Table S1. Exponents ζ_i and valence shell ionization potentials H_{ii} of Slater-type orbitals χ_i used for extended Hückel tight-binding calculation [a]

atom	χ_i	H_{ii} (eV)	ζ_i	C [b]	ζ'_i	C′ [b]
Cr	4s	-8.66	1.772	1.00		
Cr	4p	-5.24	1.300	1.00		
Cr	3d	-11.22	5.410	0.3830	2.340	0.7367
Mn	4s	-9.75	1.844	1.00		
Mn	4p	-5.89	1.350	1.00		
Mn	3d	-11.67	5.767	0.3898	2.510	0.7297
Fe	4s	-9.10	1.925	1.00		
Fe	4p	-5.32	1.390	1.00		
Fe	3d	-12.60	6.068	0.4038	2.618	0.7198
Co	4s	-9.21	2.001	1.00		
Co	4p	-5.29	1.430	1.00		
Co	3d	-13.18	6.386	0.4133	2.745	0.7126
O	2s	-32.3	2.688	0.7076	1.675	0.3745
O	2p	-14.8	3.694	0.3322	1.659 [c]	0.7448

[a] H_{ii}'s are the diagonal matrix elements $\langle\chi_i|H^{eff}|\chi_i\rangle$, where H^{eff} is the effective Hamiltonian. In our calculations of the off-diagonal matrix elements $H^{eff} = \langle\chi_i|H^{eff}|\chi_j\rangle$, the weighted formula was used. See: Ammeter, J.; Bürgi, H.-B.; Thibeault, J.; Hoffmann, R., *J. Am. Chem. Soc*. **1978**, *100*, 3686.

[b] Contraction coefficients used in the double-zeta Slater-type orbital.

[c] This value refers to the case of x = 0.