Electronic Supplementary Material (ESI) for Nanoscale

Supporting Information:

Boratabenzene-Vanadium Sandwich Molecular Wire and its properties

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System	PGS	Conformer (Degree of rotation of neighboring B atoms)	E_B / eV	TMM / μ_B
$V(HBBz)_2$	C_{2h}	180^o	7.75	2.8
$Cr(HBBz)_2$	C_{2h}	90^o	6.31	0.0
$Mn(HBBz)_2$	C_{2h}	90^o	6.15	0.0
$Fe(HBBz)_2$	C_{2h}	180^o	7.52	0.0

Table S1. Point Group Symmetry (PGS), Conformer, Binding Energies per V atom (E_B), and Total Magnetic Moment (TMM) for $M(HBBz)_2$ (M = Fe, Mn, Cr).

						Individual Magnetic Moment										
system	relative position of B atoms	ES	TMM / μ_B	S-A	ΔE / meV	HBBz1	V1	HBBz2	V2	HBBz3	V3	HBBz4	V4	HBBz5	V5	HBBz6
1,1	-	PM	3.80	↑	-	0.09	3.71									
1,2	180	PM	2.77	↑	-	0.03	2.71	0.03								
2,3	180	FM	3.59	0↑0↑↓	20.1	-0.01	1.93	-0.01	1.93	-0.25						
		AFM	-0.04	0↑0↓0	0.0	0.00	1.95	-0.04	-1.95	0.00						
3,4	180	FM	5.15	0↑↓↑↓↑0	39.0	-0.01	2.01	-0.18	1.51	-0.18	2.01	-0.01				
		FiM 1	2.33	0↑0↓0↑0	72.1	-0.04	1.91	-0.01	-1.39	-0.01	1.91	-0.04				
		FiM 2	1.22	0↑↓↑0↓0	0.0	0.00	2.06	-0.27	1.41	0.09	-2.09	0.02				
4,5	180	FM	6.56	0↑↓↑↓↑↓↑0	28.9	-0.01	2.03	-0.22	1.53	-0.10	1.53	-0.22	2.03	-0.01		
		FiM 1	3.63	0↑0↓0↑↓↑0	37.7	-0.04	1.91	0.01	-1.54	0.09	1.39	-0.25	2.06	0.00		
		FiM 2	2.71	0↑↓↑↓↑0↓0	24.2	-0.01	2.02	-0.21	1.61	-0.20	1.43	0.06	-2.02	0.03		
		AFM 1	0.00	0↑0↓0↑0↓0	96.7	-0.03	1.93	-0.03	-1.34	0.00	1.34	0.03	-1.93	0.03		
		AFM 2	-1.12	0↓0↑↓↑0↓0	10.1	0.03	-2.01	0.05	1.51	-0.28	1.51	0.05	-2.01	0.03		
		AFM 3	0.00	0↑↓↑0↓↑↓0	0.0	0.00	2.04	-0.26	1.57	0.00	-1.57	0.26	-2.04	0.00		
5,6	180	FM	7.99	0↑↓↑↓↑↓↑↓↑0	27.8	-0.01	2.02	-0.22	1.56	-0.13	1.54	-0.13	1.56	-0.22	2.02	0.00
		FiM 1	5.35	0↑0↓0↑↓↑↓↑0	64.7	-0.04	1.96	-0.03	-1.35	0.05	1.49	-0.17	1.59	-0.22	2.07	0.00
		FiM 2	4.16	0↑↓↑↓↑↓↑0↓0	23.4	0.00	2.02	-0.22	1.56	-0.13	1.63	-0.22	1.44	0.06	-2.01	0.03
		FiM 3	2.23	0↑0↓0↑0↓0↑0	12.8	-0.03	1.92	-0.03	-1.39	0.02	1.25	0.02	-1.39	-0.03	1.92	-0.03
		FiM 4	1.46	0↑↓↑↓↑0↓↑↓0	14.2	0.00	2.02	-0.21	1.60	-0.18	1.60	-0.03	-1.56	0.26	-2.04	0.00
		FiM 5	4.95	0↑↓↑0↓0↑↓↑0	12.2	0.00	2.06	-0.26	1.42	0.08	-1.65	0.08	1.42	-0.26	2.06	0.00
		FiM 6	2.39	0↑↓↑0↓↑↓0↑0	0.0	0.00	2.04	-0.27	1.51	0.04	-1.66	0.27	-1.47	-0.06	2.02	-0.03
		FiM 7	0.25	0↓0↑↓↑↓↑0↓0	17.8	0.03	-2.02	0.07	1.42	-0.22	1.69	-0.22	1.42	0.07	-2.02	0.03
		FiM 8	1.29	0↑0↓0↑↓↑0↓0	59.4	-0.04	1.89	0.01	-1.46	0.05	1.48	-0.26	1.50	0.05	-1.96	0.03
		FiM 9	1.34	0↑↓↑0↓0↑0↓0	76.4	0.00	2.04	-0.25	1.44	0.07	-1.47	0.00	1.37	0.02	-1.91	0.03

Table S2. Configuration of conformer(R), Electronic State (ES), Total Magnetic Moment (TMM), Spin Arrangement of the vanadium atoms(black arrows) and HBBz rings(red arrows, zero value denotes diamagnetism)(S-A), Energy Difference (ΔE) between each spin state and the ground state (assigned with a value of zero) and individual MMs of all assigned states for the $V_2(HBBz)_3$, $V_3(HBBz)_4$, $V_4(HBBz)_5$, and $V_5(HBBz)_6$ clusters. HBBz1-6 and V1-5 specify the BBBz rings and V atoms respectively from one end to the other end of the cluster.

					Individual MM (μ_B)			
System	ES	TMM (μ_B)	S-A	ΔE / eV	BBz1	V1	BBz2	V2
Eclipsed	FM	3.52	↑↑	0	0.01	1.75	0.01	1.75
	AFM	0	↑↓	0.057	0	1.42	0	-1.42
60°	FM	3.62	↑↑	0	0.01	1.80	0.01	1.80
	AFM	0	↑↓	0.06	0	1.43	0	-1.43
120°	FM	3.59	↑↑	0	0.01	1.79	0.01	1.78
	AFM	0	↑↓	0.057	0	1.40	0	-1.40
180° (Transoid)	FM	3.48	↑↑	0	0.01	1.73	0.01	1.73
	AFM	0	↑↓	0.054	0	1.40	0	-1.40

Table S3. Electronic State (ES), Total Magnetic Moment (TMM), Spin Arrangement of different vanadium atoms(S-A), Energy Difference (ΔE) between FM and AFM states (assigned with a value of zero) and individual MMs of FM and AFM state for the vanadium boratabenzene sandwich molecular wires in different conformations.

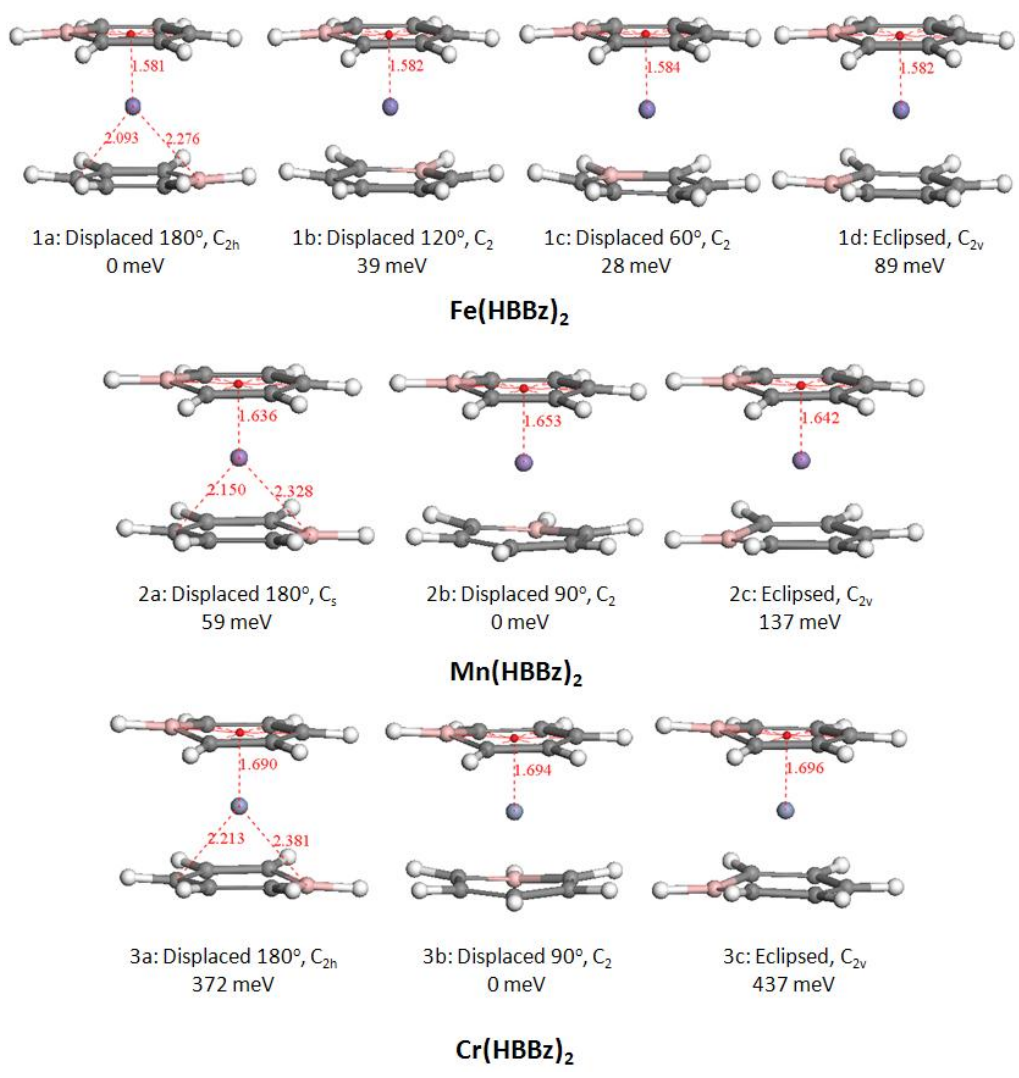

Figure S1 Optimized structures showing different conformations of $M(HBBz)_2$ (M = Fe, Mn, Cr). The labels show the symmetry and the relative energies of the clusters with respect to their ground state structures (0 eV). Purple spheres denote the transition metal atoms

(Fe, Mn, Cr), dark grey spheres denote carbon atoms, pink spheres denote boron atoms, and white spheres denote hydrogen atoms.

Selected bond distances are indicated in the figures.

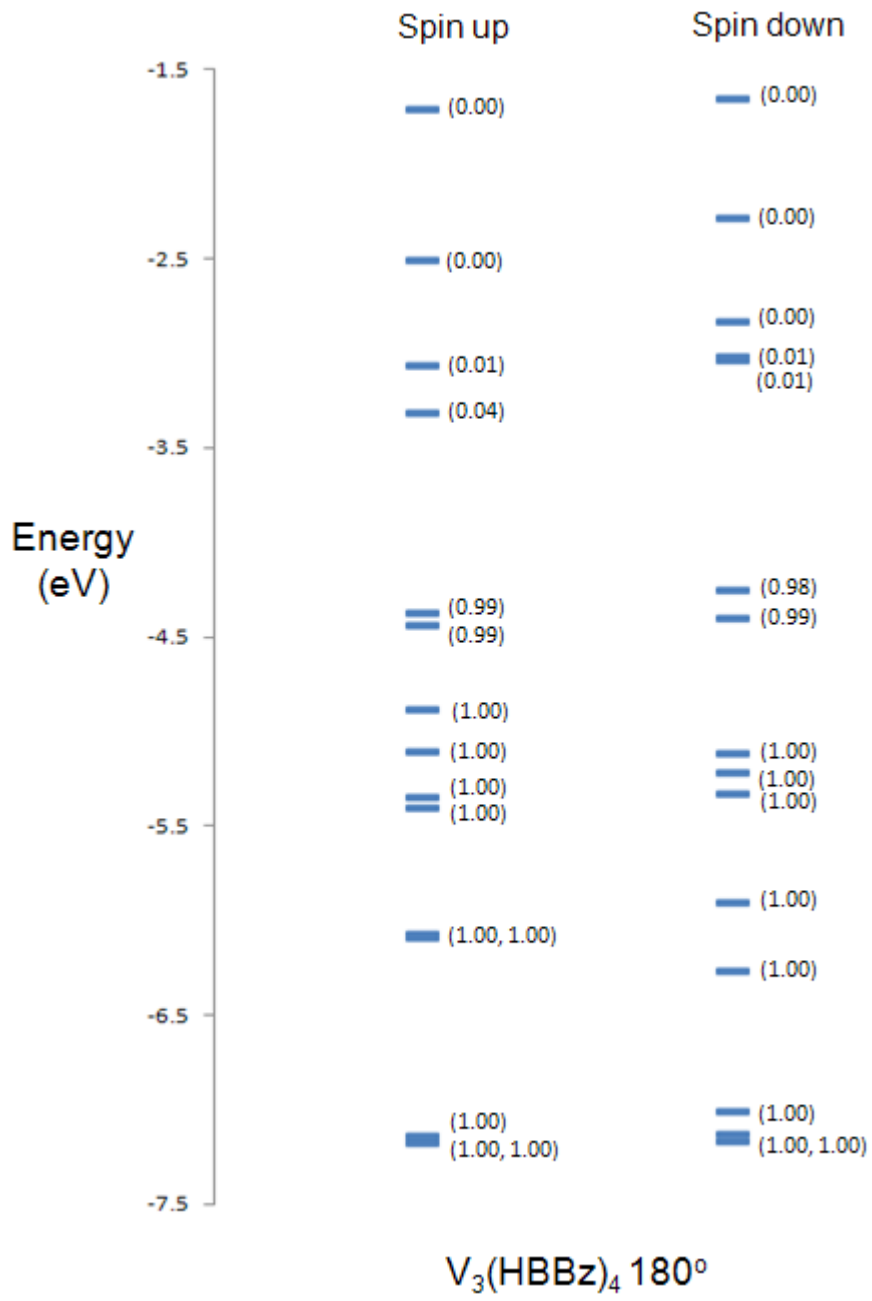

Figure S2 Molecular orbital diagram of the 180^{o} conformer of $V_3(HBBz)_4$. The numbers in parentheses are the population of the electrons in each molecular orbital.

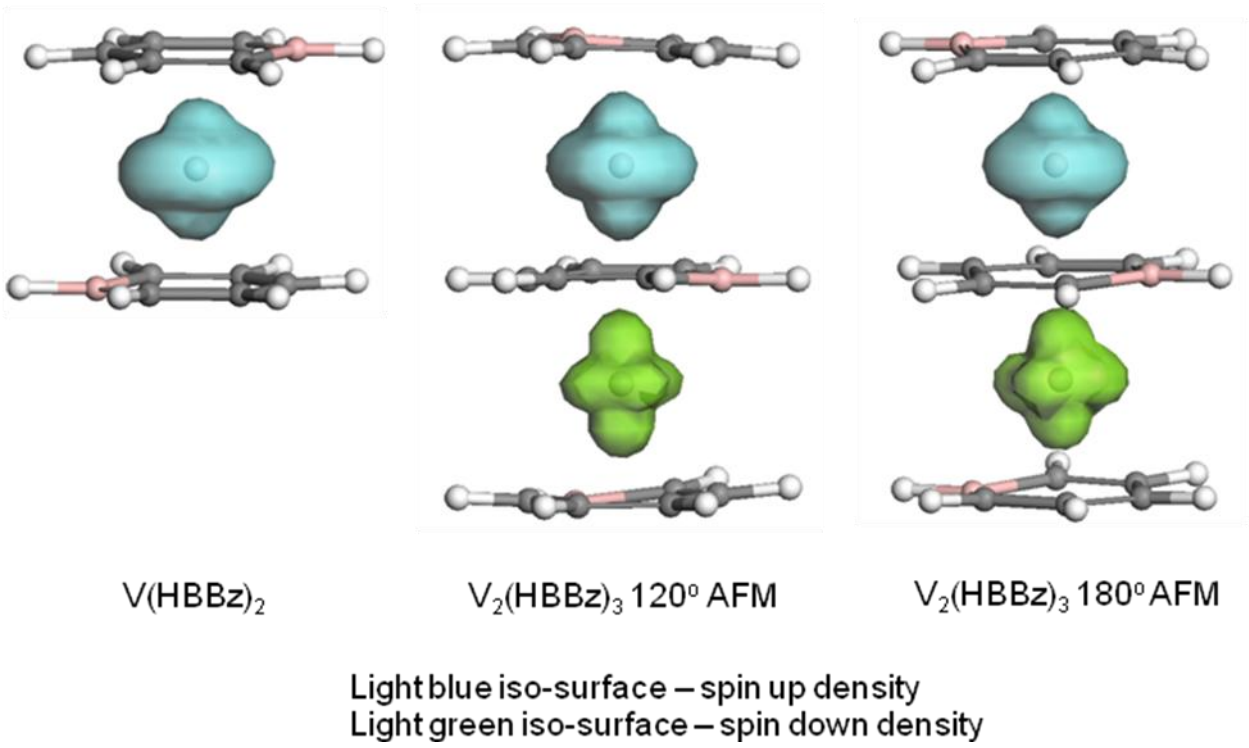

Figure S3. Spin density diagrams of the $V(HBBz)_2$, 120^{o} and 180^{o} conformers of $V_2(HBBz)_3$. Green spheres denote vanadium atoms, dark grey spheres denote carbon atoms, pink spheres denote boron atoms, and white spheres denote hydrogen atoms.