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

Supplementary Information

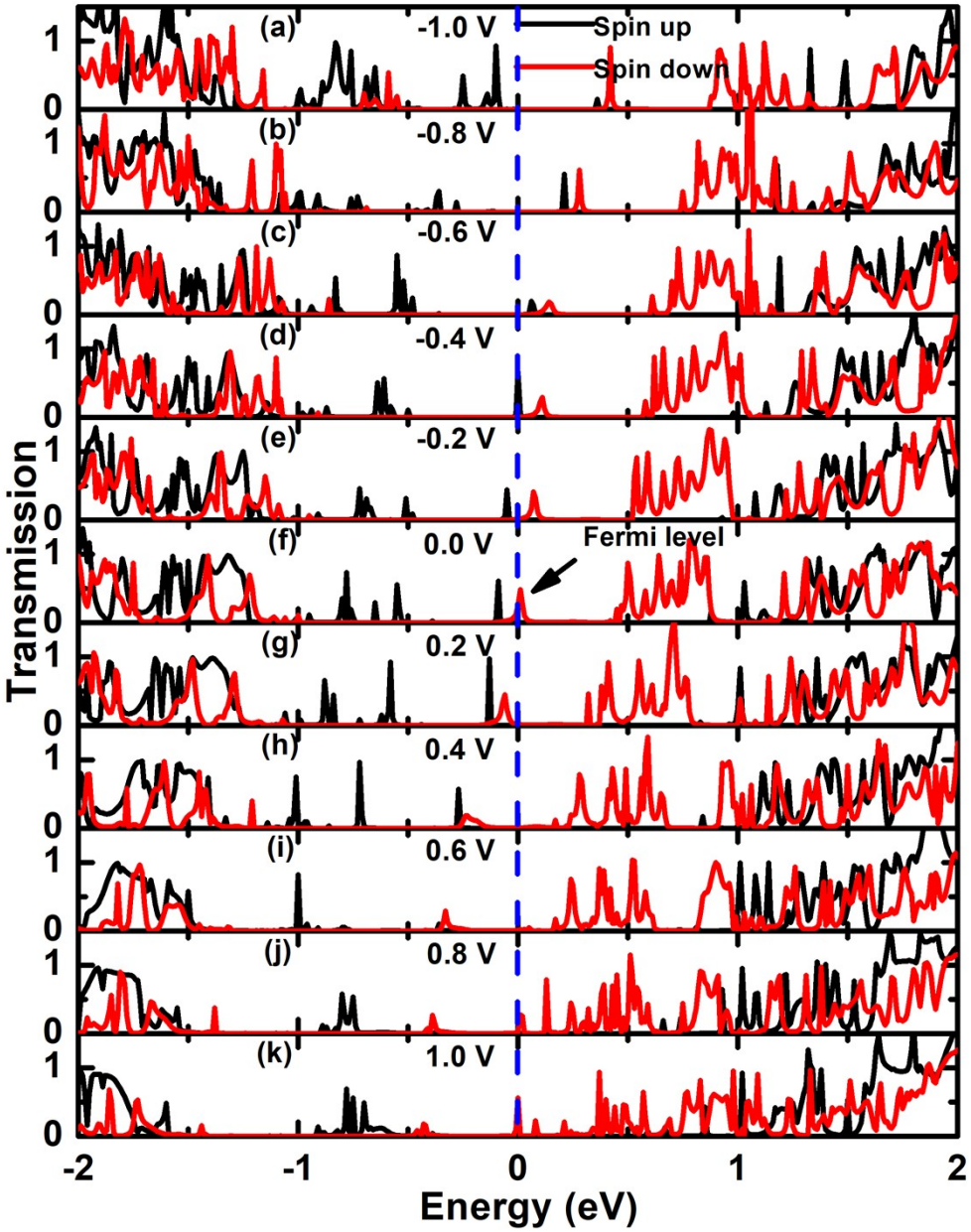

Fig. S1 (Color online) (a)-(k) Transmission spectra of ZGNR-ZGNRP22-ZGNR systems varying with gate voltage, which are denoted in the insets.

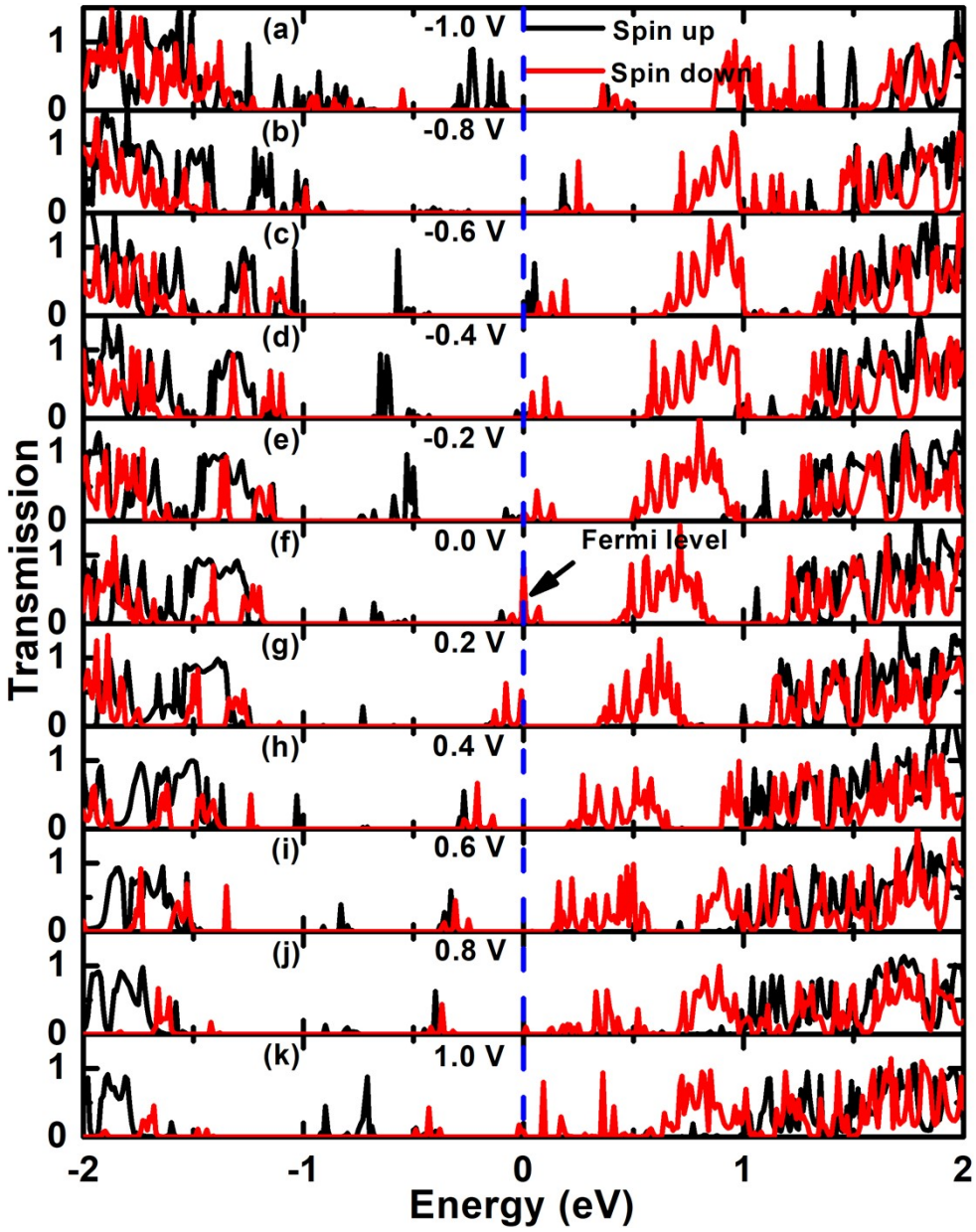

Fig. S2 (Color online) (a)-(k) Transmission spectra of ZGNR-ZGNRP24-ZGNR systems varying with gate voltage, which are denoted in the insets.

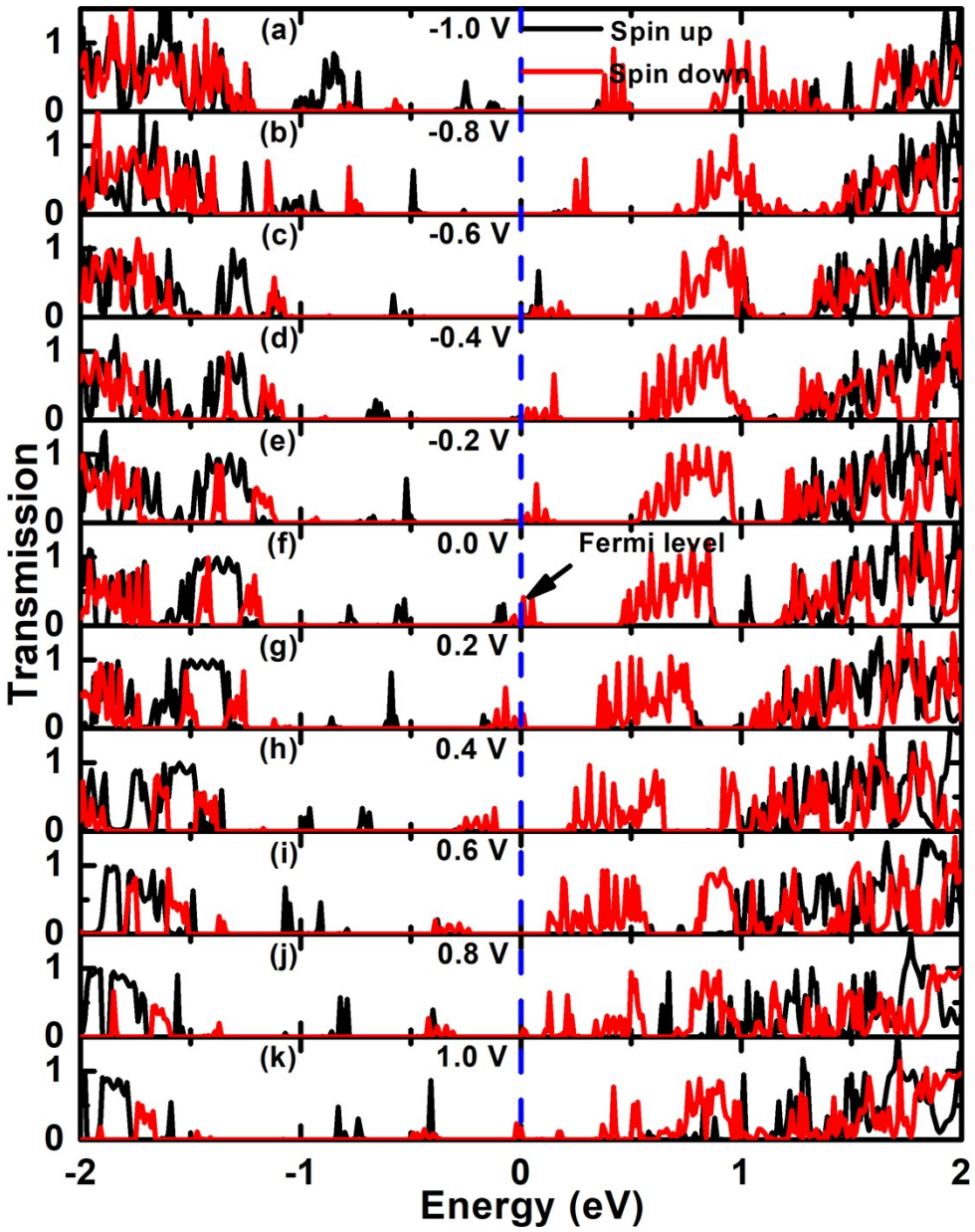

Fig. S3 (Color online) (a)-(k) Transmission spectra of ZGNR-ZGNRP26-ZGNR systems varying with gate voltage, which are denoted in the insets.

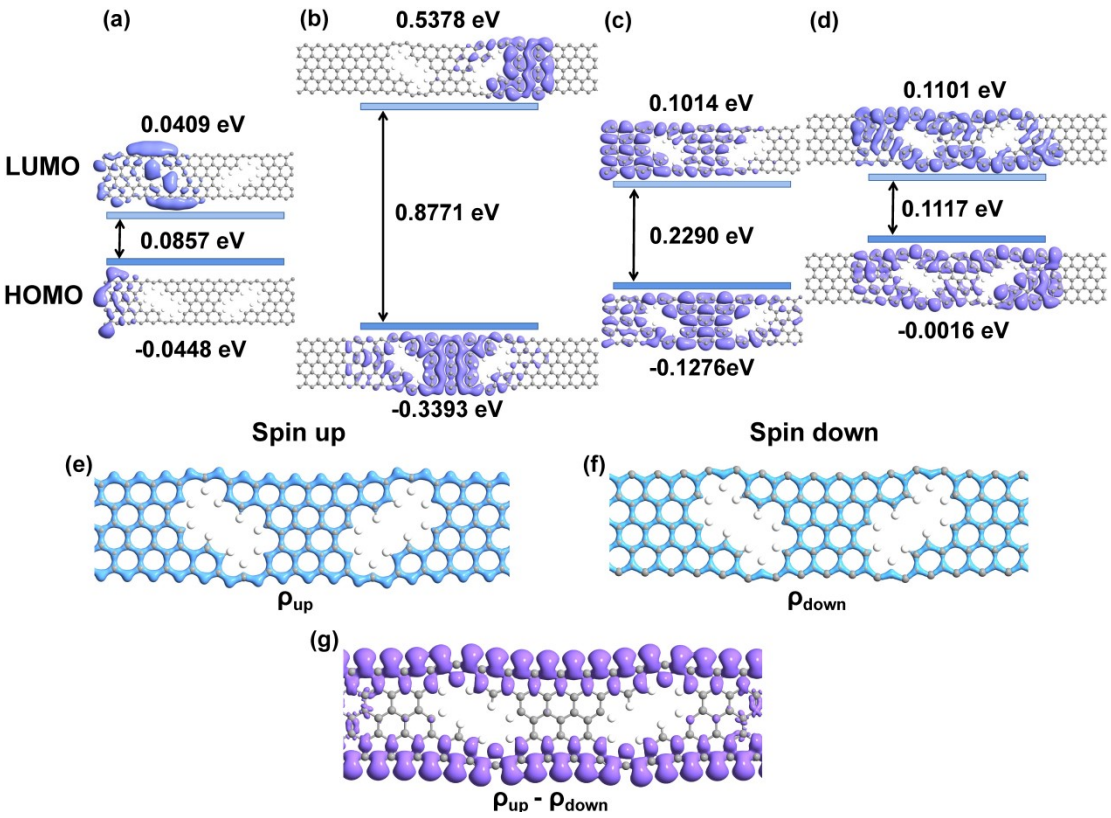

Fig. S4 (Color online) (a) The Highest Occupied Molecular Orbital / Lowest Unoccupied Molecular Orbital (HOMO/LUMO) states of isolated ZGNRP12 molecule for spin-up component. (b) The HOMO/LUMO states of the molecular projected self-consistent Hamiltonian (MPSH) of the two-probe system onto the central scattering region for spin-up component. (c)-(d) The same cases for spin-down component. (e)-(g) The spin-up and spin-down electron densities, as well as their difference (spin charge density magnetization) for ZGNR-ZGNRP12-ZGNR, respectively. The isovalues are 0.8, 0.8 and 0.02 $Å^{-3/2}$ respectively.

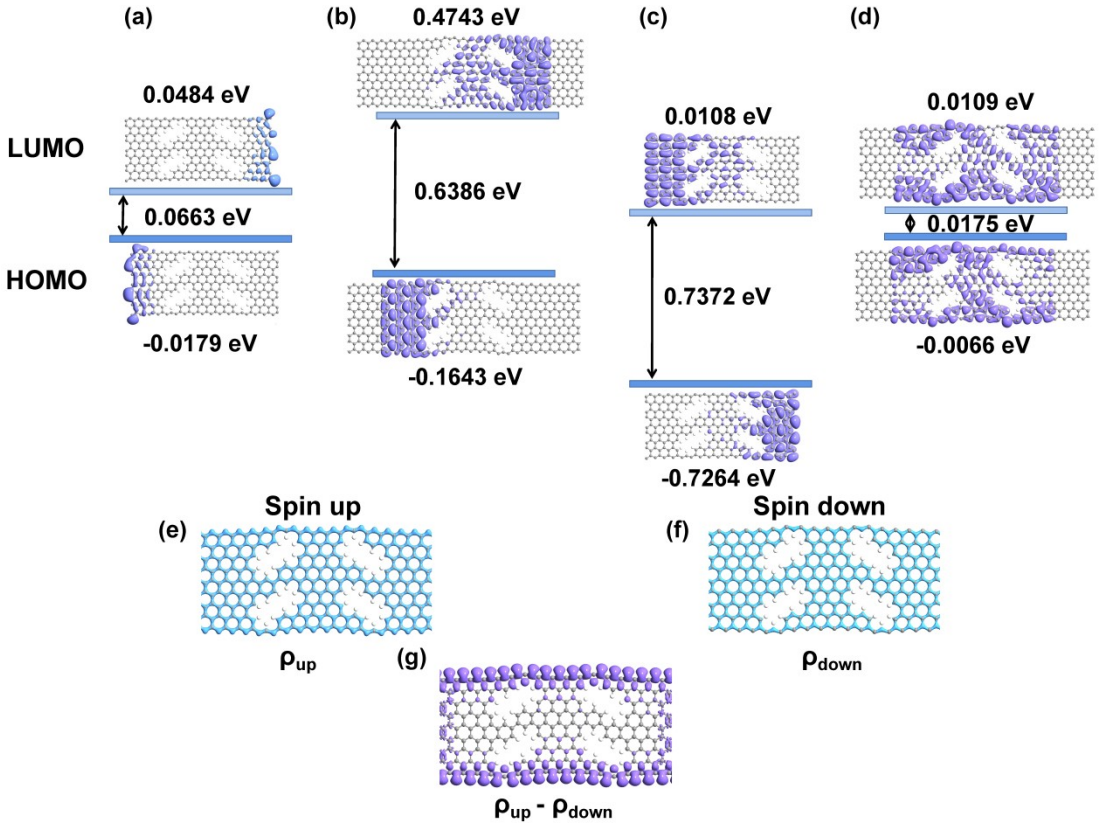

Fig. S5 (Color online) (a) The HOMO/LUMO states of isolated ZGNRP22 molecule for spin-up component. (b) The HOMO/LUMO states of the MPSH of the two-probe system onto the central scattering region for spin-up component. (c)-(d) The same cases for spin-down component. (e)-(g) The spin-up and spin-down electron densities, as well as their difference (spin charge density magnetization) for ZGNR-ZGNRP22-ZGNR, respectively. The isovalues are 0.8, 0.8 and 0.02 $Å^{-3/2}$ respectively.

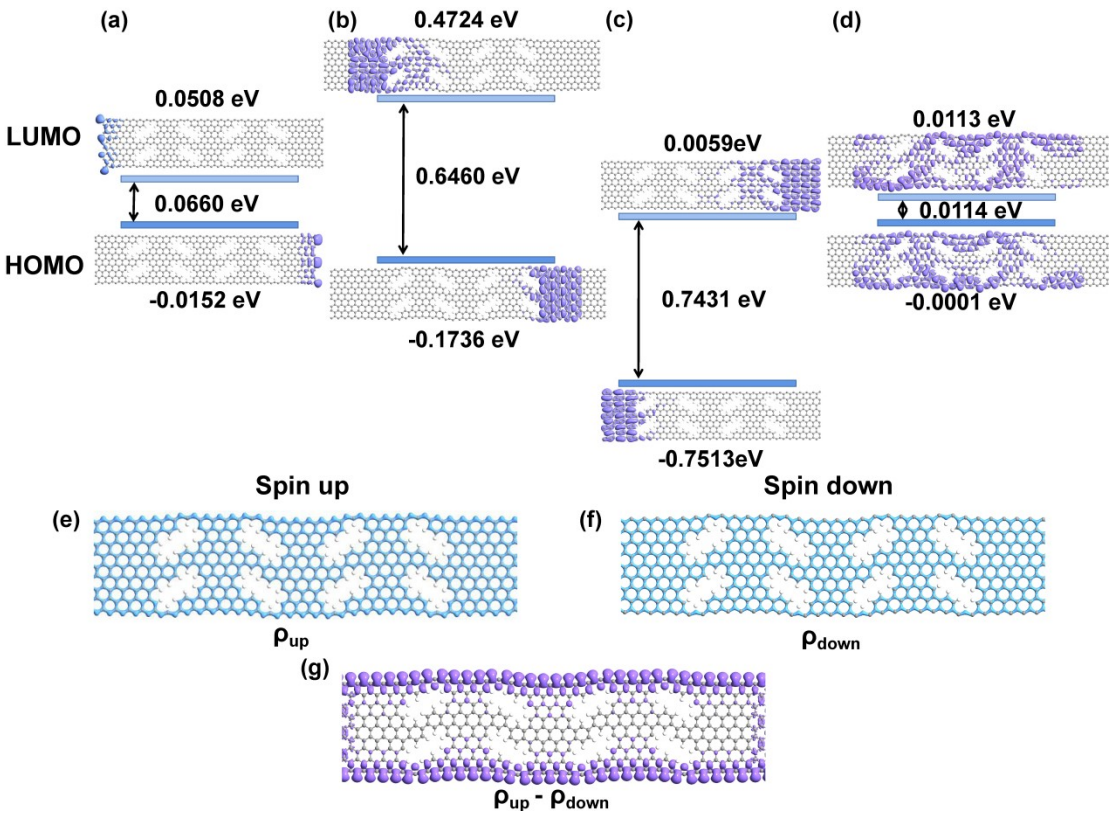

Fig. S6 (Color online) (a) The HOMO/LUMO states of isolated ZGNRP24 molecule for spin-up component. (b) The HOMO/LUMO states of the MPSH of the two-probe system onto the central scattering region for spin-up component. (c)-(d) The same cases for spin-down component. (e)-(g) The spin-up and spin-down electron densities, as well as their difference (spin charge density magnetization) for ZGNR-ZGNRP24-ZGNR, respectively. The isovalues are 0.8, 0.8 and 0.02 $Å^{-3/2}$ respectively.

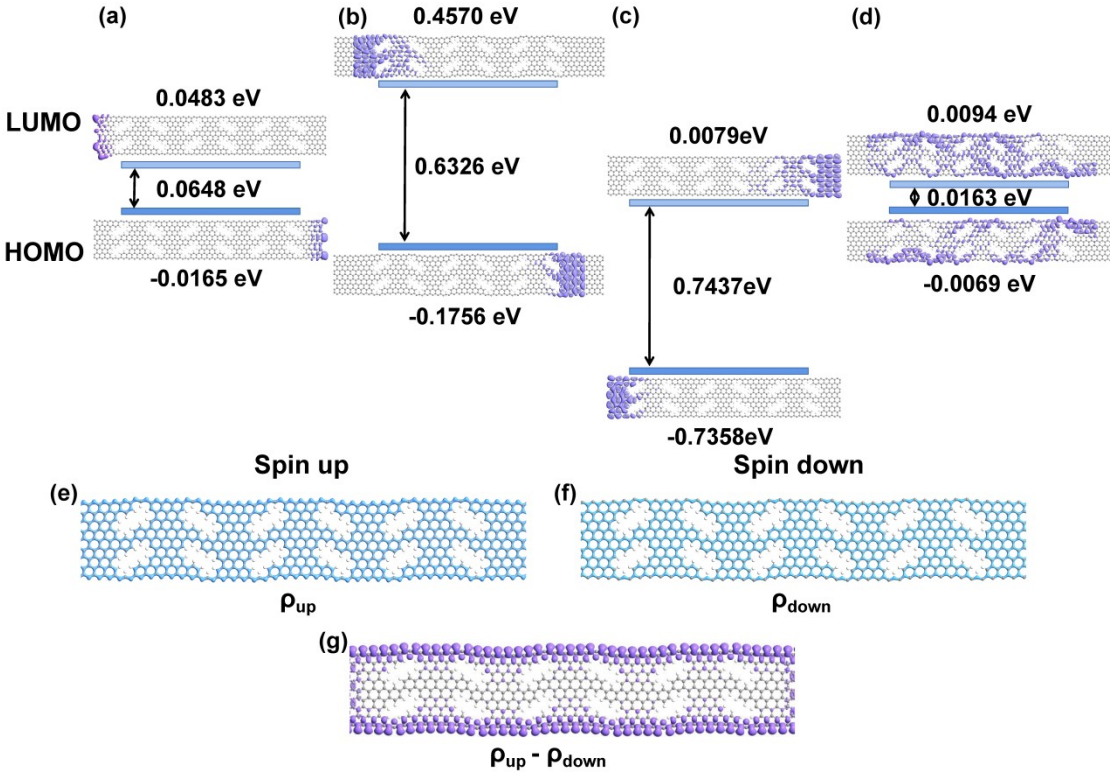

Fig. S7 (Color online) (a) The HOMO/LUMO states of isolated ZGNRP26 molecule for spin-up component. (b) The HOMO/LUMO states of the MPSH of the two-probe system onto the central scattering region for spin-up component. (c)-(d) The same cases for spin-down component. (e)-(g) The spin-up and spin-down electron densities, as well as their difference (spin charge density magnetization) for ZGNR-ZGNRP26-ZGNR, respectively. The isovalues are 0.8, 0.8 and 0.02 $Å^{-3/2}$ respectively.