Supplementary Information: Physical Chemistry Chemical Physics: Giant magnetoresistance and dual spin filtering effect in ferromagnetic $6,6,12/\gamma$-graphyne zigzag nanoribbon lateral heterojunction

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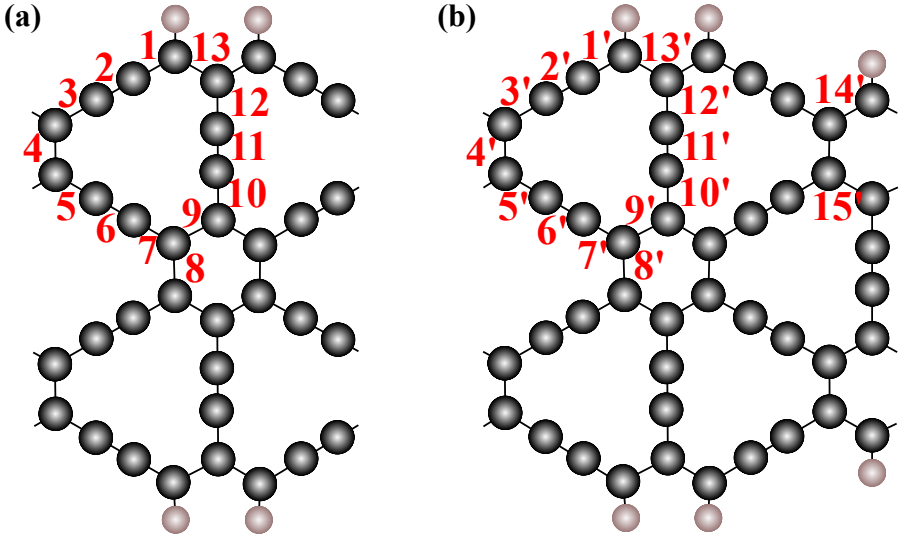

Figure S1 (a) $6,6,12$-GYZNR. (b) γ-GYZNR.

Table 1 The bond length (Å) labeled in Fig S1.

$6,6,12$-GYZNR				γ-GYZNR			
bond	bond length	bond	bond length	bond	bond length	bond	bond length
1	1.370	9	1.427	1’	1.377	9’	1.425
2	1.237	10	1.408	2’	1.237	10’	1.407
3	1.388	11	1.220	3’	1.397	11’	1.219
4	1.462	12	1.415	4’	1.451	12’	1.415
5	1.393	13	1.414	5’	1.399	13’	1.415
6	1.232			6’	1.228	14’	1.407
7	1.394			7’	1.401	15’	1.426
8	1.447			8’	1.437		

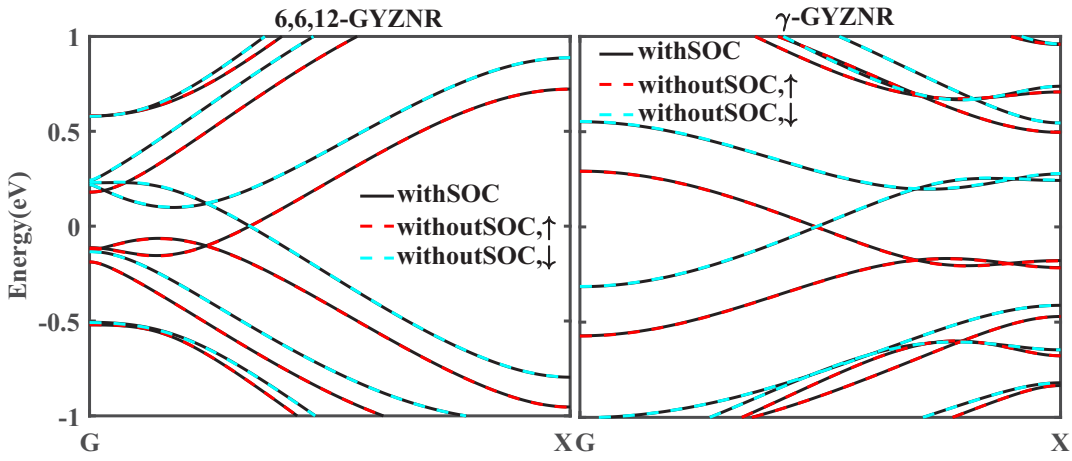

Figure S2 Band structure of $6,6,12$- and γ-GYZNR with (without) SOC, magnetic moment **m**=↑.

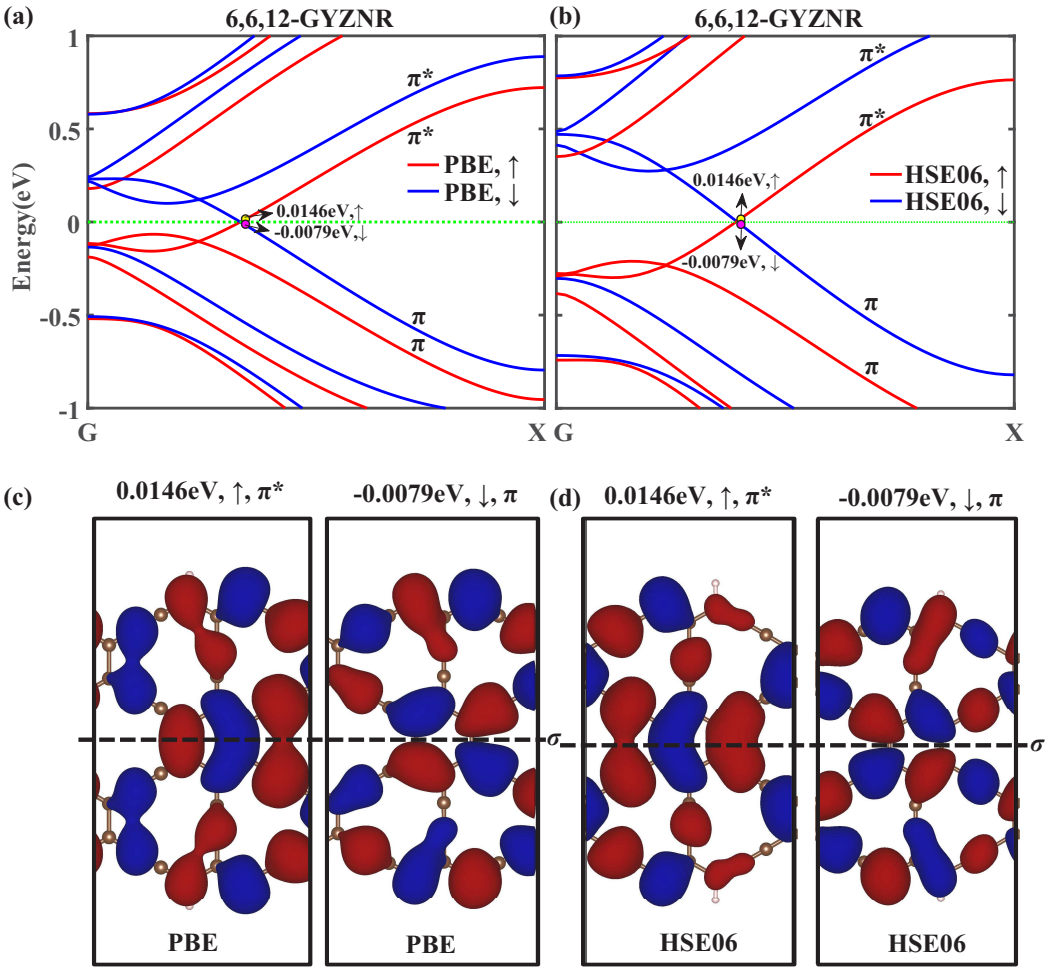

Figure S3 (a) Band structure of the $6,6,12$-GYZNR from PBE calculation. (b) Band structure of the $6,6,12$-GYZNR from HSE06 calculation. (c) Isosurface plot of real part of wave functions with spin up/spin down when E=0.0146 eV/-0.0079 eV from PBE calculation. (d) Isosurface plot of real part of wave functions with spin up/spin down when E=0.0146 eV/-0.0079 eV from HSE06 calculation.

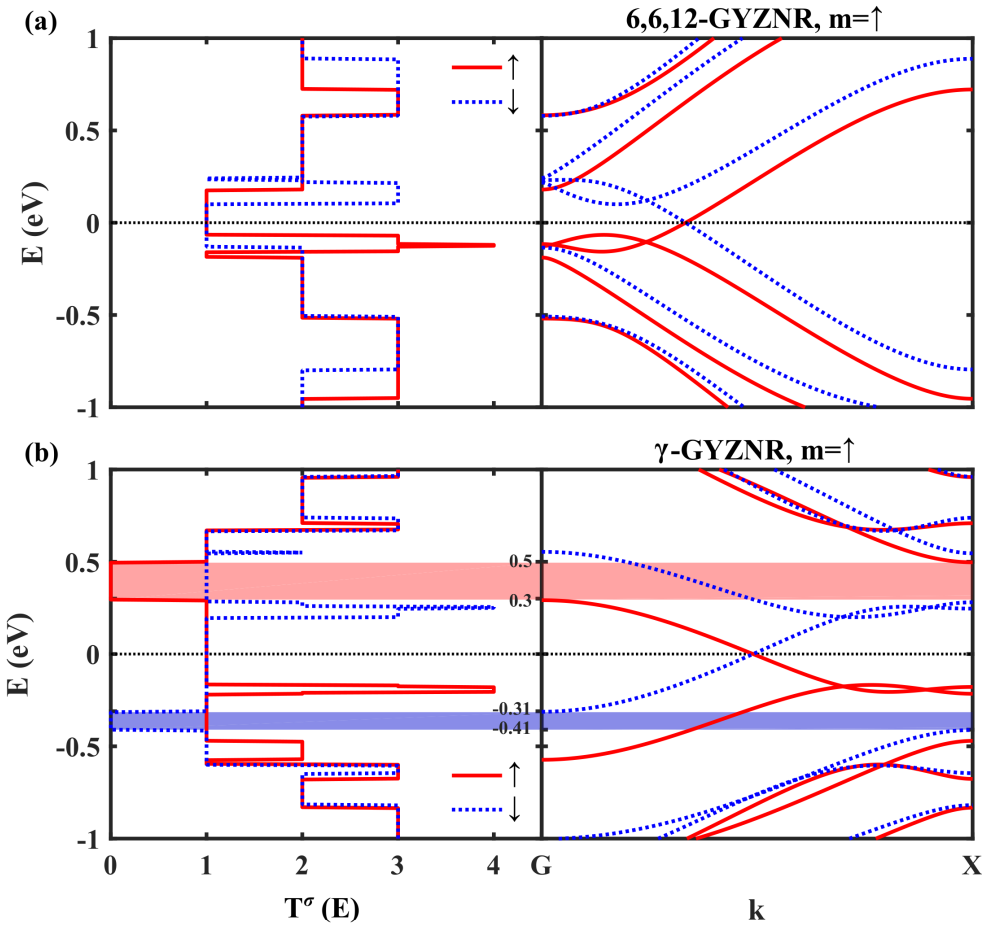

Figure S4 (a) Spin dependent transmission channel $T^{\sigma}(E)$ versus energy E (left column) when $V_b = 0$ V, $V_g = 0$ V and band structures (right column) of 6,6,12-GYZNR with spin magnetic moment $m =\uparrow$. (b) Spin dependent transmission channel $T^{\sigma}(E)$ versus energy E (left column) when $V_b = 0$ V, $V_g = 0$ V and band structures (right column) of γ-GYZNR with spin magnetic moment $m =\uparrow$. The red solid lines and blue dashed lines represent the spin up and spin down component, respectively. The red and blue regions represent transmission gap regions of spin up and spin down in γ-GYZNR, respectively.

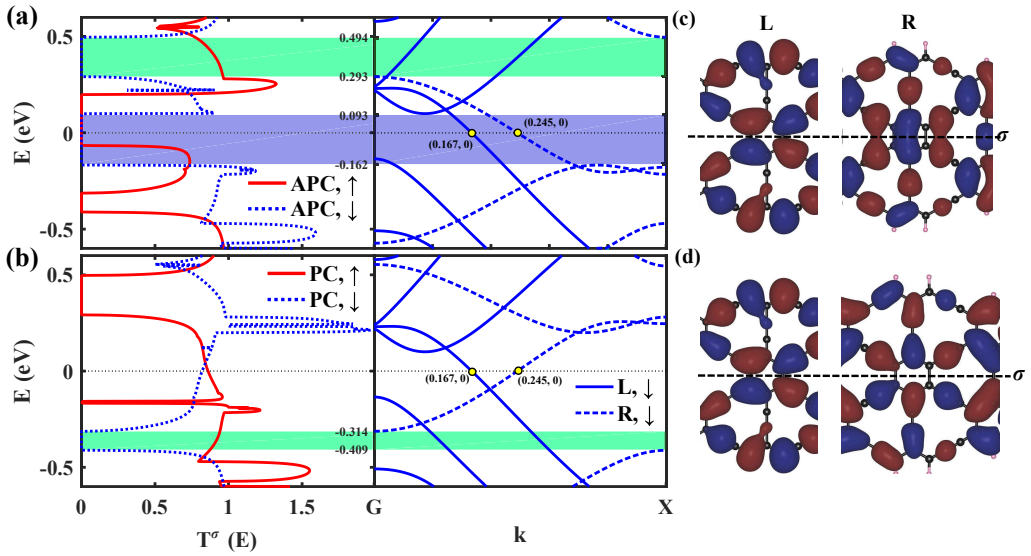

Figure S5 Spin dependent transmission coefficients $T^{\sigma}(E)$ versus energy E (left column) when $V_b = 0$ V, $V_g = 0$ V and band structures (right column) of spin down component in left and right leads for (a) APC and (b) PC, respectively. The red solid and blue dashed lines (left column) represent the spin up and spin down transmission components, respectively. The blue solid and dashed lines (right column) represent bandstructure of left and right lead, respectively. The blue and green regions represent transmission gap regions of spin down component. (c,d) Isosurface plot of real part of wave functions in unit cell of left and right leads when $E = 0$ eV (denoted by the yellow circles in band structures) in APC and PC, respectively. σ indicates the symmetry axis along the longitudinal direction.

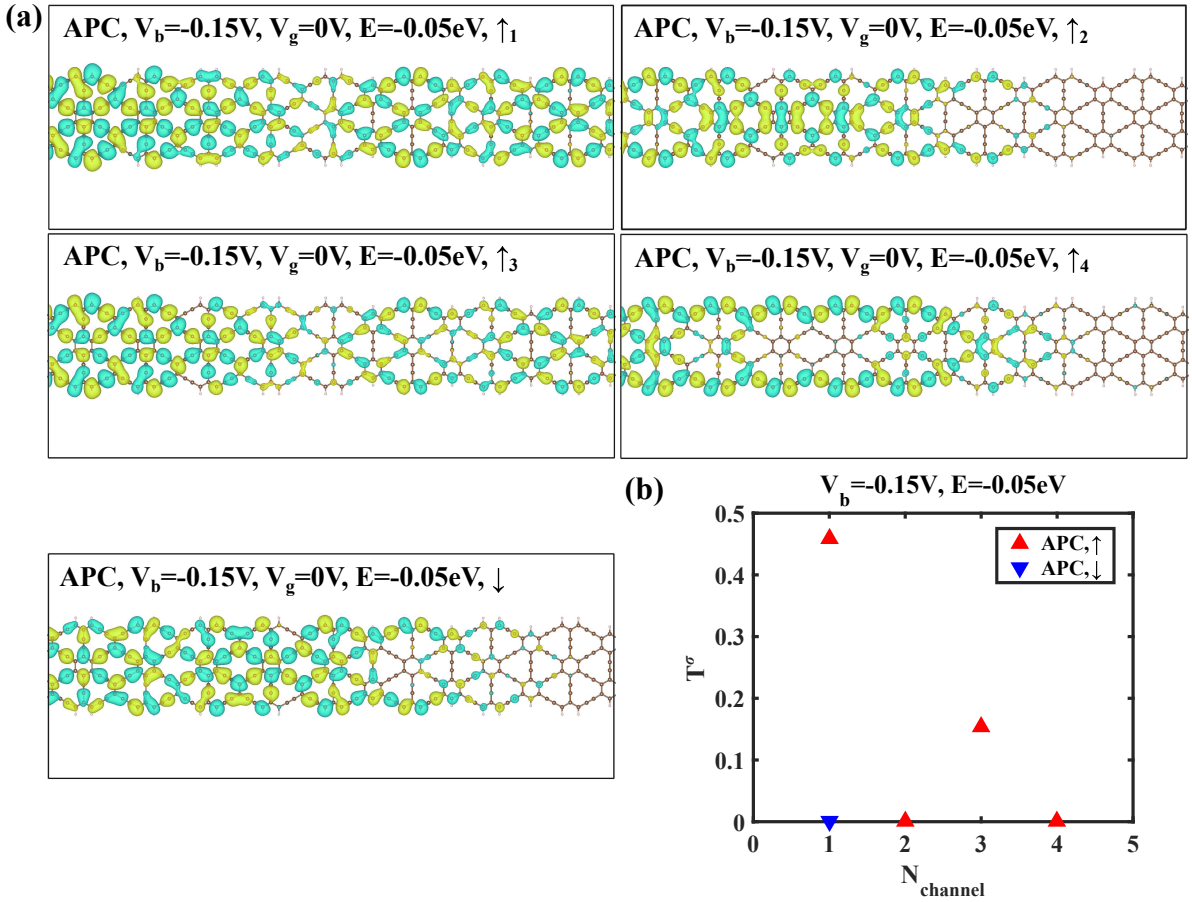

Figure S6 (a) Isosurface plot of real part of scattering wave functions with spin up/down component in APC ($V_b = -0.15$ V, $E = -0.05$ eV). (b) The spin dependent transmission T^σ of the corresponding channels in APC ($V_b = -0.15$ V, $E = -0.05$ eV). The isosurface value is fixed as 0.05 in (a).