

Tunable Electronic and Magnetic Properties of Transition Metal-Cyclopentadiene Sandwich Molecule Wires Functionalized Narrow Single Wall Carbon Nanotubes

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**Supporting Information**

Table S1. The Systems, the lattice parameter per unit cell of [TMCp] $_{\infty}$ ,  $C_1(\text{\AA})$  and SWCNTs,  $C_2(\text{\AA})$ , the ratio of  $pC_1/qC_2$  ( $R$ ) and the mismatch degree ( $M_{is}\%$ ),  $M_{is}\% = |pC_1(\text{\AA}) - qC_2(\text{\AA})|/qC_2(\text{\AA}) \times 100\%$ , the diameters of selected SWCNTs ( $D(\text{\AA})$ ).

Systems	$C_1(\text{\AA})^1$	$C_2(\text{\AA})$	$R$	Mis(%)	$D(\text{\AA})$
[Co <sub>2</sub> Cp <sub>2</sub> /3(7,7)] $_{\infty}$	3.50 <sup>30</sup>	2.46	2:3	0.42	9.58
[Sc <sub>3</sub> Cp <sub>3</sub> /5(7,7)] $_{\infty}$	4.08 <sup>30</sup>	2.46	3:5	0.5	9.58
[Mn <sub>3</sub> Cp <sub>3</sub> /4(7,7)] $_{\infty}$	3.32 <sup>30</sup>	2.46	3:4	1.2	9.58
[Mn <sub>5</sub> Cp <sub>5</sub> /4(10,0)] $_{\infty}$	3.32 <sup>30</sup>	4.26	5:4	2.6	7.91
[Mn <sub>5</sub> Cp <sub>5</sub> /4(11,0)] $_{\infty}$	3.32 <sup>30</sup>	4.26	5:4	2.6	8.70
[Fe <sub>5</sub> Cp <sub>5</sub> /4(10,0)] $_{\infty}$	3.41 <sup>30</sup>	4.26	5:4	0.06	7.91
[Fe <sub>5</sub> Cp <sub>5</sub> /4(11,0)] $_{\infty}$	3.41 <sup>30</sup>	4.26	5:4	0.06	8.70
[V <sub>7</sub> Cp <sub>7</sub> /6(10,0)] $_{\infty}$	3.62 <sup>30</sup>	4.26	7:6	0.9	7.91
[V <sub>7</sub> Cp <sub>7</sub> /6(11,0)] $_{\infty}$	3.62 <sup>30</sup>	4.26	7:6	0.9	8.70

- (1) Shen, L.; Yang, S. W.; Ng, M. F.; Ligatchev, V.; Zhou, L. P.; Feng, Y. P. Charge-transfer-based Mechanism for Half-Metallicity and Ferromagnetism in One-Dimensional Organometallic Sandwich Molecular Wires. *J. Am. Chem. Soc.* **2008**, 130, 13956-13960.

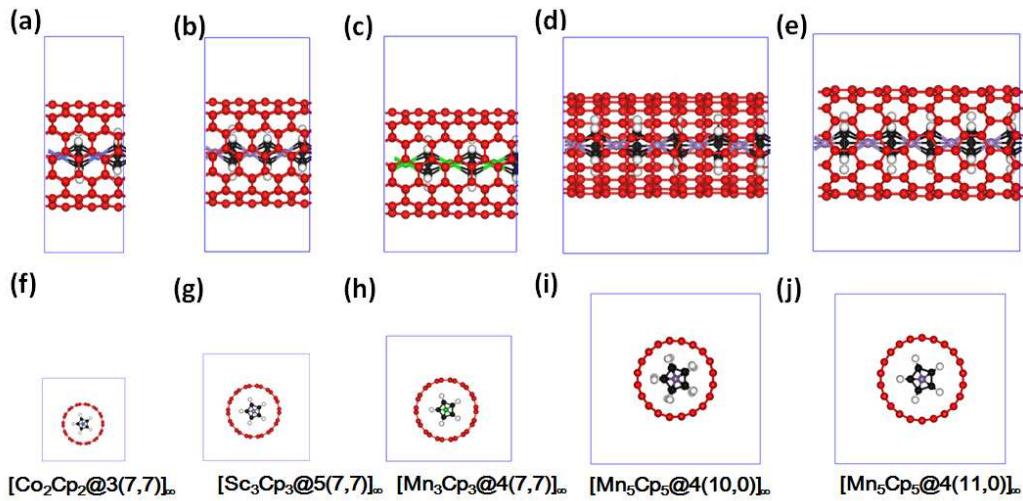


Figure S1. Top and side view of the optimized structures of (a, f) [Co<sub>2</sub>Cp<sub>2</sub>@3(7,7)]<sub>∞</sub>, (b, g) [Mn<sub>3</sub>Cp<sub>3</sub>@4(7,7)]<sub>∞</sub>, (c, h) [Sc<sub>3</sub>Cp<sub>3</sub>@5(7,7)]<sub>∞</sub>, (d, i) [Fe<sub>5</sub>Cp<sub>5</sub>@4(10,0)]<sub>∞</sub> and (e, j) [Fe<sub>5</sub>Cp<sub>5</sub>@4(11,0)]<sub>∞</sub>.

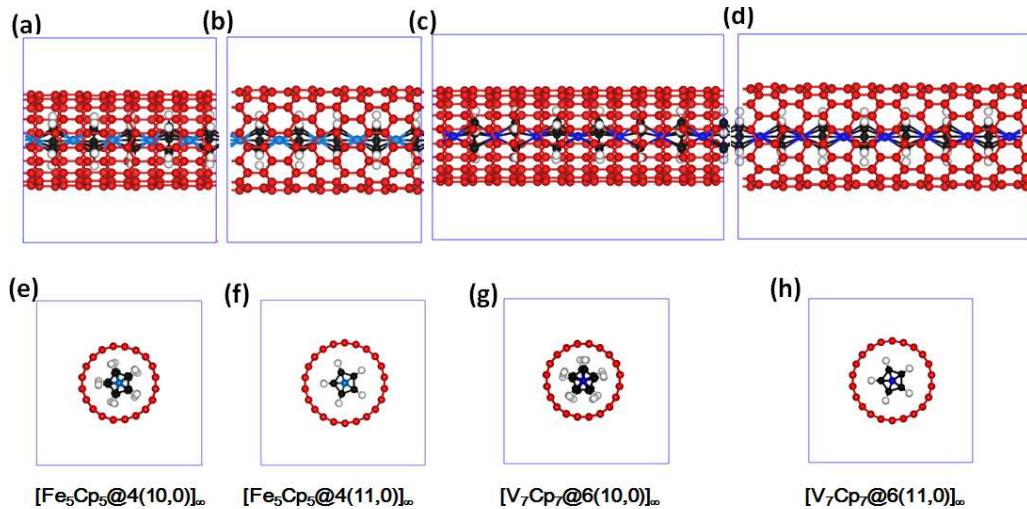


Figure S2. Top and side view of the optimized structures of (a, e) [Fe<sub>5</sub>Cp<sub>5</sub>@4(10,0)]<sub>∞</sub>, (b, f) [Fe<sub>5</sub>Cp<sub>5</sub>@4(11,0)]<sub>∞</sub>, (c, g) [V<sub>7</sub>Cp<sub>7</sub>@6(10,0)]<sub>∞</sub> and (d, h) [V<sub>7</sub>Cp<sub>7</sub>@6(11,0)]<sub>∞</sub>.

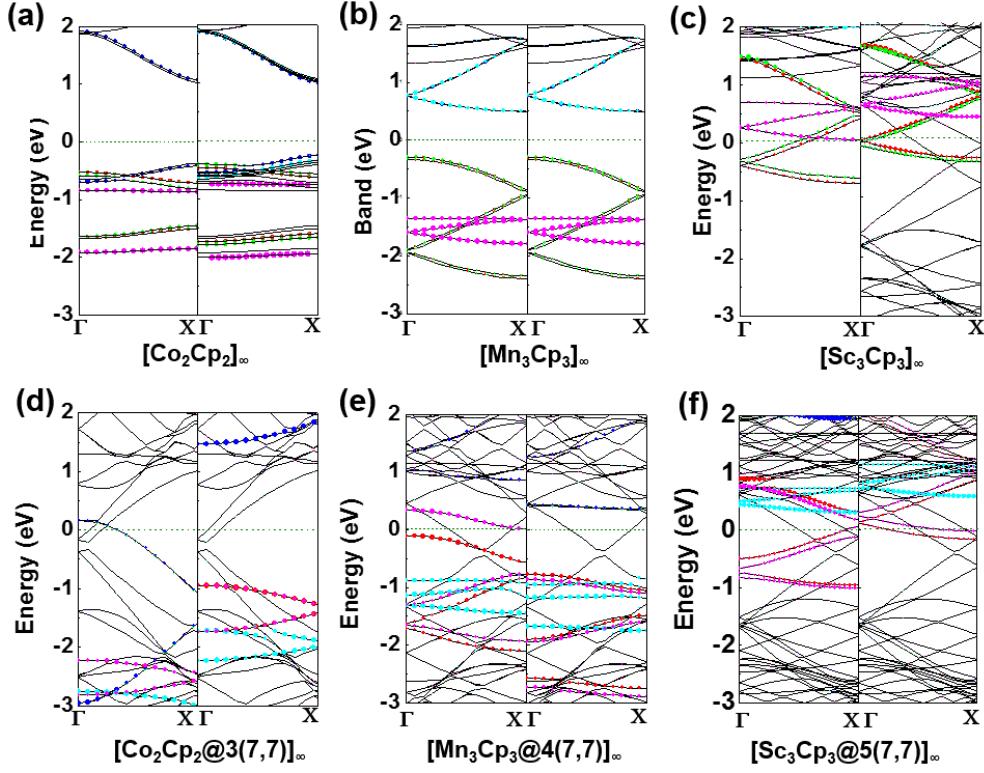


Figure S3. (a-f) Band structures of 1D  $[\text{Co}_2\text{Cp}_2]_\infty$ ,  $[\text{Mn}_3\text{Cp}_3]_\infty$ ,  $[\text{Sc}_3\text{Cp}_3]_\infty$  and  $[\text{Co}_2\text{Cp}_2@3(7,7)]_\infty$ ,  $[\text{Mn}_3\text{Cp}_3@4(7,7)]_\infty$ ,  $[\text{Sc}_3\text{Cp}_3@5(7,7)]_\infty$ .

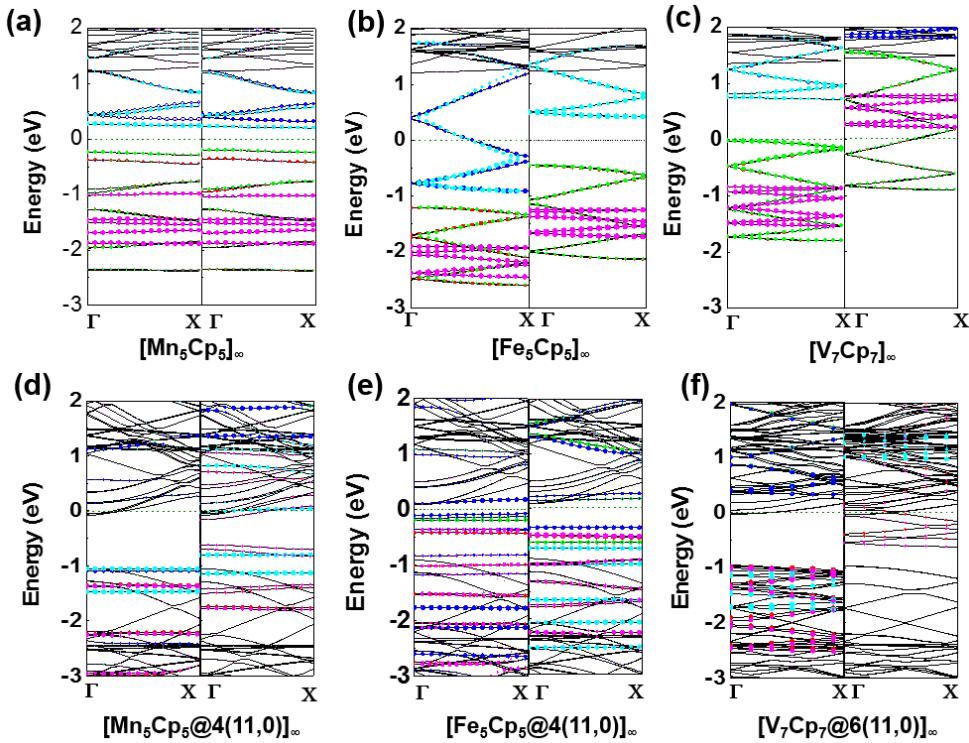


Figure S4. (a-f) Bandstructures of 1D  $[\text{Mn}_5\text{Cp}_5]_\infty$ ,  $[\text{Fe}_5\text{Cp}_5]_\infty$ ,  $[\text{V}_7\text{Cp}_7]_\infty$  wires and 1D  $[\text{Mn}_5\text{Cp}_5@4(11,0)]_\infty$ ,  $[\text{Fe}_5\text{Cp}_5@4(11,0)]_\infty$ ,  $[\text{V}_7\text{Cp}_7@6(11,0)]_\infty$ .

$[\text{Mn}_5\text{Cp}_5@4(11,0)]_\infty$ ,  $[\text{Fe}_5\text{Cp}_5@4(11,0)]_\infty$ ,  $[\text{V}_7\text{Cp}_7@6(11,0)]_\infty$ .

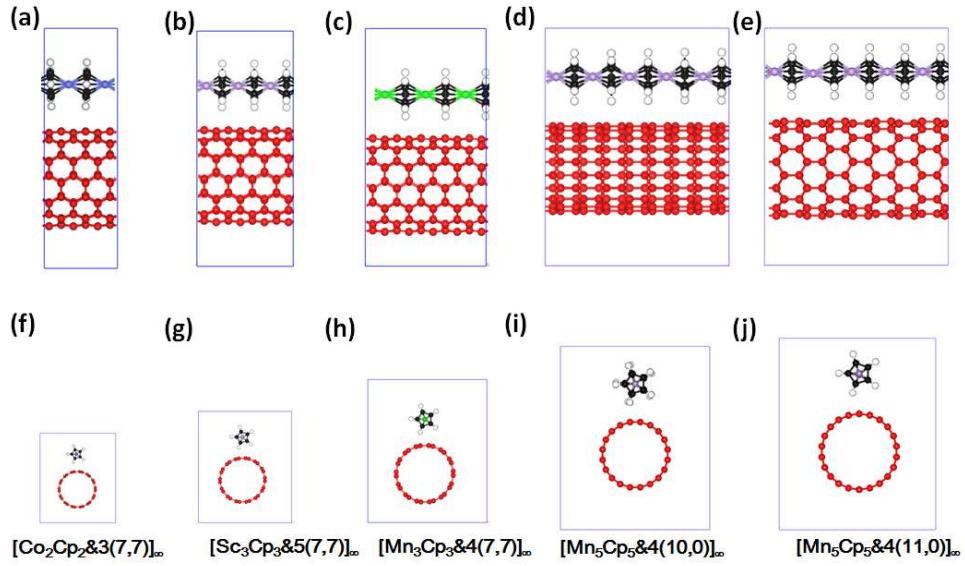


Figure S5. Top and side view of the optimized structures of (a, f)  $[\text{Co}_2\text{Cp}_2&3(7,7)]_\infty$ , (b, g)  $[\text{Mn}_3\text{Cp}_3&4(7,7)]_\infty$ , (c, h)  $[\text{Sc}_3\text{Cp}_3&5(7,7)]_\infty$ , (d, i)  $[\text{Mn}_5\text{Cp}_5&4(10,0)]_\infty$  and (e, j)  $[\text{Mn}_5\text{Cp}_5&4(11,0)]_\infty$ .

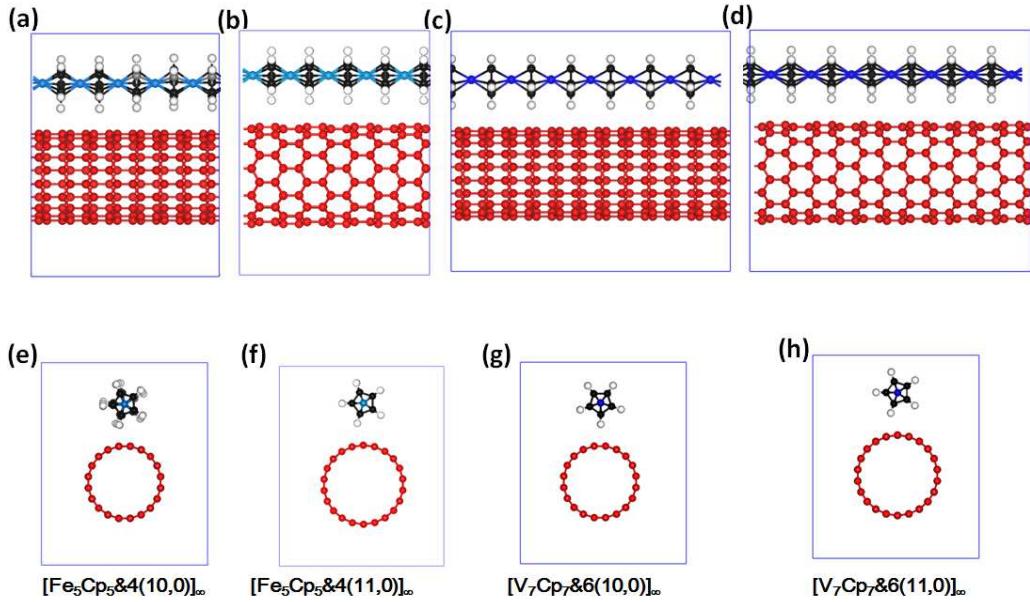


Figure S6. Top and side view of the optimized structures of (a, e)  $[\text{Fe}_5\text{Cp}_5&4(10,0)]_\infty$ , (b, f)  $[\text{Fe}_5\text{Cp}_5&4(11,0)]_\infty$ , (c, g)  $[\text{V}_7\text{Cp}_7&6(10,0)]_\infty$  and (d, h)  $[\text{V}_7\text{Cp}_7&6(11,0)]_\infty$ .

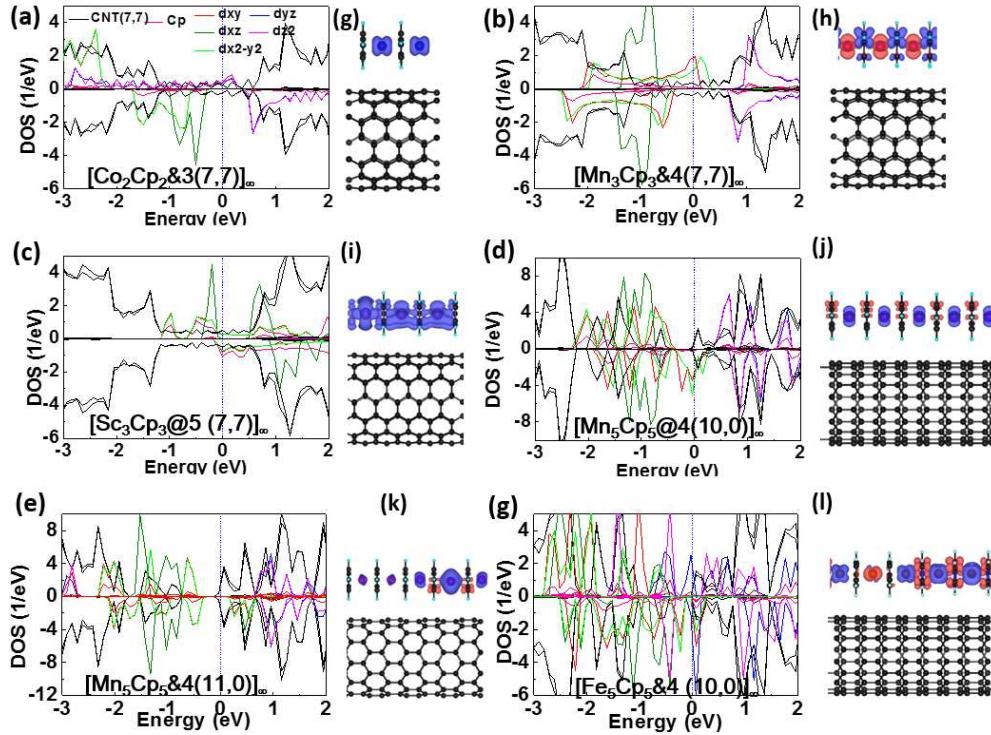


Figure S7. (a-f) Plots of density of states and (g-l) spin densities of 1D ISMW&N( $n, m$ )s.

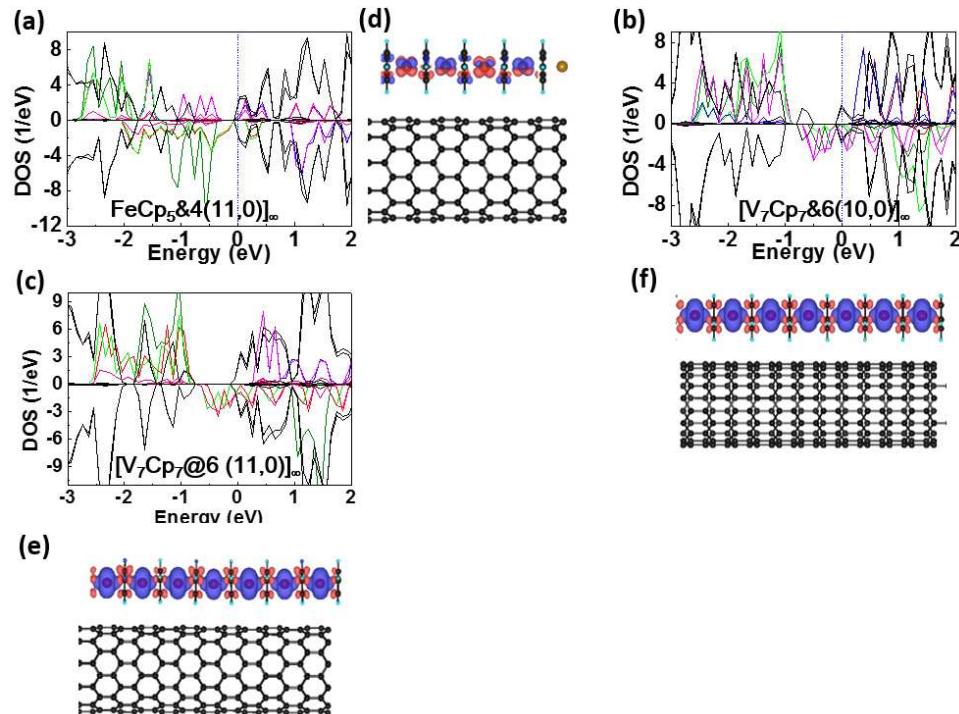


Figure S8. (a-c) Plots of density of states and (d-f) spin densities of 1D [Fe<sub>5</sub>Cp<sub>5</sub>&4(11,0)]<sub>∞</sub> and [V<sub>7</sub>Cp<sub>7</sub>&6(10,0)]<sub>∞</sub> and [V<sub>7</sub>Cp<sub>7</sub>&6(11,0)]<sub>∞</sub>.

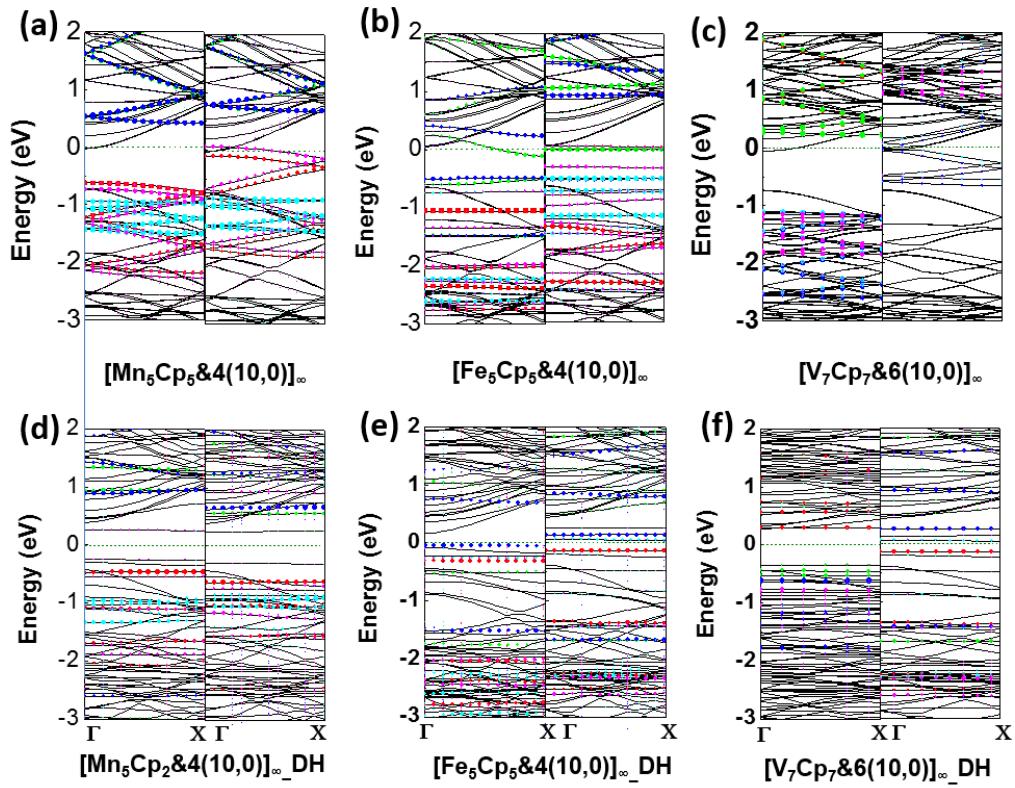


Figure S9. (a-f) Bandstructures of 1D  $[\text{Mn}_5\text{Cp}_5\&4(10,0)]_\infty$ ,  $[\text{Fe}_5\text{Cp}_5\&4(10,0)]_\infty$ ,  $[\text{V}_7\text{Cp}_7\&6(10,0)]_\infty$  wires and 1D  $[\text{Mn}_5\text{Cp}_5\&4(10,0)]_\infty\text{-DH}$ ,  $[\text{Fe}_5\text{Cp}_5\&4(10,0)]_\infty\text{-DH}$ ,  $[\text{V}_7\text{Cp}_7\&6(10,0)]_\infty\text{-DH}$

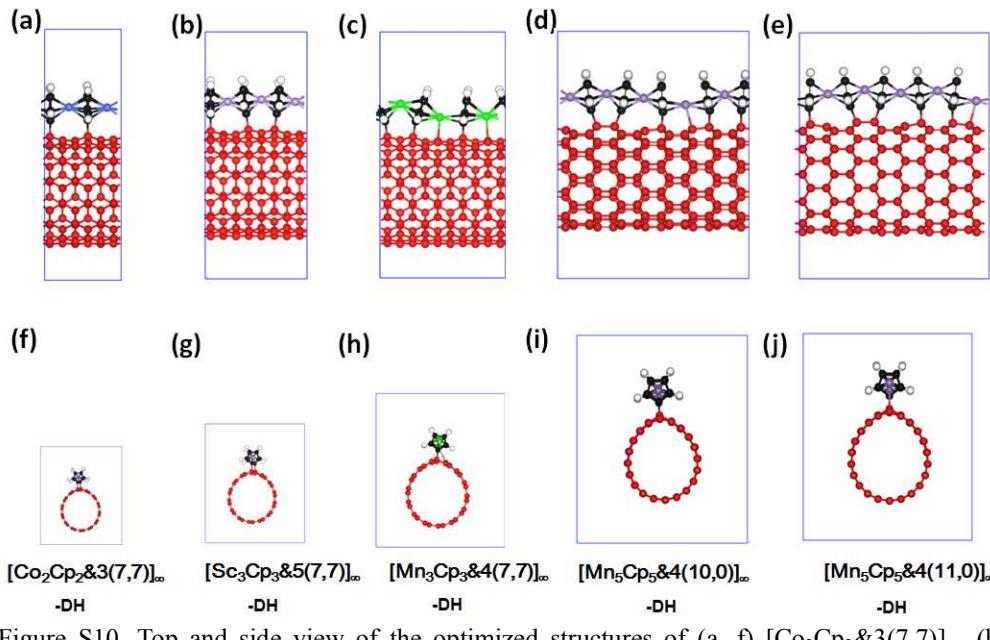


Figure S10. Top and side view of the optimized structures of (a, f)  $[\text{Co}_2\text{Cp}_2\&3(7,7)]_\infty$ , (b, g)  $[\text{Mn}_3\text{Cp}_3\&4(7,7)]_\infty\text{-DH}$ , (c, h)  $[\text{Sc}_3\text{Cp}_3\&5(7,7)]_\infty\text{-DH}$ , (d, i)  $[\text{Mn}_5\text{Cp}_5\&4(10,0)]_\infty\text{-DH}$  and (e, j)  $[\text{Mn}_5\text{Cp}_5\&4(11,0)]_\infty\text{-DH}$ .

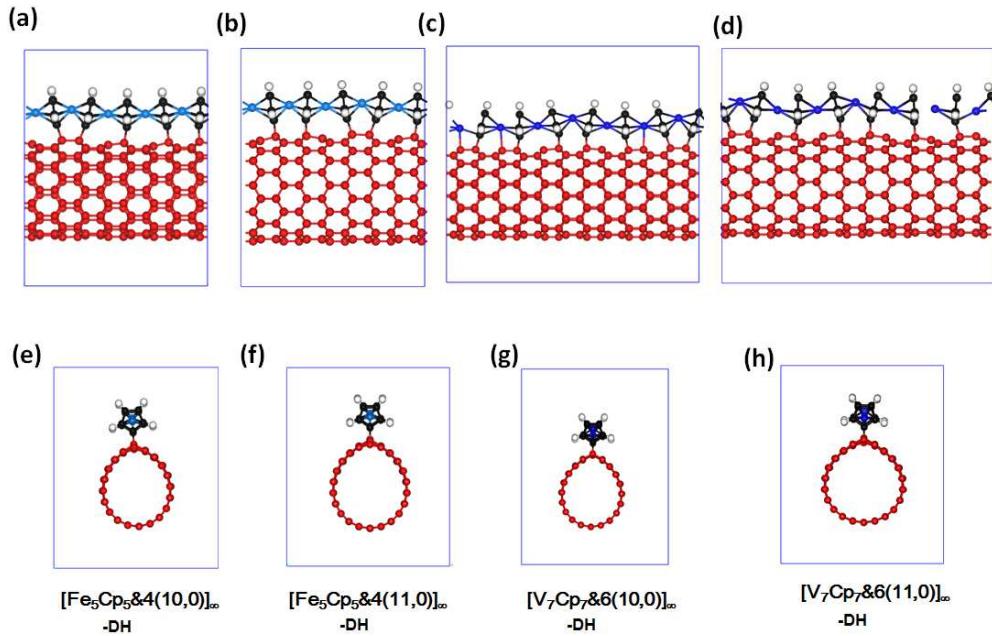


Figure S11. Top and side view of the optimized structures of (a, e)  $[\text{Fe}_5\text{Cp}_5\&4(10,0)]_\infty$ , (b, f)  $[\text{Fe}_5\text{Cp}_5\&4(11,0)]_\infty$ , (c, g)  $[\text{V}_7\text{Cp}_7\&6(10,0)]_\infty$  and (d, h)  $\text{V}_7\text{Cp}_7\&6(11,0)]_\infty$ .

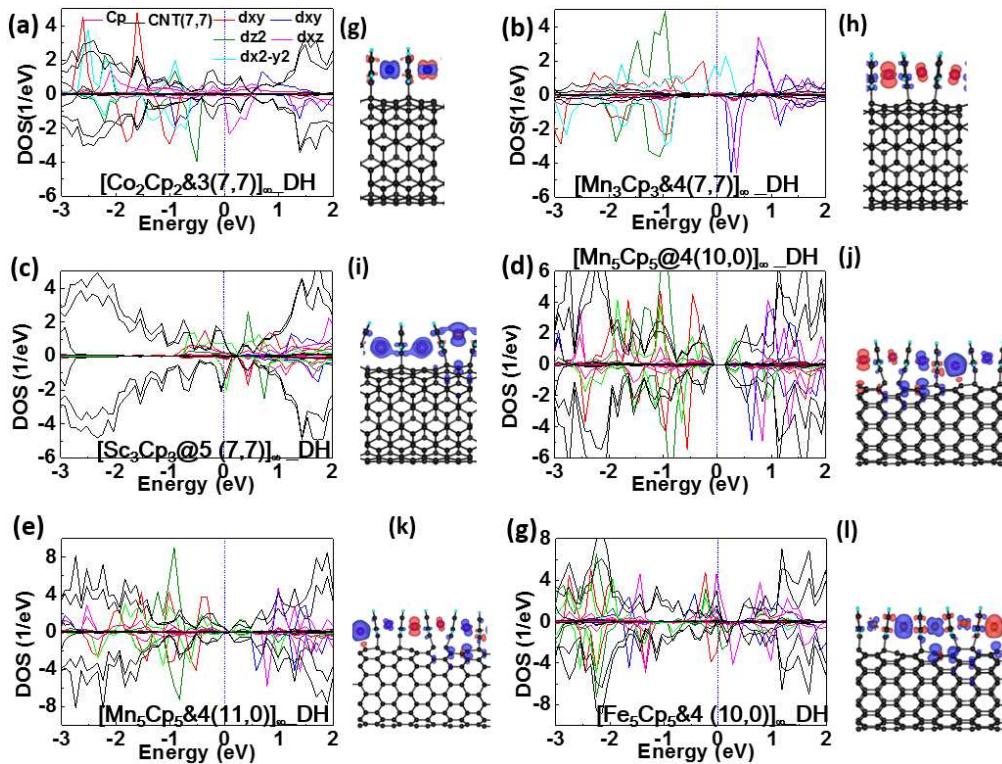


Figure S12. (a-f) Plots of density of states and (g-k) spin densities of 1D ISMW&N( $n, m$ )\_DHs.

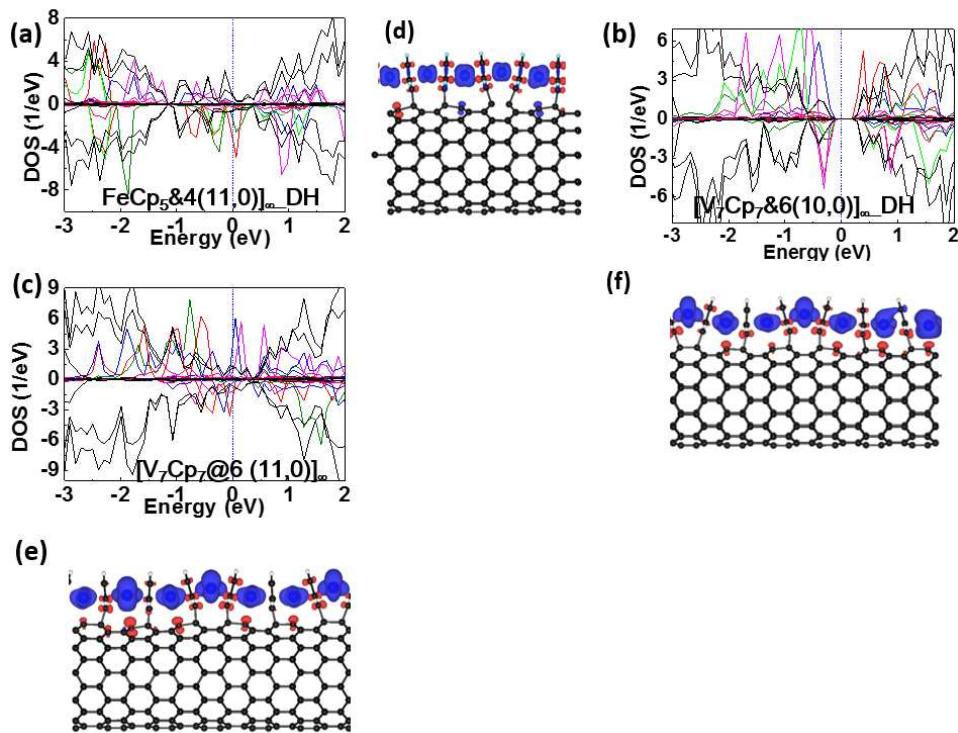


Figure S13. (a-c) Plots of density of states and (d-f) spin densities of 1D ISMW&N( $n, m$ )\_DHs.

Table S2. The Systems, C-C bond lengths  $L_{C-C(1)}(\text{\AA})$  and diameters (D) of SWCNTs, C-C ( $L_{C-C(2)}$ ) (C)/C-H ( $L_{C-H}$ ) bond lengths, the TM-Cp ( $D_{TM-Cp}$ ) distance of 1D ISMWs, the distance of TM chain to the tube wall of SWCNTs ( $D_{W-T}$ ) of 1D ISMW&SWCNTs\_DH.

System	$L_{C-C(1)}(\text{\AA})$	D (Å)	$L_{C-C(2)}(\text{\AA})$	$L_{C-H}(\text{\AA})$	$D_{TM-Cp}(\text{\AA})$	$D_{W-T}(\text{\AA})$
[Co <sub>2</sub> Cp <sub>2</sub> &3(7,7)] <sub>∞</sub> _DH	1.434-1.461	9.21-9.84	1.400-1.536	1.085,1.086	1.852,1.853	2.95
[Sc <sub>3</sub> Cp <sub>3</sub> &5(7,7)] <sub>∞</sub> _DH	1.418-1.514	9.00-10.63	1.427-1.466	1.086-1.089	2.067-2.311	2.52
[Mn <sub>3</sub> Cp <sub>3</sub> &4(7,7)] <sub>∞</sub> _DH	1.376-1.542	9.16-9.97	1.464-1.477	1.085-1.088	1.595-1.690	3.02
[Mn <sub>5</sub> Cp <sub>5</sub> &4(10,0)] <sub>∞</sub> _DH	1.419-1.606	7.22-9.542	1.441-1.480	1.087,1.088	1.597-2.149	3.59
[Mn <sub>5</sub> Cp <sub>5</sub> &4(11,0)] <sub>∞</sub> _DH	1.410-1.607	8.03-9.51	1.450-1.482	1.087-1.088	1.593-1.698	3.23
[Fe <sub>5</sub> Cp <sub>5</sub> &4(10,0)] <sub>∞</sub> _DH	1.398-1.600	7.29-8.54	1.447-1.467	1.086-1.088	1.577-1.860	3.22
[Fe <sub>5</sub> Cp <sub>5</sub> &4(11,0)] <sub>∞</sub> _DH	1.406-1.595	8.06-9.38	1.455-1.470	1.086,1.087	1.573-2.174	2.84
[V <sub>7</sub> Cp <sub>7</sub> &6(10,0)] <sub>∞</sub> _DH	1.390-1.588	7.14-9.76	1.440-1.493	1.086-1.088	1.758-2.207	2.03
[V <sub>7</sub> Cp <sub>7</sub> &6(11,0)] <sub>∞</sub> _DH	1.390-1.590	8.21-9.24	1.442-1.4	1.085-1.086	1.784-2.229	2.80

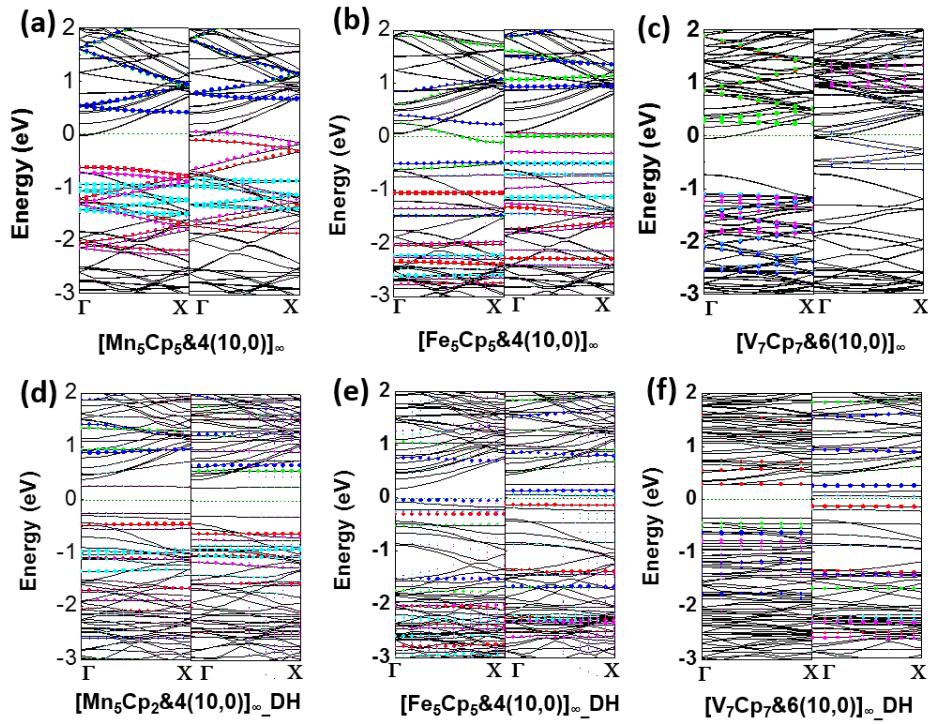


Figure S14. Band structures of (a-c) 1D  $[\text{Mn}_5\text{Cp}_5 \& 4(10,0)]_\infty$ ,  $[\text{Fe}_5\text{Cp}_5 \& 4(10,0)]_\infty$  and  $[\text{V}_7\text{Cp}_7 \& 6(10,0)]_\infty$ ; (d-f) 1D  $[\text{Mn}_5\text{Cp}_5 \& 4(10,0)]_\infty\text{-DH}$ ,  $[\text{Fe}_5\text{Cp}_5 \& 4(10,0)]_\infty\text{-DH}$  and  $[\text{V}_7\text{Cp}_7 \& 6(10,0)]_\infty\text{-DH}$ , respectively