

## Designing Bifunctional Molecular Devices with Metallocporphyrin Dimer

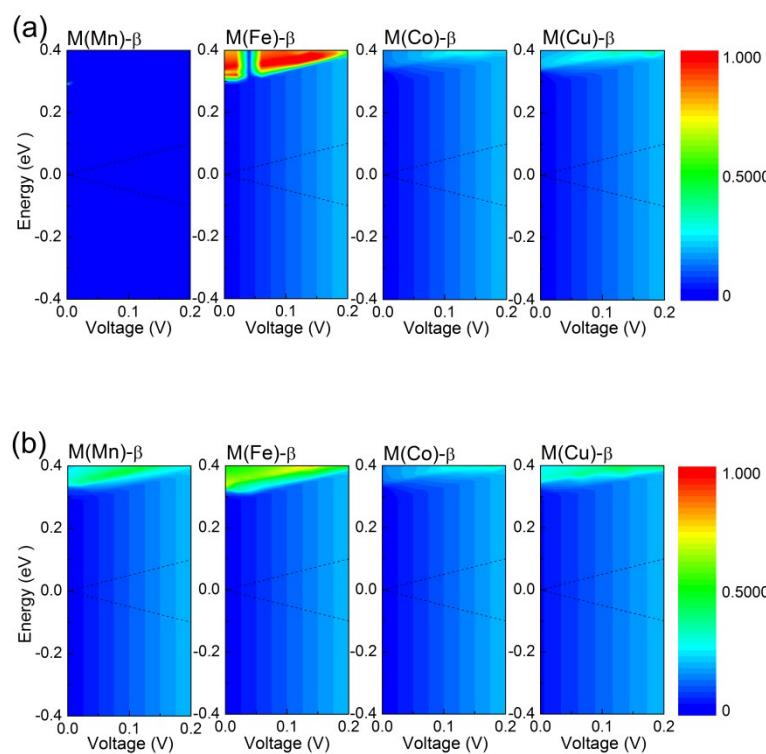
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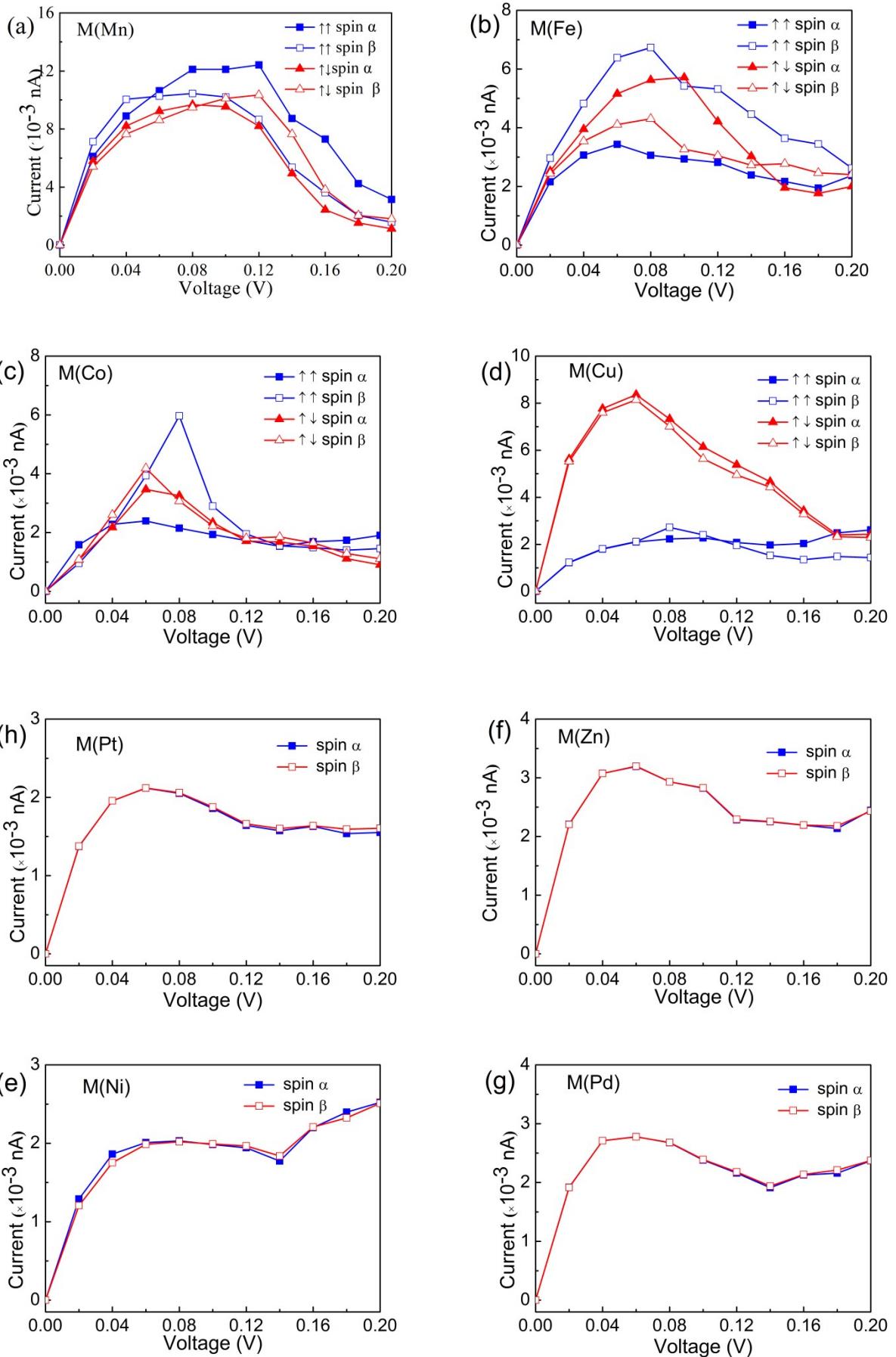
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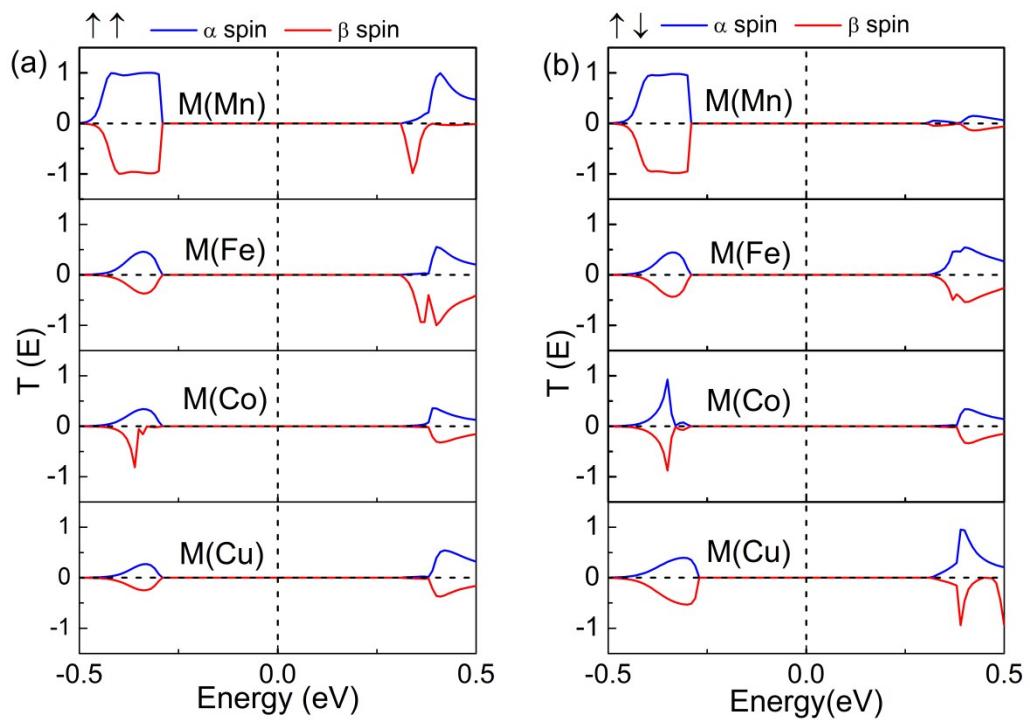
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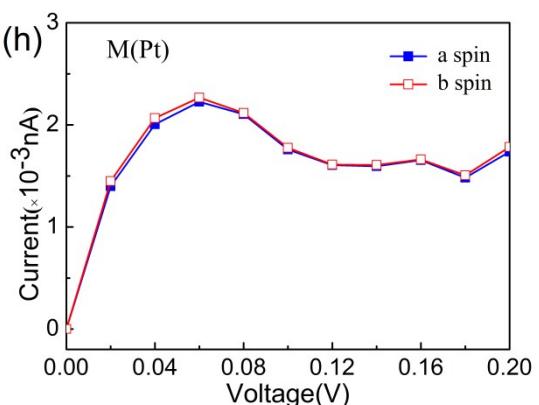
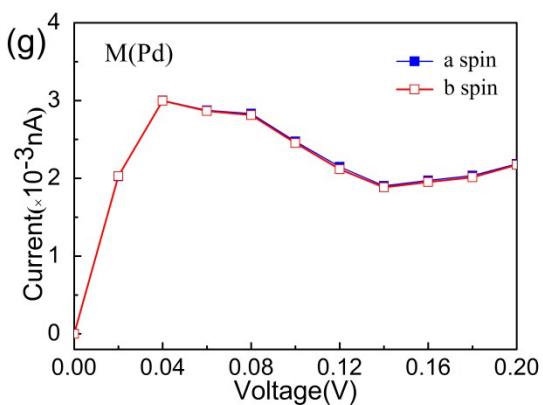
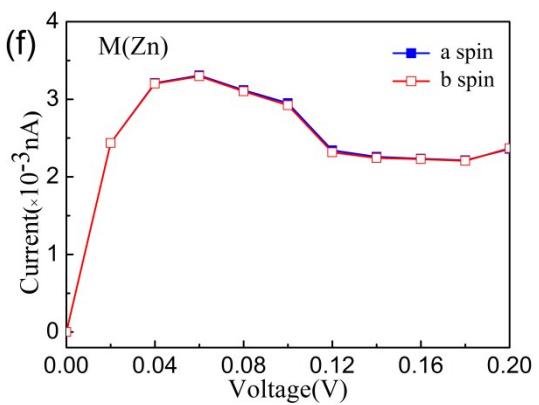
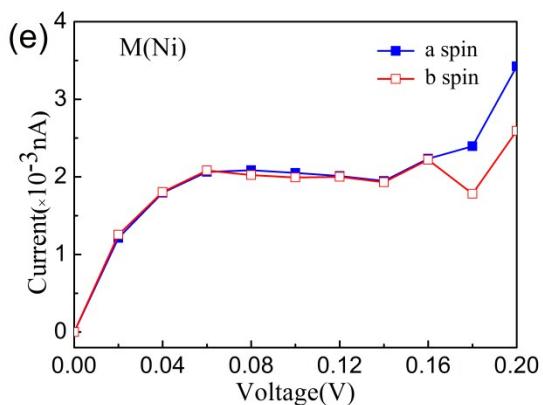
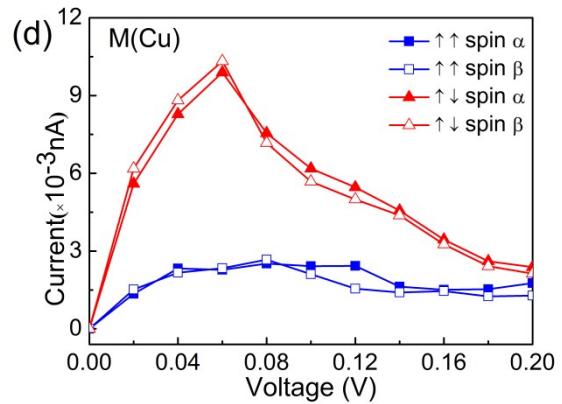
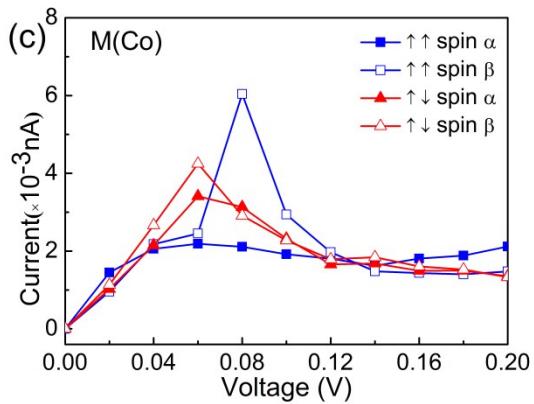
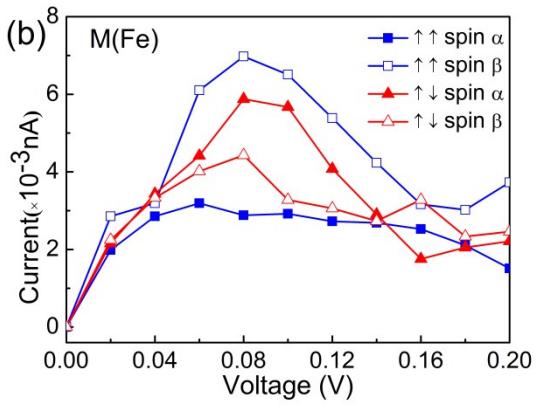
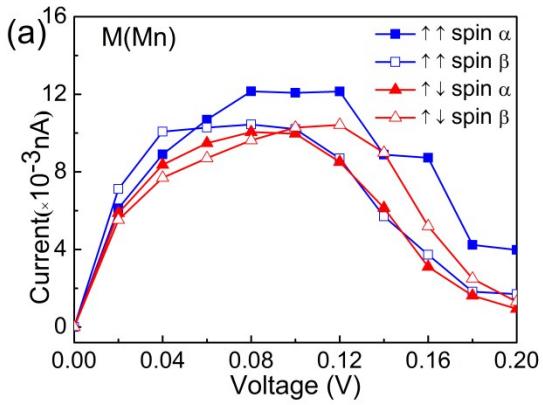
**Fig. S1.** Spin-resolved contour maps of  $\beta$  spin transmission spectra for M(Mn), M(Fe), M(Co), and M(Cu) in the bias range from 0 to 0.2V, respectively. The black dash lines designate the region of the bias window. The Fermi level is set at zero in the energy scale.



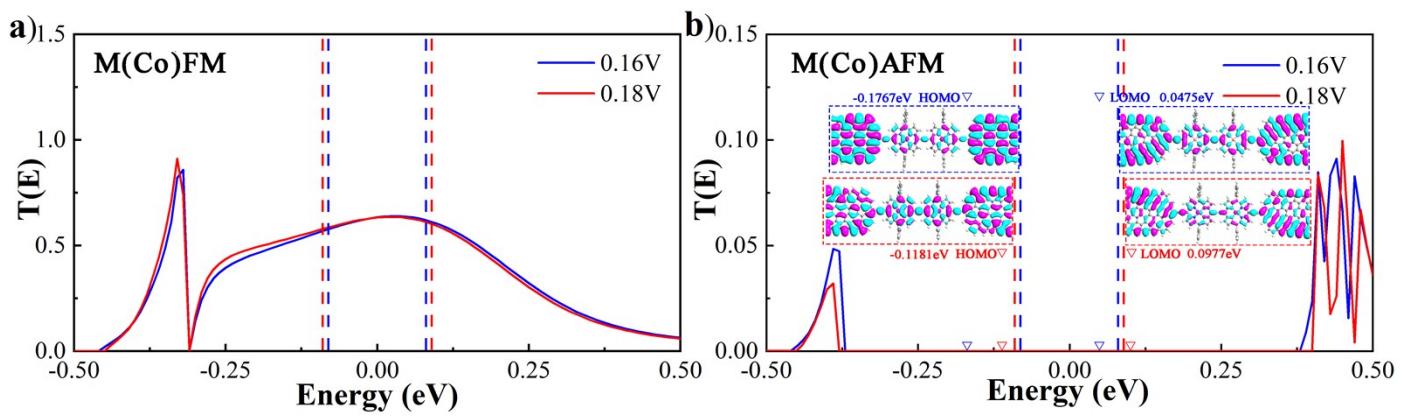
**Fig. S2.** (a)-(h) The IV curves of M(Mn), M(Fe), M(Co), M(Cu), M(Ni), M(Zn), M(Pd), and M(Pt) in AFM.



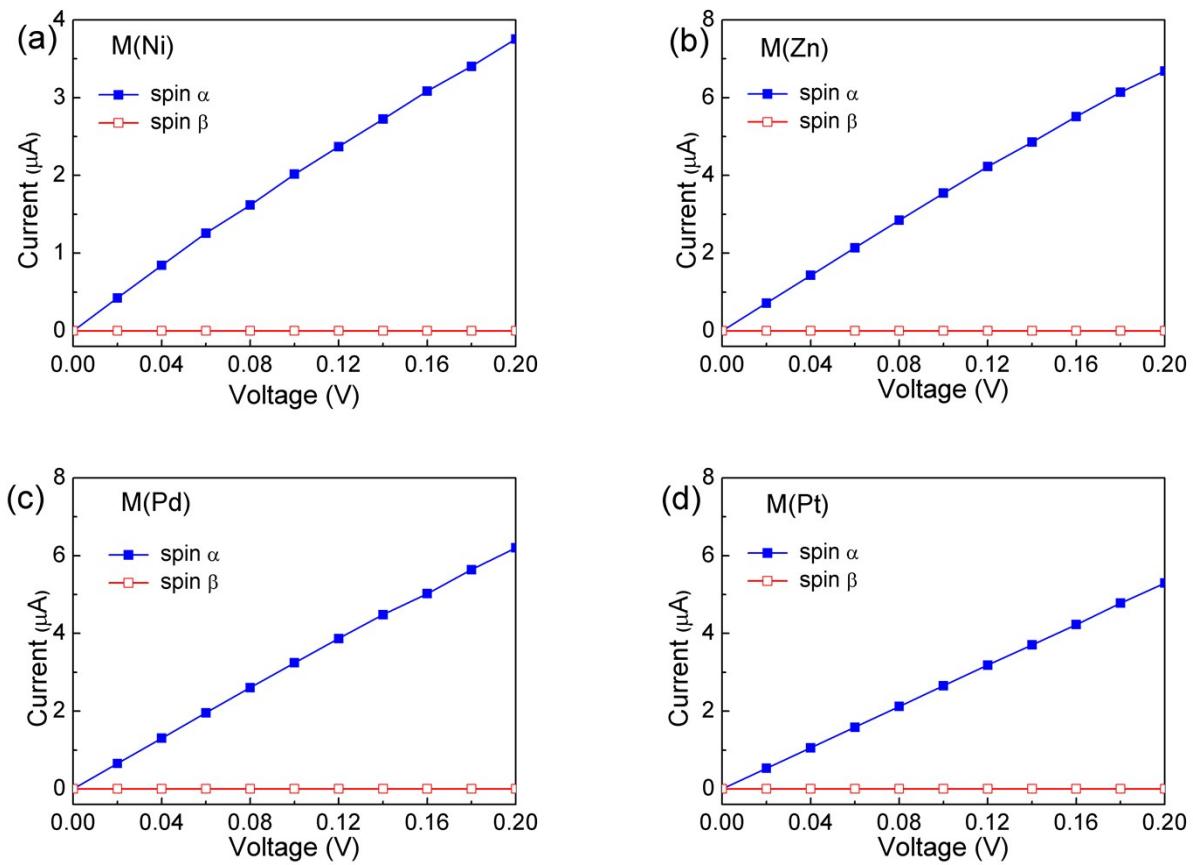
**Fig. S3.** The transmission spectra of M(Mn), M(Fe), M(Co) and M(Cu) in the AFM at zero bias.



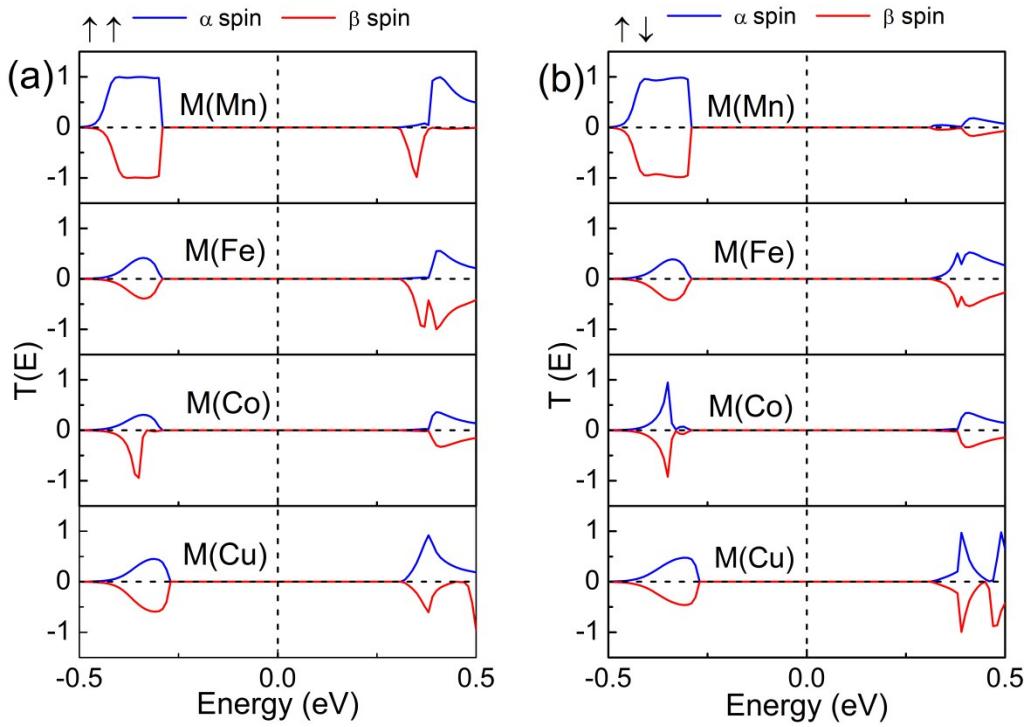
**Fig. S4.** (a)-(h) The IV curves of M(Mn), M(Fe), M(Co), M(Cu), M(Ni), M(Zn), M(Pd), and M(Pt) in AP.



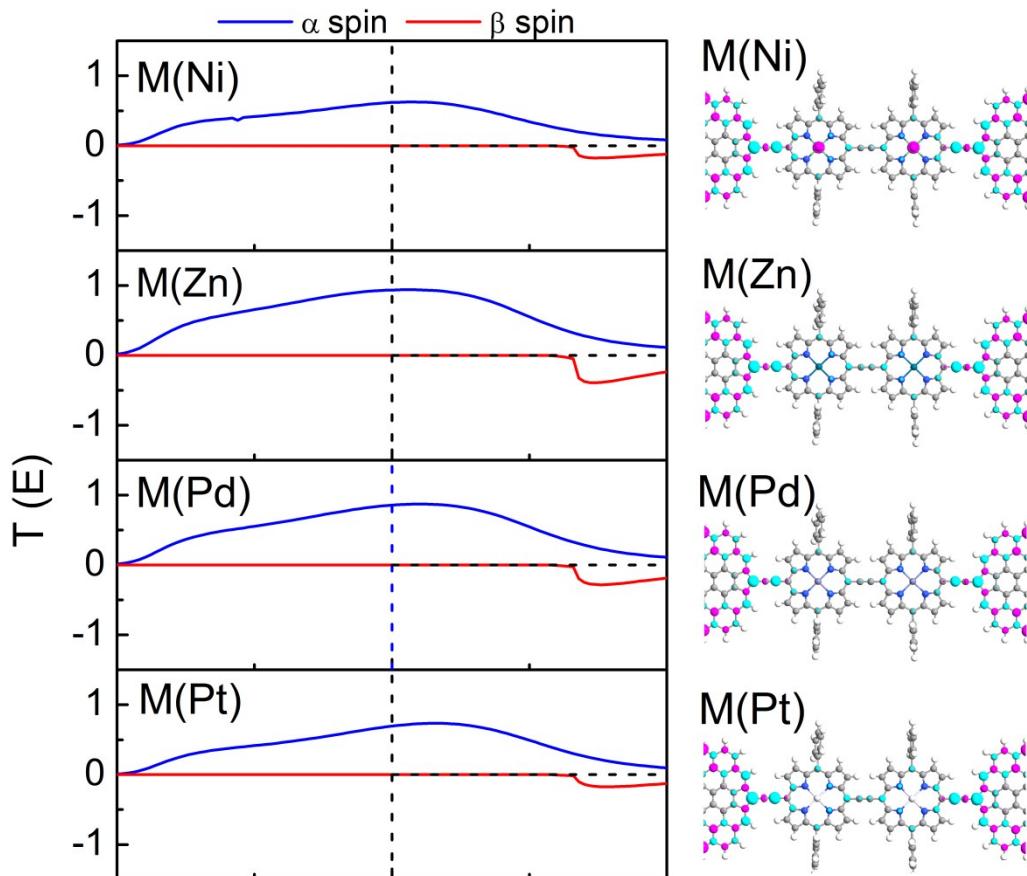
**Fig.S5** The transmission spectra of M(Co) at 0.16 and 0.18V bias under  $\uparrow\downarrow$  magnetic configurations, (a) in the FM ground state and (b) in the AFM ground state. The insets show the MPSHs of HOMO and LUMO of each bias voltage.



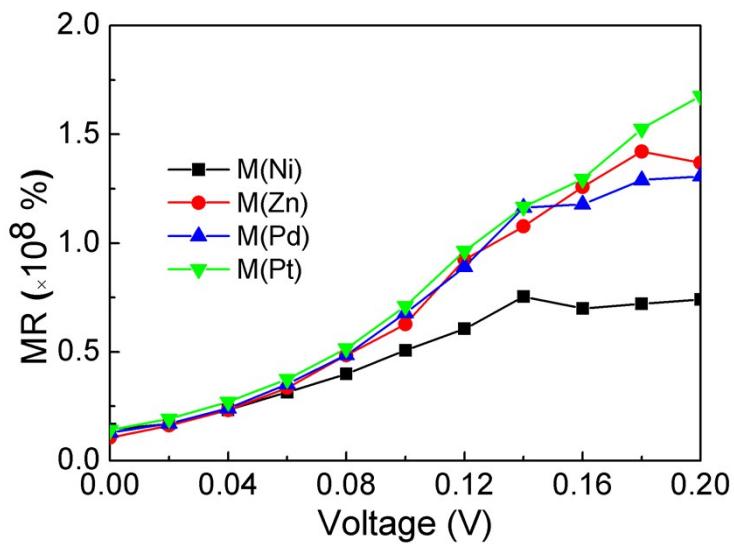
**Fig. S6.** (a)-(d) The IV curves of M(Ni), M(Zn), M(Pd) and M(Pt) in FM.



**Fig. S7.** The transmission spectra of M(Mn), M(Fe), M(Co) and M(Cu) in the AP at zero bias.



**Fig. S8.** The transmission spectra and spin electron densities of M(Ni), M(Zn), M(Pd), and M(Pt) in FM.



**Fig. S9.** The magnetoresistance of M(Ni), M(Zn), M(Pd), and M(Pt).