Supporting information for

Designing molecular rectifiers and spin valves using metallocene-functionalized undecanethiolates: one transition metal atom matters

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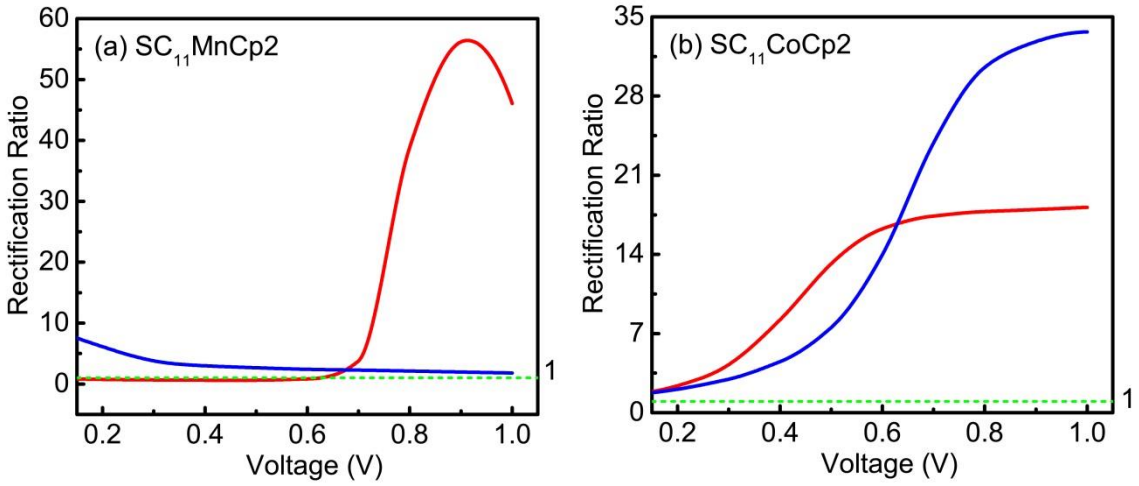

Figure S1. Spin-resolved rectification ratios of the spin-up current-voltage curve (red line) and spin-down current-voltage curve (blue line) for (a) SC_{11}MnCp2 junction and (b) SC_{11}CoCp2 junction.

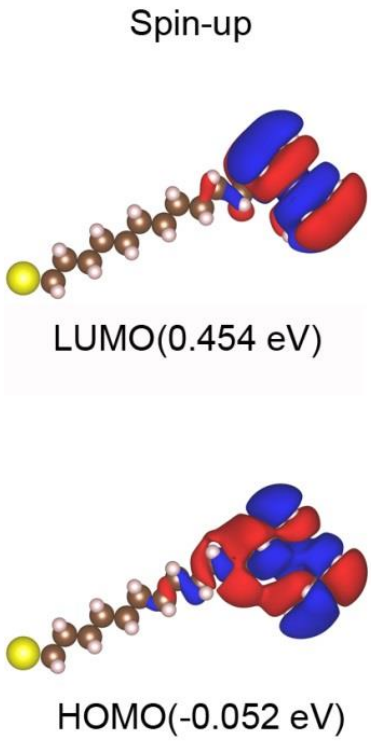

Figure S2. Spatial distributions of frontier MPSH molecular orbitals at zero bias voltage for $SC_{11}CrCp2$ junction (the isovalue is 0.002).

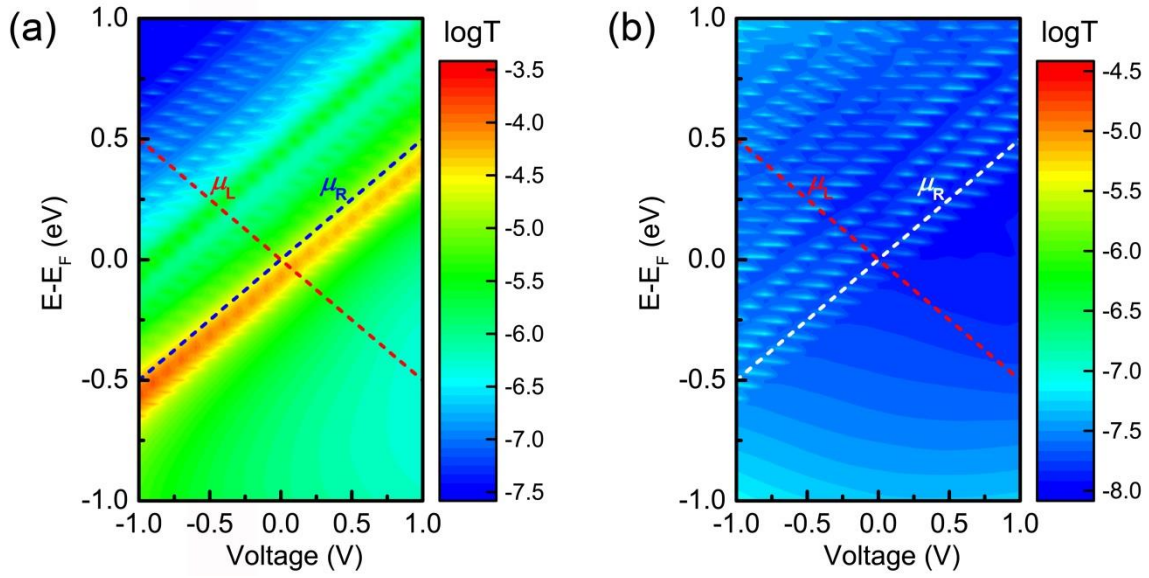

Figure S3. (a) Spin-up and (b) spin-down electronic transmission spectra in logarithmic scale at different bias voltages for $SC_{11}CrCp2$ junction. The dashed lines indicate the chemical potentials of the electrodes, and the energy range between them is the bias window.

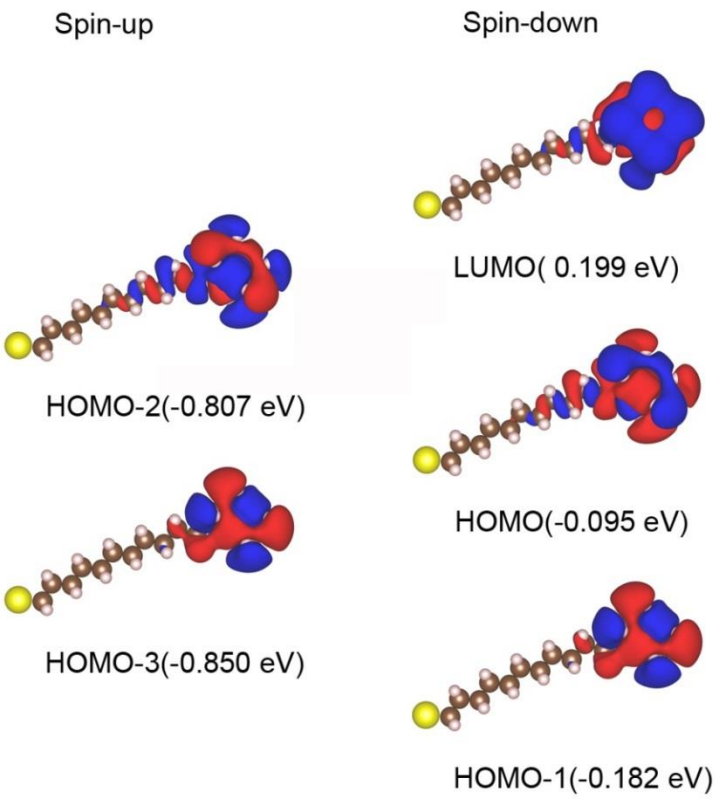

Figure S4. Spatial distributions of frontier MPSH molecular orbitals at zero bias voltage for SC_{11}MnCp2 junction (the isovalue is 0.002).

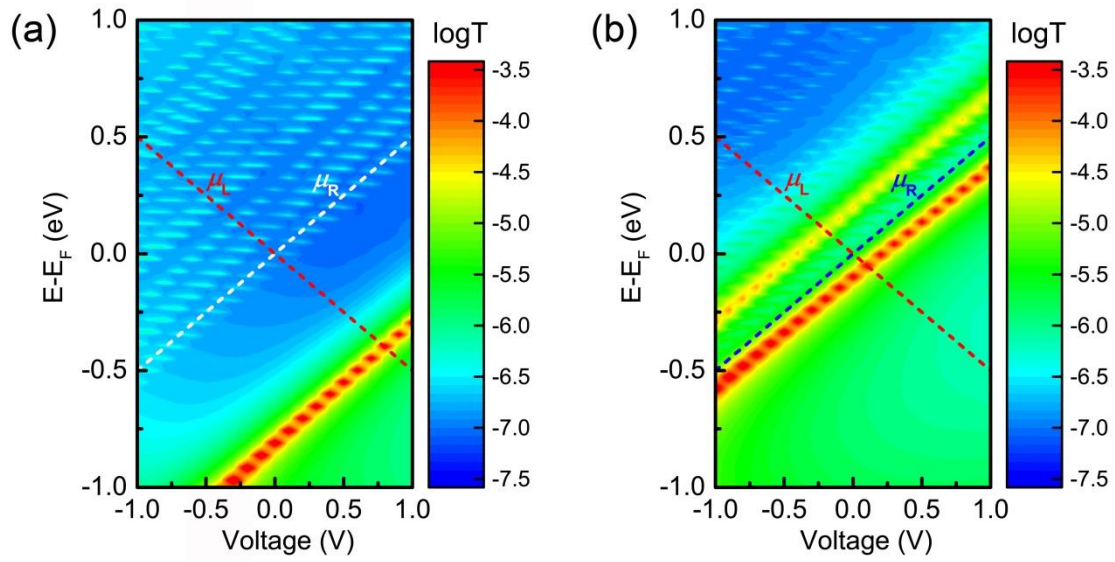

Figure S5. (a) Spin-up and (b) spin-down electronic transmission spectra in logarithmic scale at different bias voltages for SC_{11}MnCp2 junction. The dashed lines indicate the chemical potentials of the electrodes, and the energy range between them is the bias window.

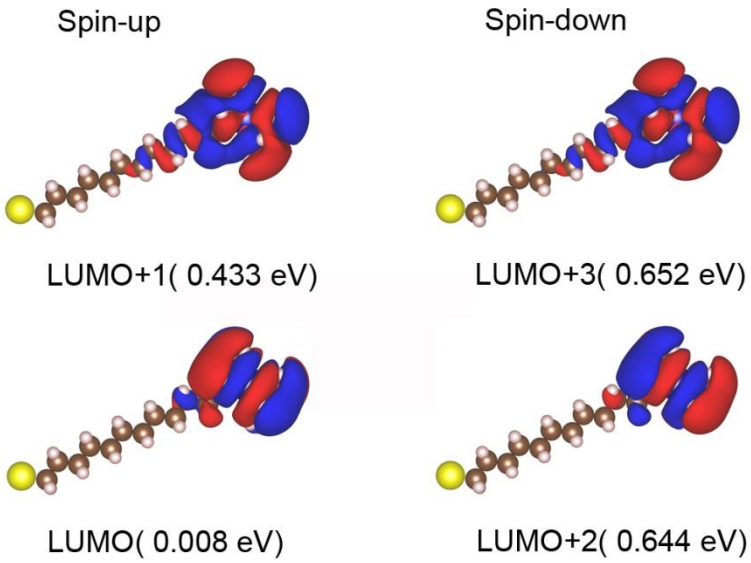

Figure S6. Spatial distributions of frontier MPSH molecular orbitals at zero bias voltage for SC_{11}CoCp2 junction (the isovalue is 0.002).

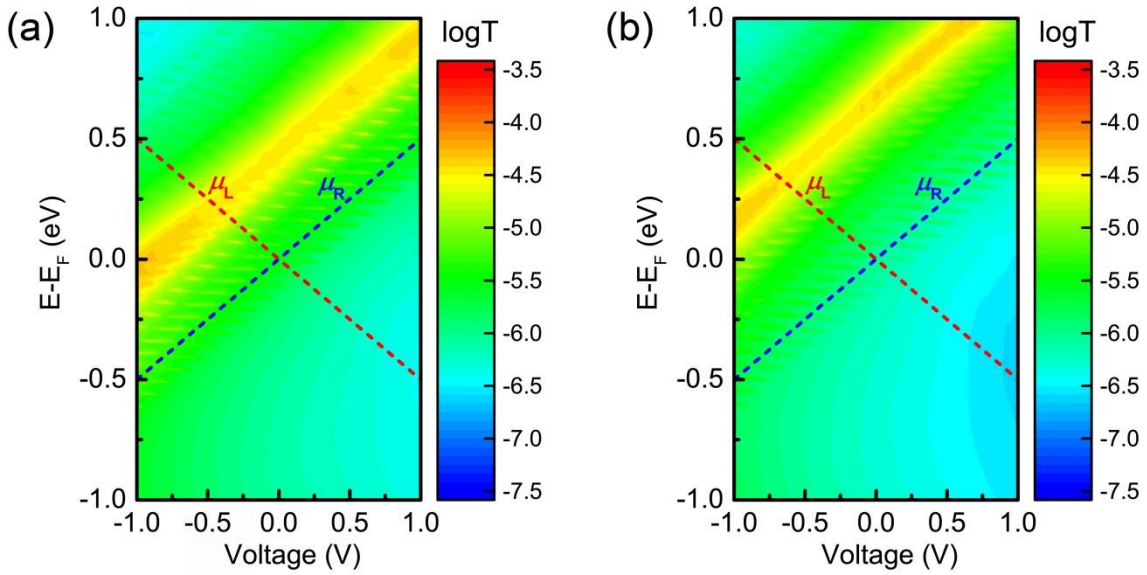

Figure S7. (a) Spin-up and (b) spin-down electronic transmission spectra in logarithmic scale at different bias voltages for SC_{11}CoCp2 junction. The dashed lines indicate the chemical potentials of the electrodes, and the energy range between them is the bias window.

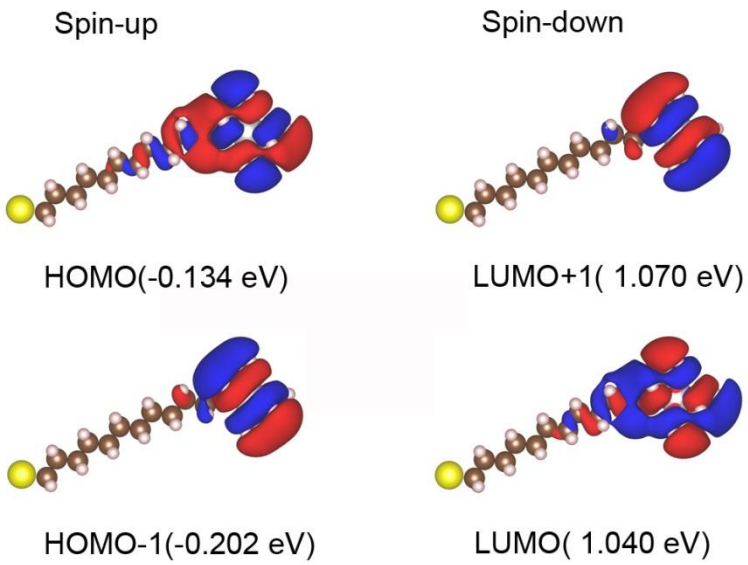

Figure S8. Spatial distributions of frontier MPSH molecular orbitals at zero bias voltage for $SC_{11}NiCp2$ junction (the isovalue is 0.002).

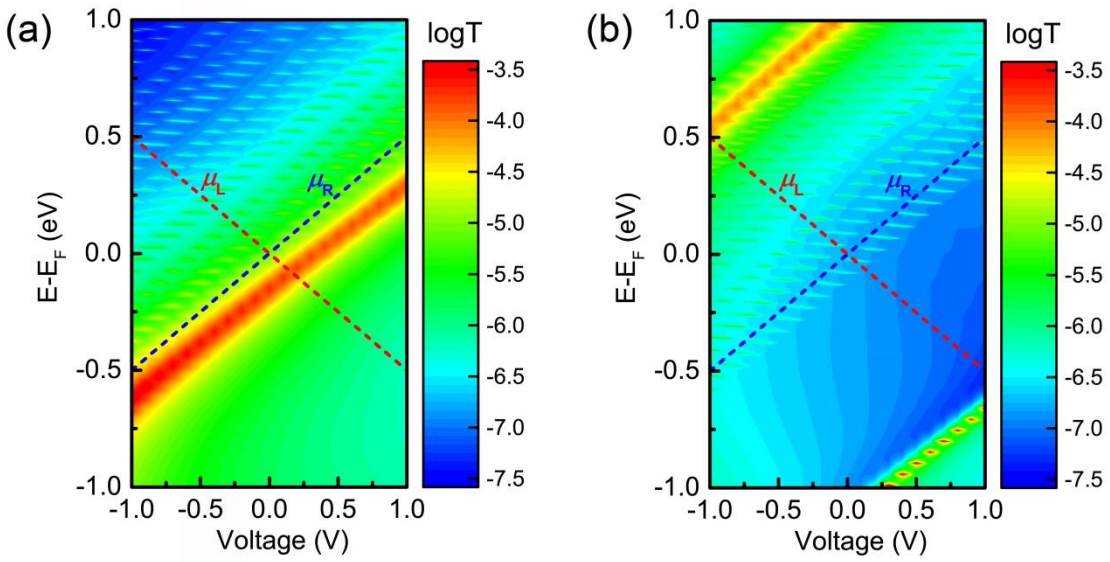

Figure S9. (a) Spin-up and (b) spin-down electronic transmission spectra in logarithmic scale at different bias voltages for $SC_{11}NiCp2$ junction. The dashed lines indicate the chemical potentials of the electrodes, and the energy range between them is the bias window.