Electronic Supplementary Material (ESI) for RSC Advances.

Theoretical Exploration on the Electronic and Magnetic Properties of $(FeCp)_n^-$ (n=1, 2) Ligands Functionalized Graphene

Supporting Information

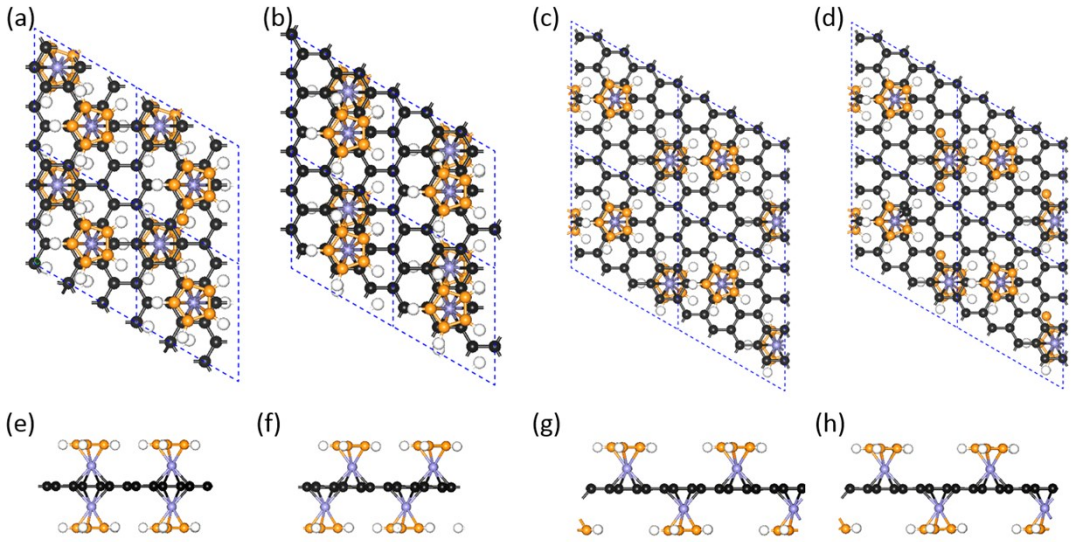

Figure S1. 2x2 supercell of $(FeCp)_2@G_{33}$-D_1(a,e), $(FeCp)_2@G_{33}$-D_2(b,f), $(FeCp)_2@G_{44}$-D_4(c,g) and $(FeCp)_2@G_{44}$-D_5(d,h). Black, Orange balls represents carbon atoms; white, purple balls represent H atoms and Fe atoms.

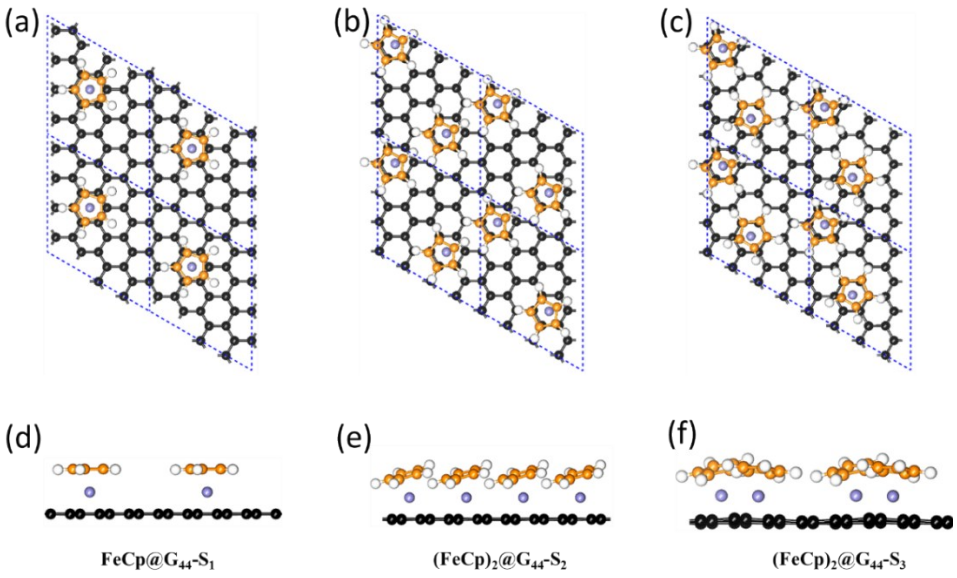

Figure S2. Scheme of $(FeCp)_n@G_{33,}$ n=1, 2. Optimized structure of $FeCp@G_{44}$-S_1, $(FeCp)_2@G_{44}$-S_2 and $(FeCp)_2@G_{44}$-S_3, respectively. Black, Orange balls represents carbon atoms; white, purple balls represent H atoms and Fe atoms.

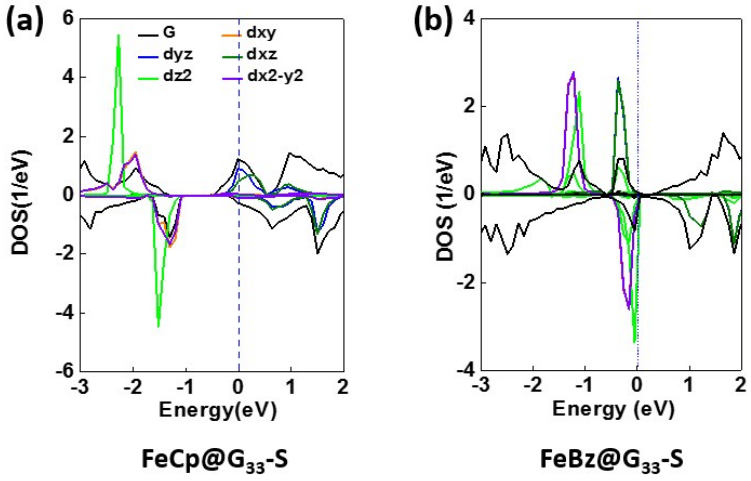

Figure S3. Density of states plots of FeCp@G_{33}-S and FeCp@G_{44}-S.

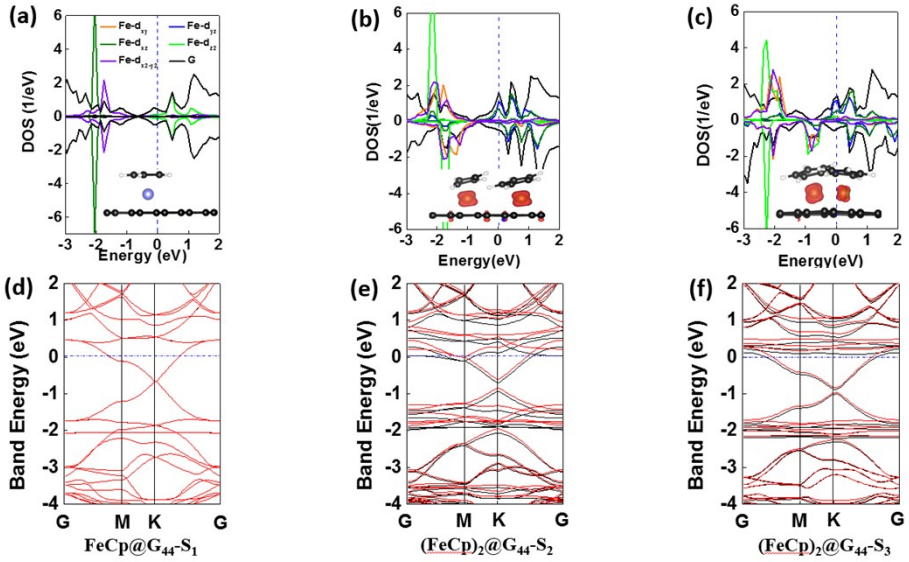

Figure S4. Band structure and the density of states of FeCp@G_{44}-S_1, $(FeCp)_2$@G_{44}-S_2 and $(FeCp)_2$@G_{44}-S_3.

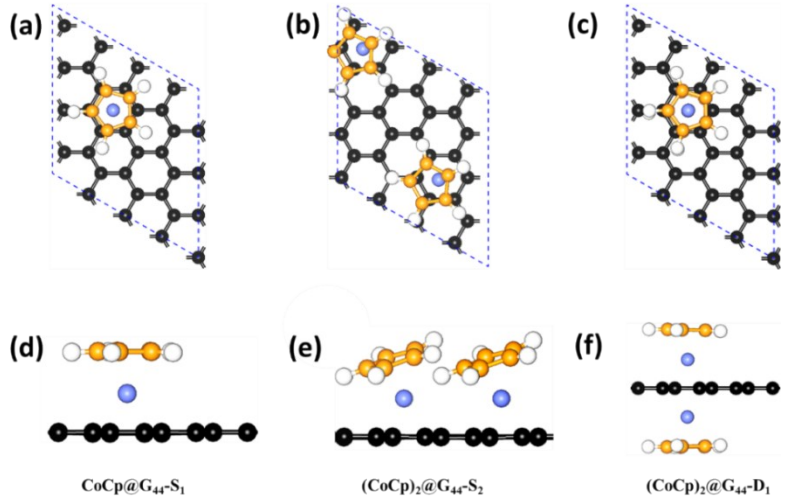

Figure S5. Top and side view of CoCp@G_{44}-S_1, $(CoCp)_2$@G_{44}-S_1 and $(CoCp)_2$@G_{44}-D_1.

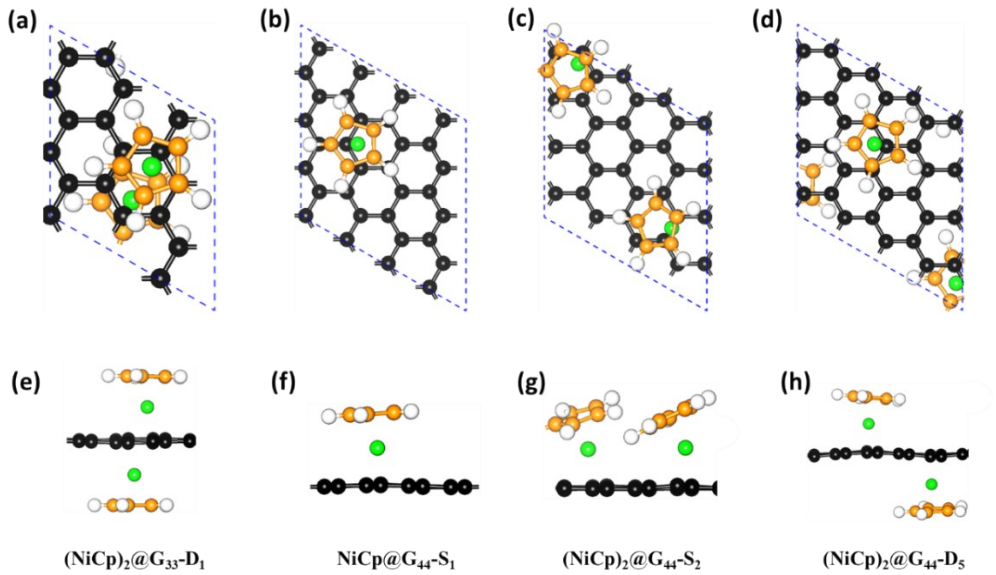

Figure S6. Top and side view of $(NiCp)_2$@G_{33}-D_1, NiCp@G_{44}-S_1, $(NiCp)_2$@G_{44}-S_2, $(NiCp)_2$@G_{44}-D_5, CoCp@G_{44}-S_1, $(CoCp)_2$@G_{44}-S_1 and $(CoCp)_2$@G_{44}-D_1.

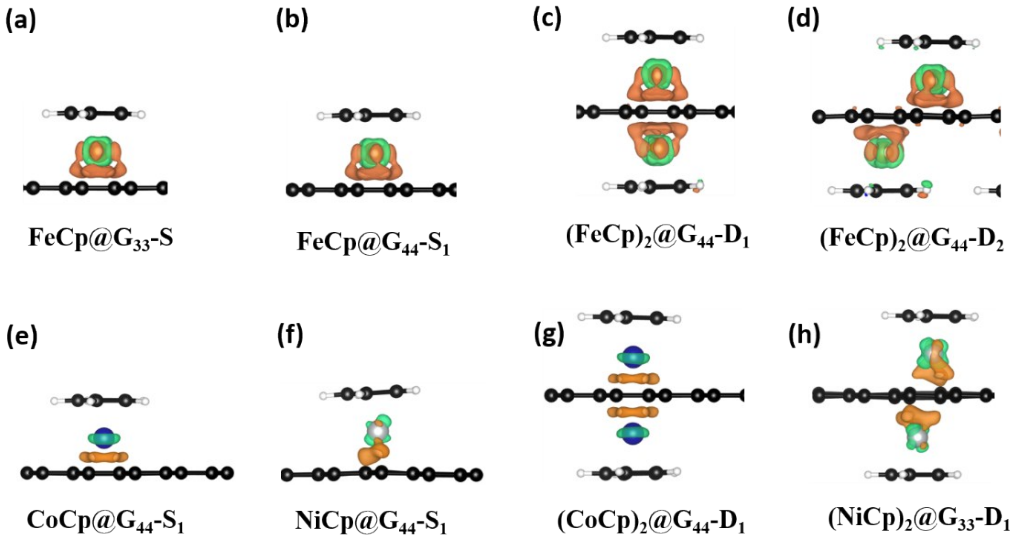

Figure S7. The CDD plots of FeBz@G_{33}(a), FeBz@G_{44}-S(b), $(FeCp)_2$@G_{44}-D_1(c), $(FeCp)_2$@G_{44}-D_2 (d), CoCp@G_{44}-S_1(e), $(NiCp)_2$@G_{44}-S_1(f), $(CoCp)_2$@G_{44}-D_1, $(NiCp)_2$@G_{33}-D_1,respectively.

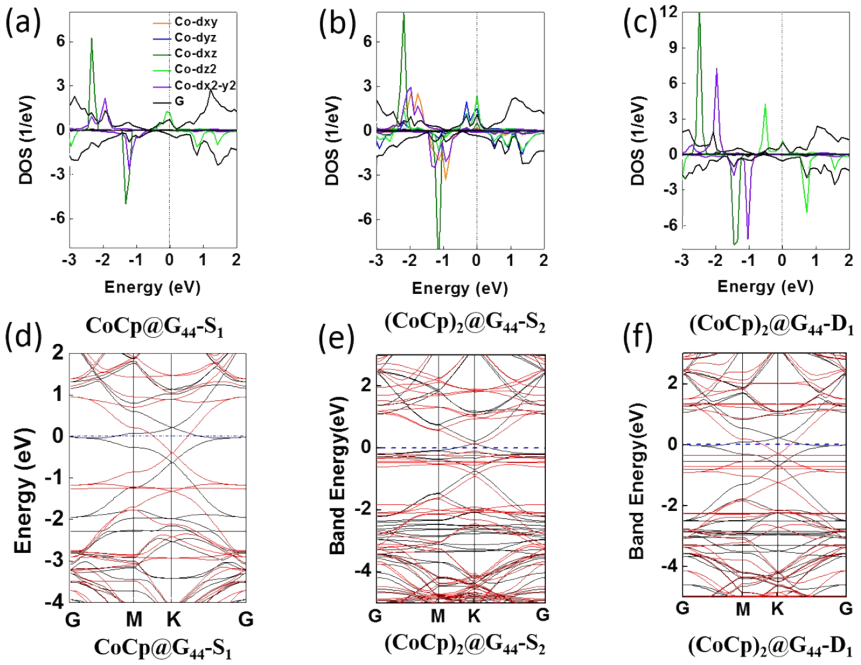

Figure S8. The density of states and bandstructures of CoCp@G_{44}-S_1, $(CoCp)_2$@G_{44}-S_1 and $(CoCp)_2$@G_{44}-D_1.

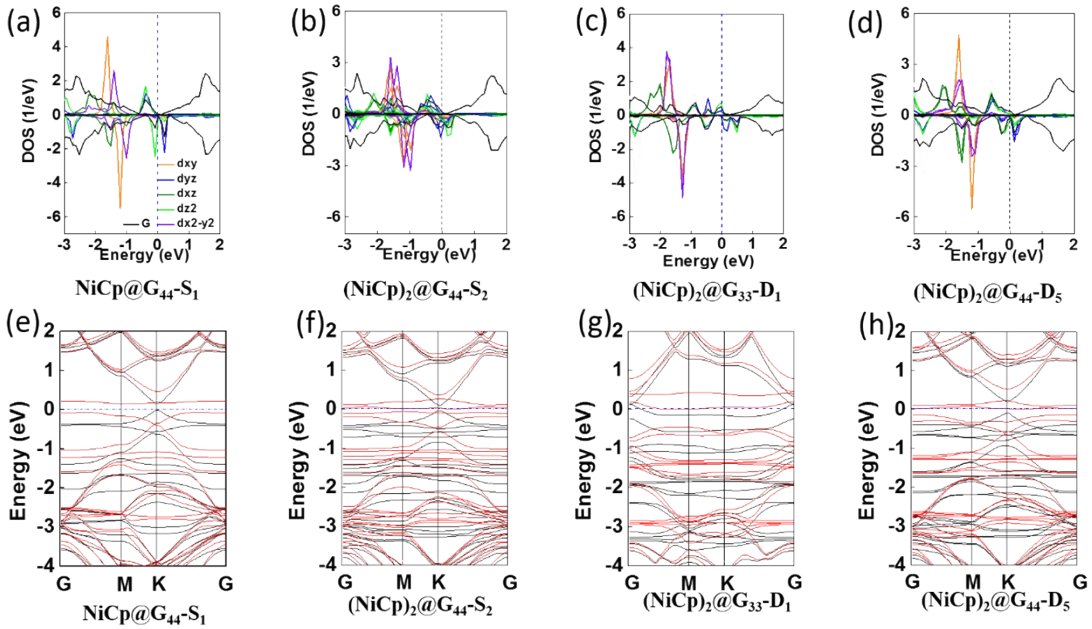

Figure S9. Band structure and the density of states of CoCp@G44-S1NiCp@G_{44}-S_1, $(NiCp)_2$@G_{44}-S_2, $(NiCp)_2$@G_{44}-D_1 and $(NiCp)_2$@G_{44}-D_5.

Table S1. Systems (sys), C-C (D_{C-C}(Cp)) and C-H bond length (D_{C-H}) of Cp ligands, C-C bond length of graphene (D_{C-C}(G)) of FeCp@G_{33}s and FeCp@G_{44}s.

Sys	D_{C-C}(Cp)(Å)	D_{C-C}(G) (Å)	D_{C-H} (Å)
FeCp@G33-S	1.43	1.42-1.43	1.09
$Fe_2Cp_2@G_{33}$-D_1	1.43-1.44	1.41-1.44	1.09
$Fe_2Cp_2@G_{33}$-D_2	1.43-1.44	1.41-1.44	1.09
$Fe_2Cp_2@G_{33}$-D_3	1.43	1.42-1.44	1.09
FeCp@G_{44}-S_1	1.43	1.42-1.44	1.09
$(FeCp)_2@G_{44}$-S_2	1.42-1.44	1.41-1.44	1.08-1.09
$(FeCp)_2@G_{44}$-S_3	1.42-1.43	1.41-1.44	1.08-1.09
$(FeCp)_2$@G44-D_1	1.42-1.44	1.41-1.45	1.09
$(FeCp)_2$@G44-D_2	1.43-1.44	1.41-1.44	1.09
$(FeCp)_2$@G44-D_3	1.43	1.41-1.45	1.09
$(FeCp)_2$@G44-D_4	1.43	1.41-1.44	1.09
$(FeCp)_2$@G44-D_5	1.43-1.44	1.41-1.44	1.09