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

Supporting Information

Highly Sensitive, Selective and Low-Power Consumption MetalloporphyrinBased Junctions for Nitrogen Monoxide Detection with Excellent Recovery

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Table S1: Calculated relative adsorption energy (E_{ads}, eV) of various configurations of NO binding over studied MPors. The considered configurations are shown in Figure S2.

Device	E_A	E_B	E_T
Sc	3×10^{-4}	0.00	0.053
Ti	3×10^{-4}	0.00	0.144
V	0.21	0.00	0.014
Cr	1.09	0.00	0.001
Mn	0.001	0.00	0.001
Fe	12×10^{-4}	0.00	8×10^{-4}
Co	0.001	0.00	0.003
Ni	0.001	0.00	1×10^{-4}
Cu	0.001	0.00	0.023
Zn	0.007	0.00	0.012

Table S2: Calculated adsorption energy (E_{ads}, eV), bond length (d, Å), and difference in Hirshfeld charge (CT) of central ion-magnet after NO adsorption.

Device	E_{ads}	d	CT
Sc	-2.09	1.79	-0.61
Ti	-2.04	1.83	-1.02
V	-1.78	1.90	-0.53
Cr	-0.56	1.79	-0.32
Mn	-0.36	1.91	-0.19
Fe	-1.33	1.66	-0.63
Co	-1.18	1.75	-0.58
Ni	-0.09	2.03	-0.03
Cu	-0.25	1.81	-0.15
Zn	-0.41	1.29	-0.28

Table S3: Calculated recovery time (τ, s) of NO gas from MPor based devices.

Device	τ
Sc	1.5×10^{18}
Ti	8.3×10^{17}
V	7.58×10^{17}
Cr	25×10^{-2}
Mn	1×10^{-7}
Fe	$2.17\times10^{+5}$
Co	$6.37\times10^{+5}$
Ni	32×10^{-12}
Cu	16×10^{-8}
Zn	0.76×10^{-5}

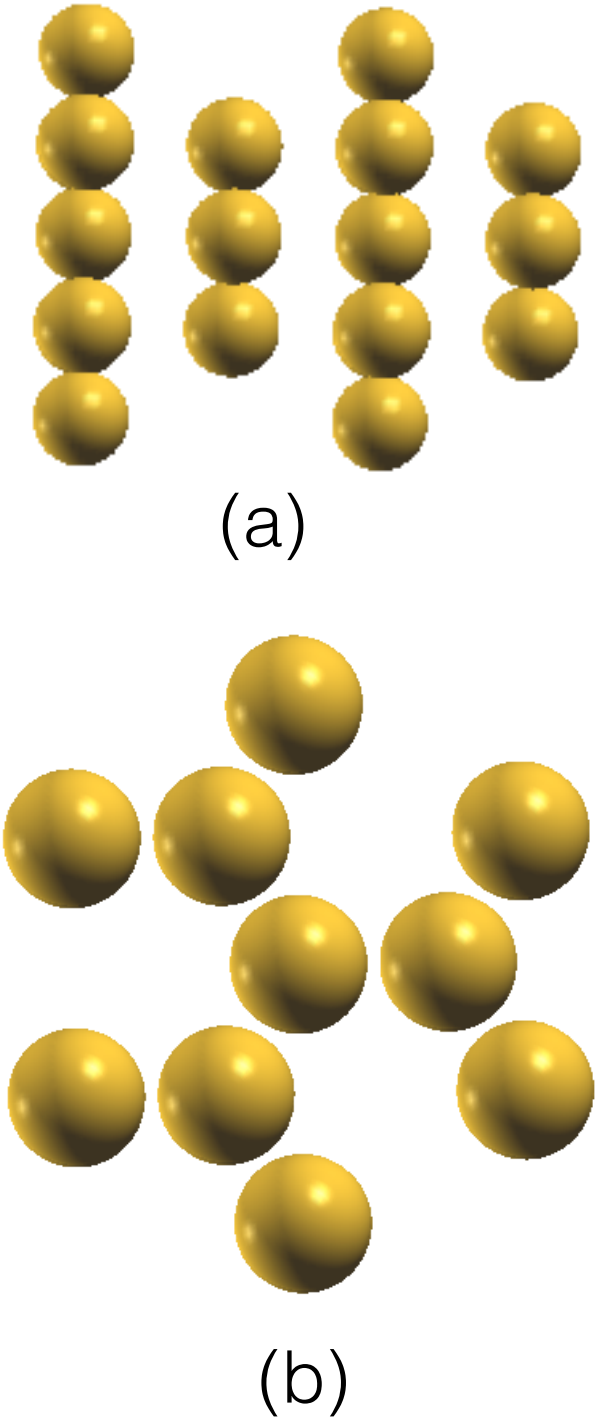

Figure S1: (a) Side and (b) Top view Au electrodes used for device designing in this study.

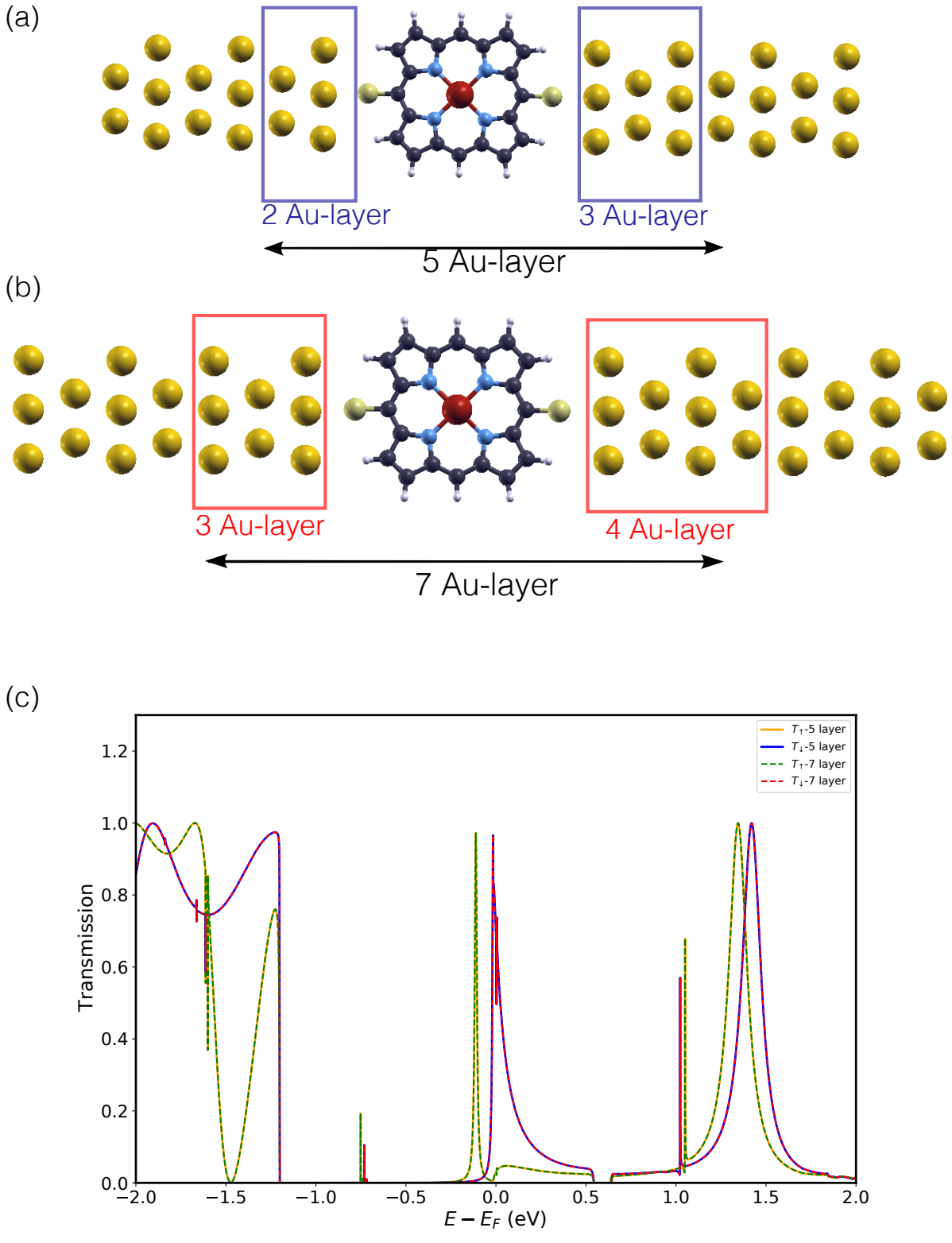

Figure S2: The structure of Au−S−FeP−S−Au device with (a) 5 Au layer and (b) 7 Au layer in extended scattering region to screen the suitable number of Au layer should be included in extended central region to avoid lateral molecule interaction and direct electrode-electrode transmission. (c) The spin-polarized transmission spectra of devices are shown in panel (a) and (b). The transmission spectra for major and minor-spins do not change by extending the central region from 5 to 7 (sum of left and right layers) Au layer.

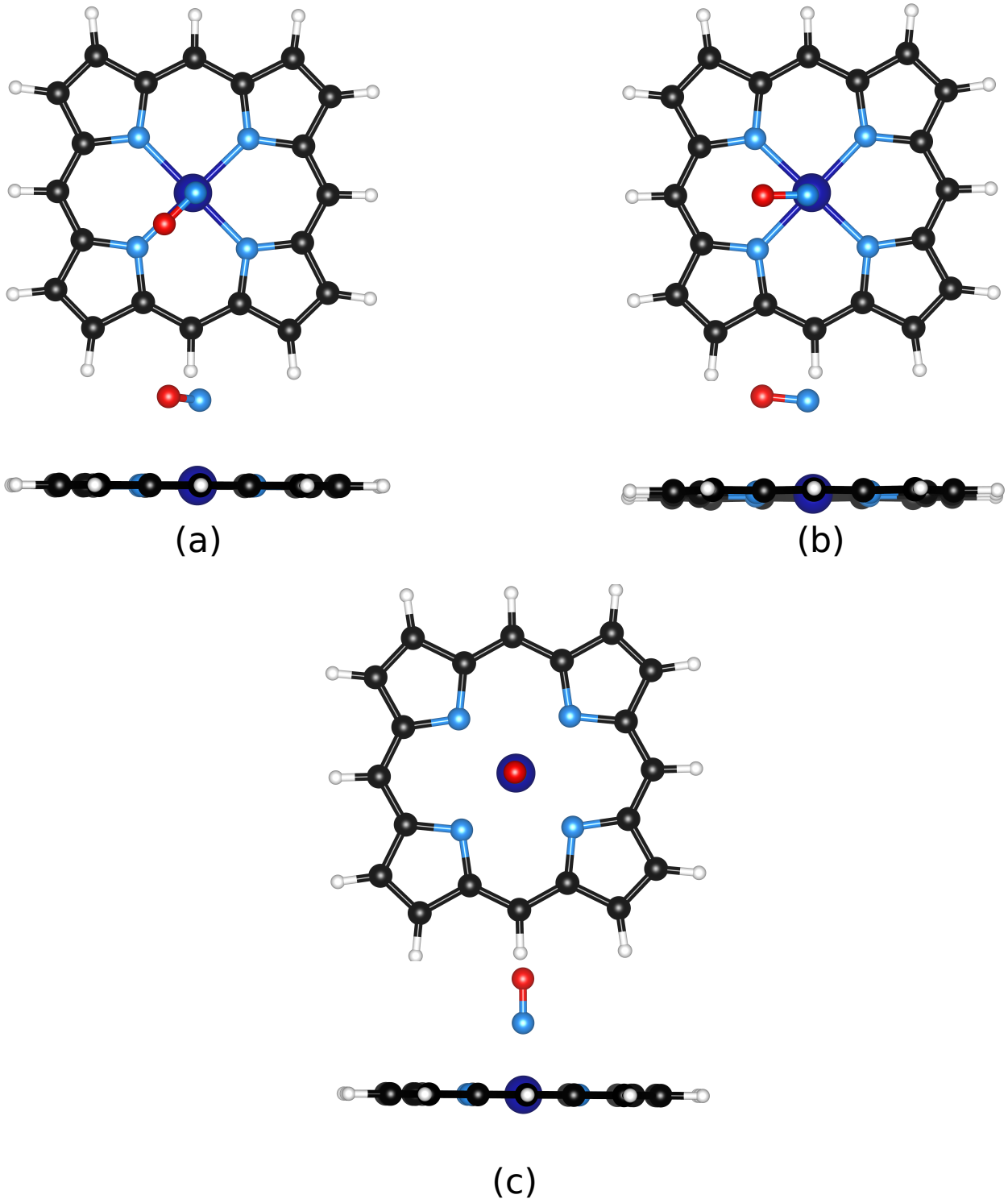

Figure S3: Different NO adsorption configurations: (a) The NO gas is placed along the two pyrrole rings: A-configuration. (b) The NO gas is posited between the two pyrrole rings: B-configuration. (c) The NO gas is placed on the top of the central ion-magnet: C-configuration. In all three configurations the NO gas is bonded through the nitrogen atom.

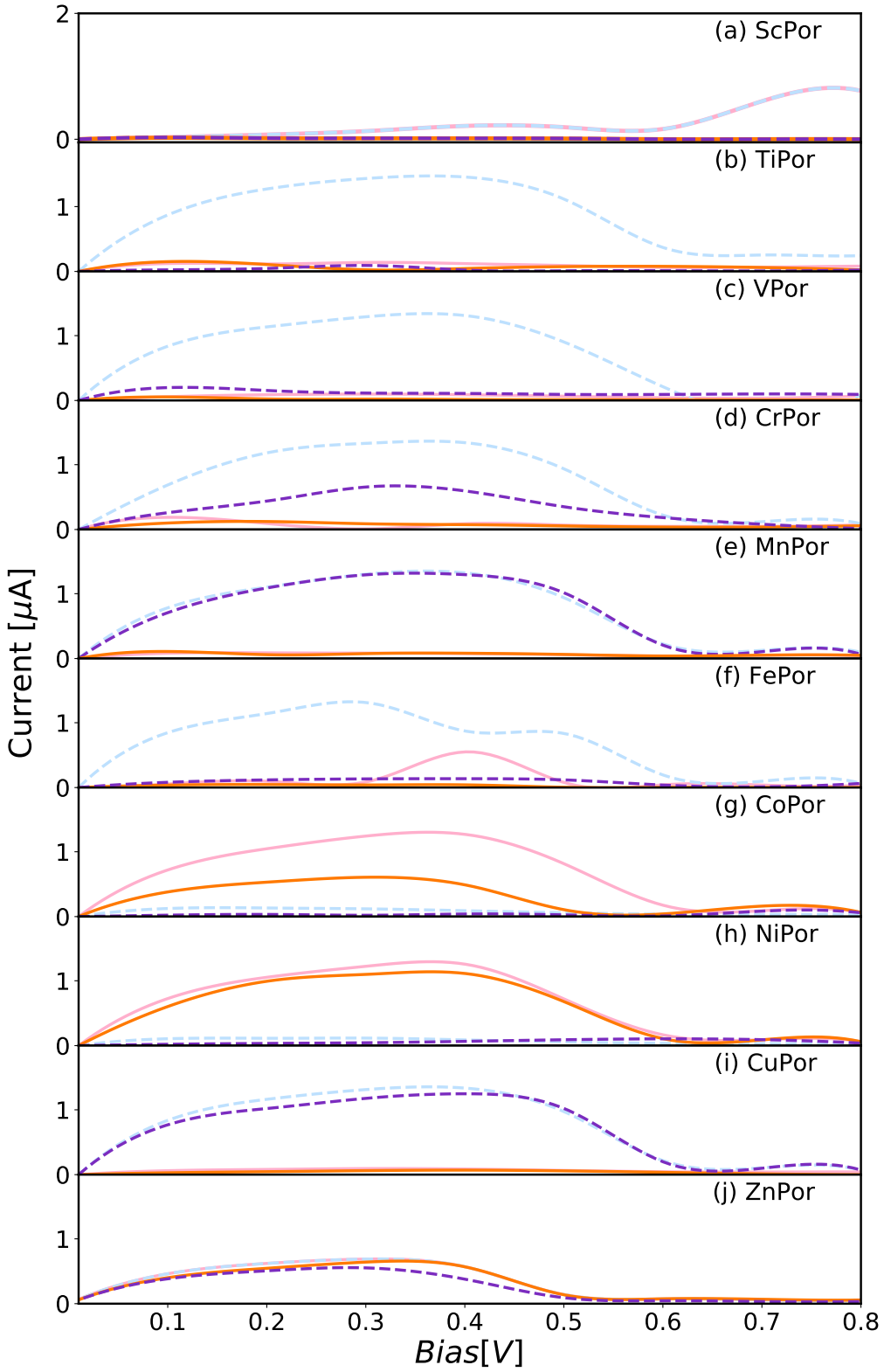

Figure S4: Calculated spin-resolved $I-V$ curves of the pristine Au−MPor−Au and Au−NO@MPor−Au devices. The light pink and light blue colors represent the obtained $I_{\uparrow}$ and $I_{\downarrow}$ for Au−MPor−Au devices. The $I_{\uparrow}$ and $I_{\downarrow}$ of NO adsorbed devices are shown by orange and purple. The dashed curves represent the $I_{\downarrow}$ of devices before and after NO adsorption. For simplicity, each plot is labeled by the device centered molecule

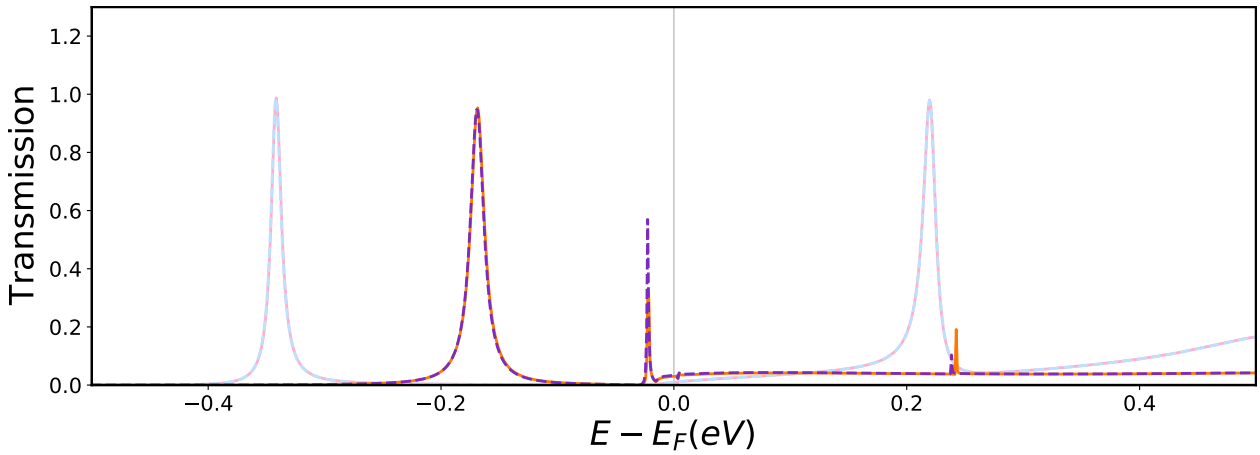

Figure S5: Spin-resolved transmission functions of Au−ScPor−Au and Au−NO@ScPor−Au at 0.0 bias voltages. The light pink and light blue colors represent the obtained $T_\uparrow$ and $T_\downarrow$ for Au−MPor−Au devices. The $T_\uparrow$ and $T_\downarrow$ of NO adsorbed devices are shown by orange and purple. The dashed curves represent the $T_\downarrow$ of devices before and after NO adsorption.

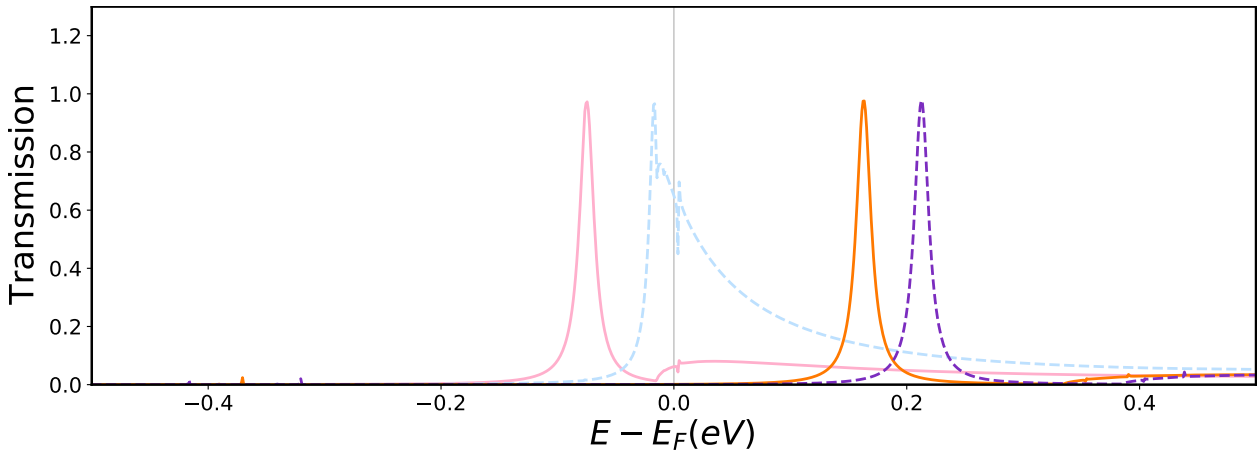

Figure S6: Spin-resolved transmission functions of Au−TiPor−Au and Au−NO@TPor−Au at 0.0 bias voltages. The light pink and light blue colors represent the obtained $T_\uparrow$ and $T_\downarrow$ for Au−MPor−Au devices. The $T_\uparrow$ and $T_\downarrow$ of NO adsorbed devices are shown by orange and purple. The dashed curves represent the $T_\downarrow$ of devices before and after NO adsorption.

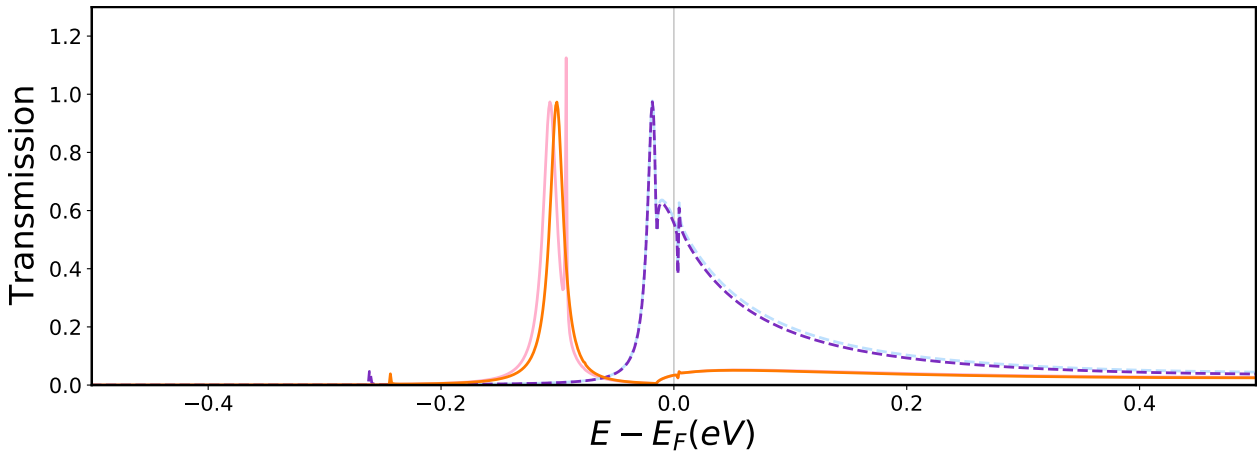

Figure S7: Spin-resolved transmission functions of Au−MnPor−Au and Au−NO@MnPor−Au at 0.0 bias voltages. The light pink and light blue colors represent the obtained $T_\uparrow$ and $T_\downarrow$ for Au−MPor−Au devices. The $T_\uparrow$ and $T_\downarrow$ of NO adsorbed devices are shown by orange and purple. The dashed curves represent the $T_\downarrow$ of devices before and after NO adsorption.

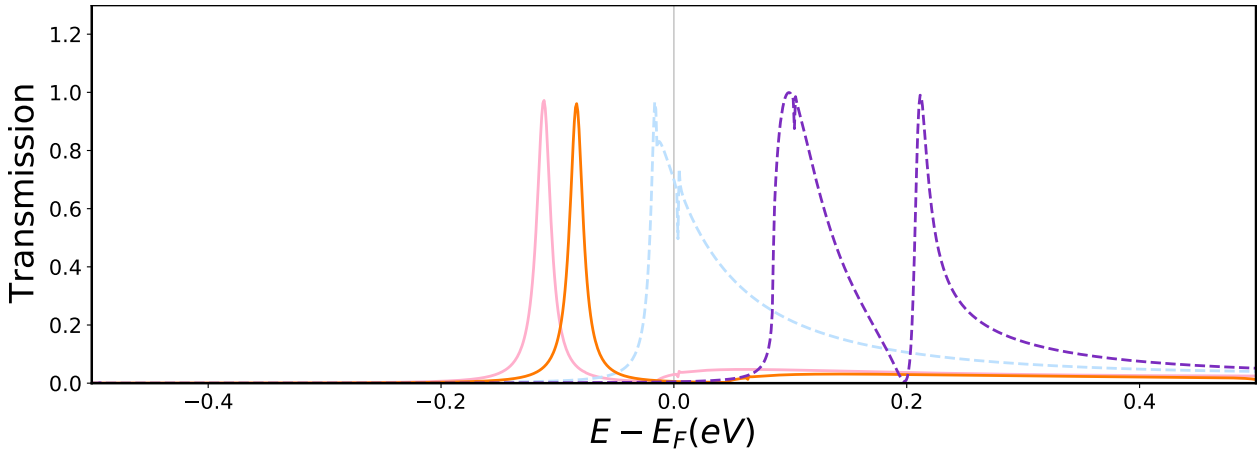

Figure S8: Spin-resolved transmission functions of Au−FePor−Au and Au−NO@FePor−Au at 0.0 bias voltages. The light pink and light blue colors represent the obtained $T_\uparrow$ and $T_\downarrow$ for Au−MPor−Au devices. The $T_\uparrow$ and $T_\downarrow$ of NO adsorbed devices are shown by orange and purple. The dashed curves represent the $T_\downarrow$ of devices before and after NO adsorption.

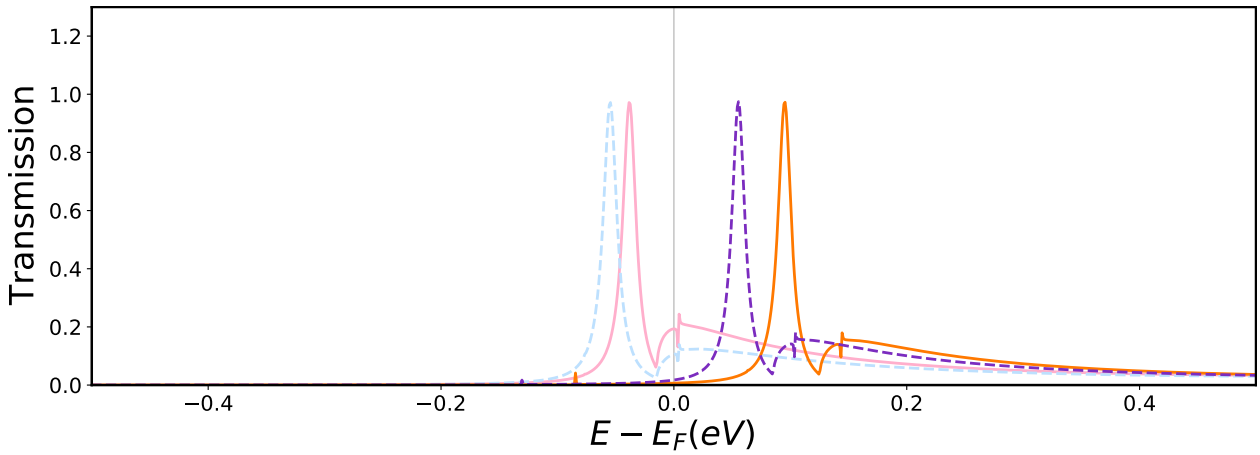

Figure S9: Spin-resolved transmission functions of Au−CoPor−Au and Au−NO@CoPor−Au at 0.0 bias voltages. The light pink and light blue colors represent the obtained $T_\uparrow$ and $T_\downarrow$ for Au−MPor−Au devices. The $T_\uparrow$ and $T_\downarrow$ of NO adsorbed devices are shown by orange and purple. The dashed curves represent the $T_\downarrow$ of devices before and after NO adsorption.

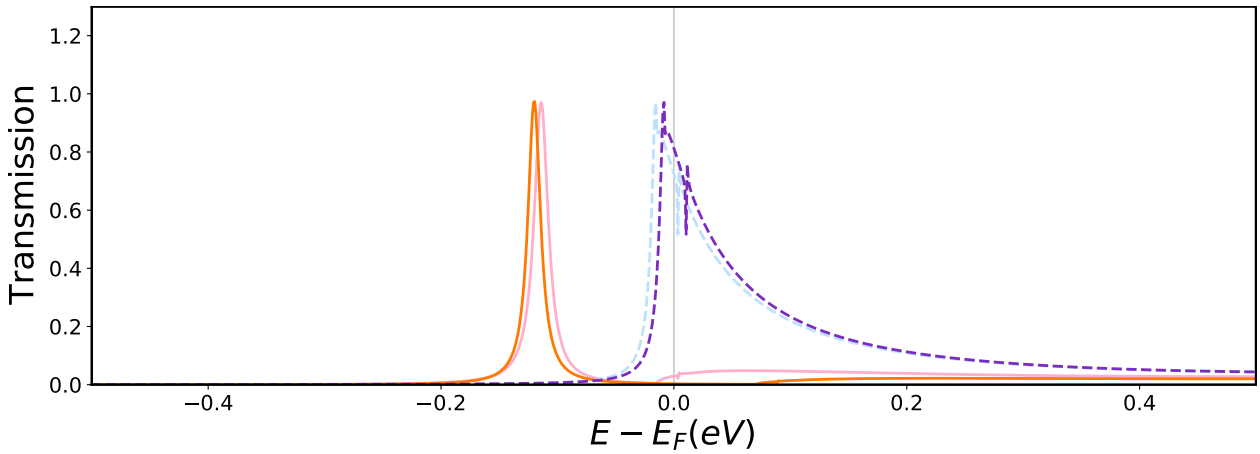

Figure S10: Spin-resolved transmission functions of Au−CuPor−Au and Au−NO@CuPor−Au at 0.0 bias voltages. The light pink and light blue colors represent the obtained $T_\uparrow$ and $T_\downarrow$ for Au−MPor−Au devices. The $T_\uparrow$ and $T_\downarrow$ of NO adsorbed devices are shown by orange and purple. The dashed curves represent the $T_\downarrow$ of devices before and after NO adsorption.

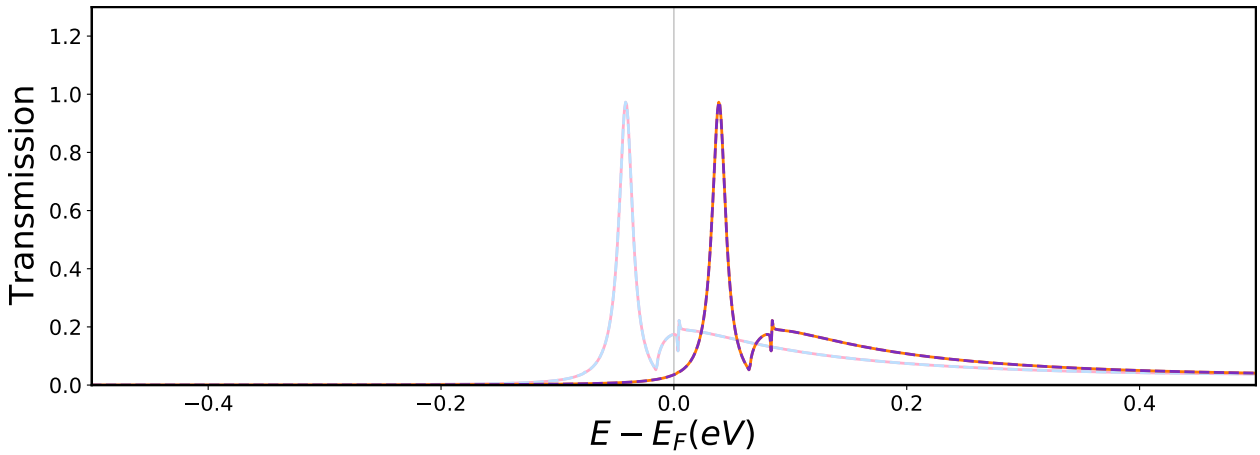

Figure S11: Spin-resolved transmission functions of Au−ZnPor−Au and Au−NO@ZnPor−Au at 0.0 bias voltages. The light pink and light blue colors represent the obtained $T_\uparrow$ and $T_\downarrow$ for Au−MPor−Au devices. The $T_\uparrow$ and $T_\downarrow$ of NO adsorbed devices are shown by orange and purple. The dashed curves represent the $T_\downarrow$ of devices before and after NO adsorption.

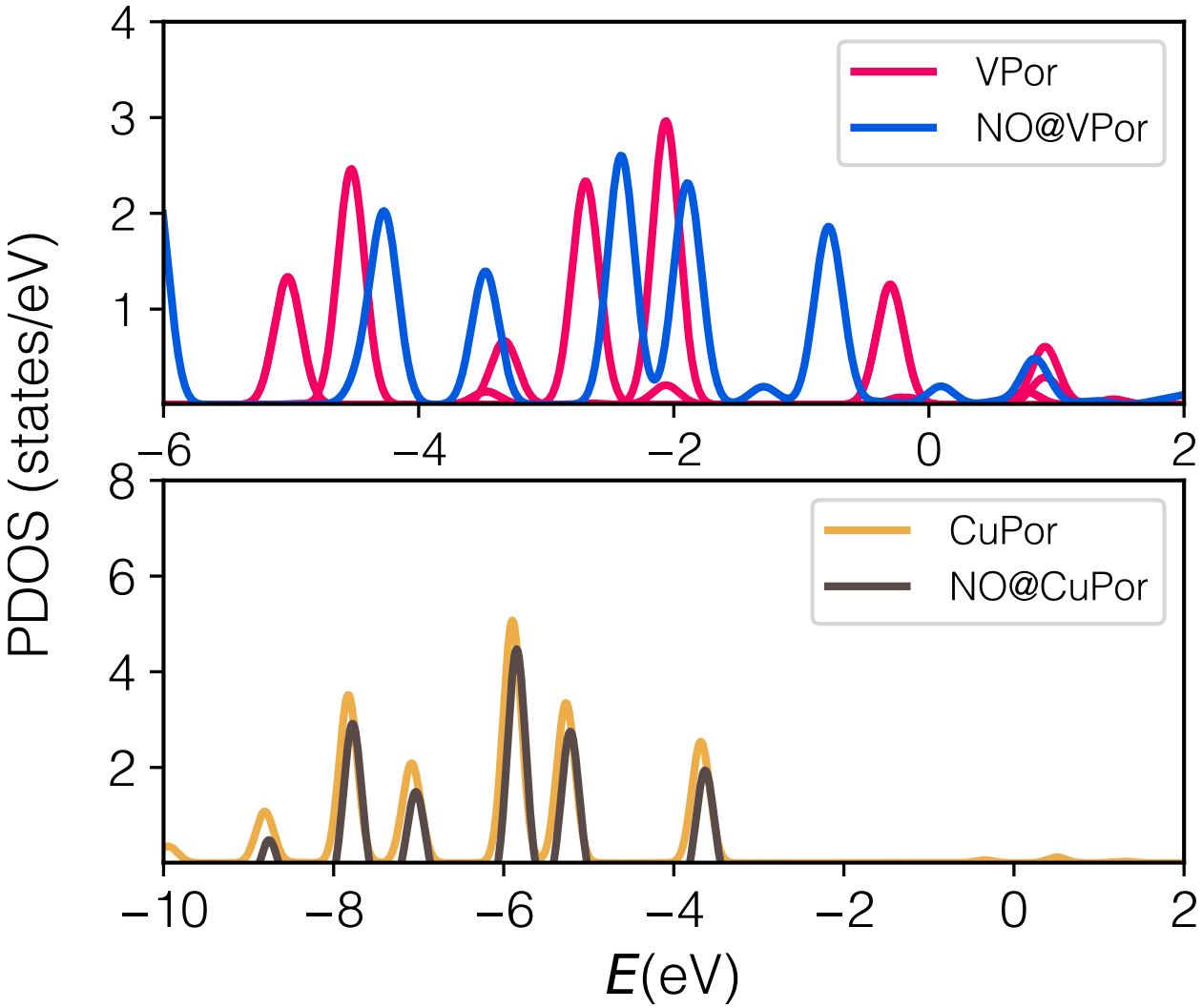

Figure S12: Projected density of states (PDOS) of M $3d$ orbital of VPor (top) and CuPor (bottom) before and after NO adsorption.