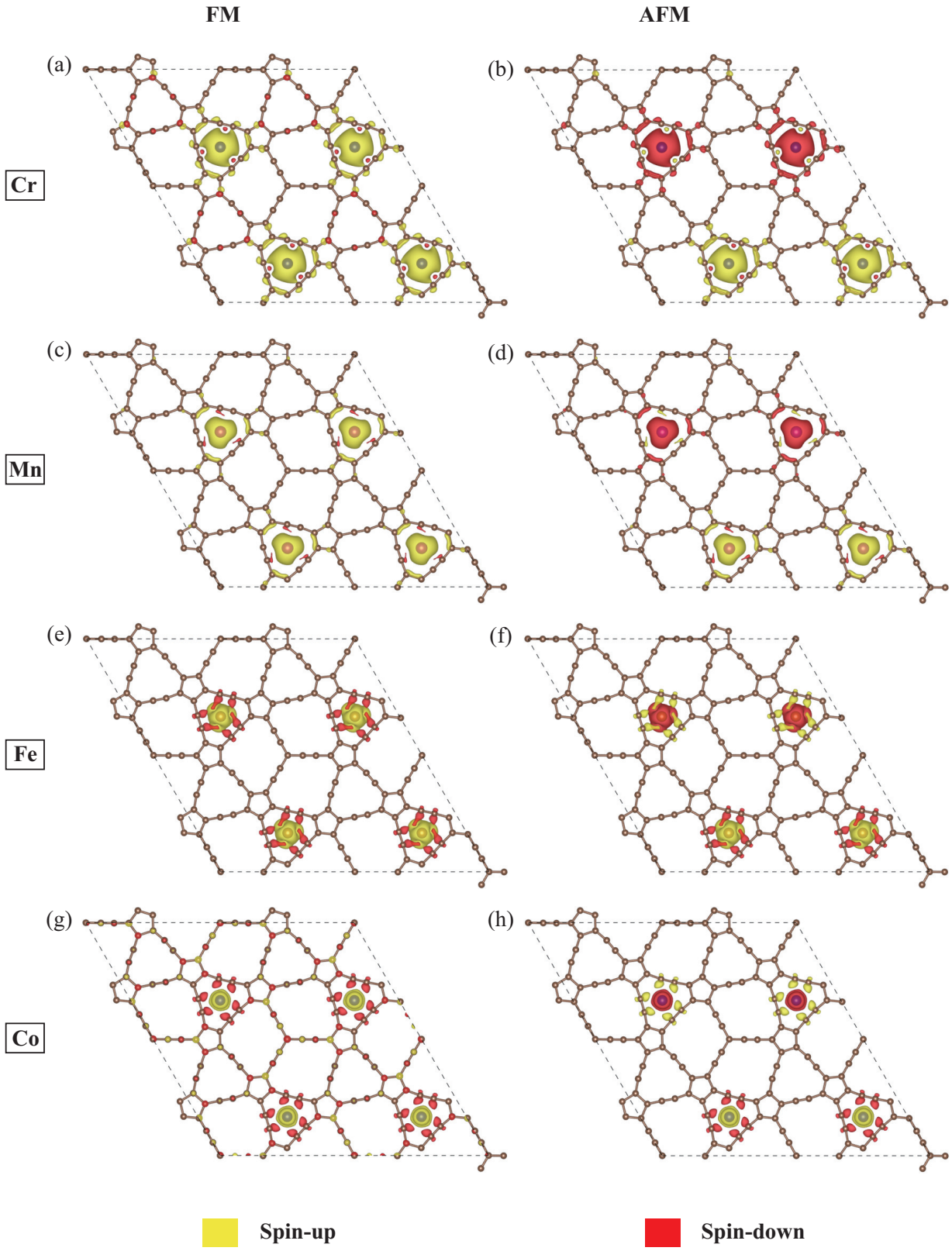

Figure S5. Spin density distribution of TM@B-GY in the ferromagnetic and antiferromagnetic states, where yellow and red colors represent spin-up and spin-down charge densities, respectively. The isosurface is set to 0.002 e/Bohr^3. The left side is the ferromagnetic state and the right side is the antiferromagnetic state. (a)-(b) Cr@B-GY, (c)-(d) Mn@B-GY, (e)-(f) Fe@B-GY and (g)-(h) Co@B-GY.