Supplementary Information of

Revealing Intrinsic Spin Coupling in Transition Metal-Doped Graphene

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Supplementary Figures

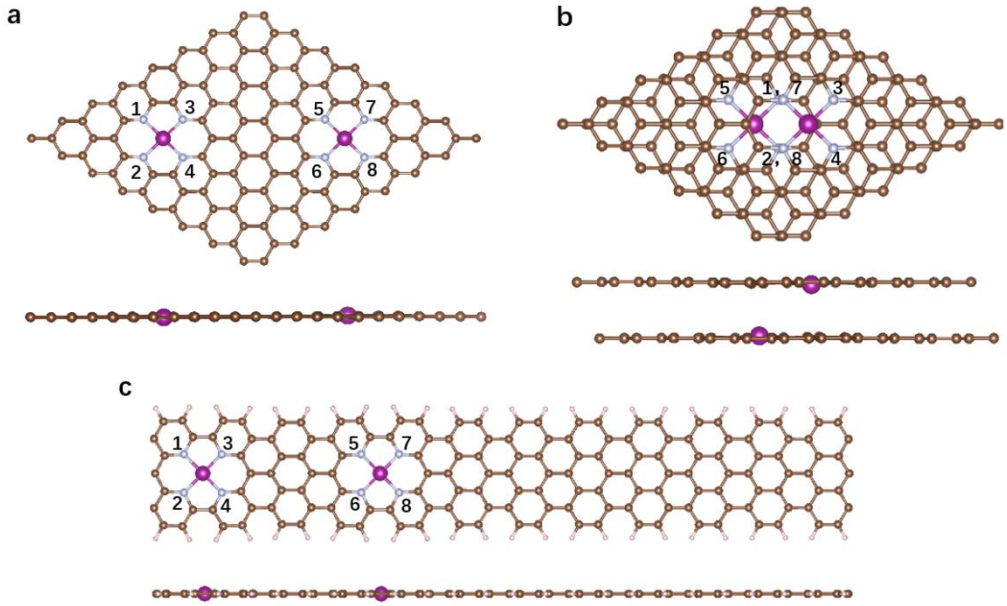

Figure S1. Top and side representations of (a) TMN_4-TMN_4 (b) double-layer TMN_4-TMN_4 and (c) TMN_4-TMN_4 in GNR. The numbers 1-8 distinguish the different N atoms. For the overlap of top view in Figure (b), 1 and 2 represent the upper N atoms, and 7 and 8 represent the lower N atoms.

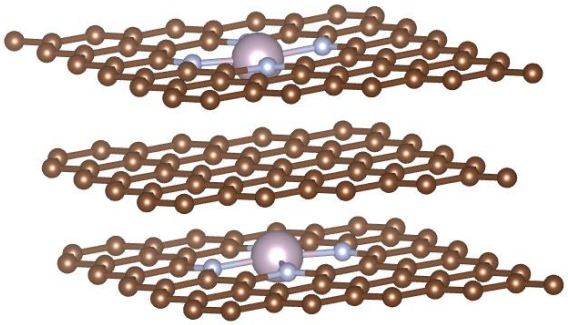

Figure S2. The side representation of triple-layer TMN_4-TMN_4.

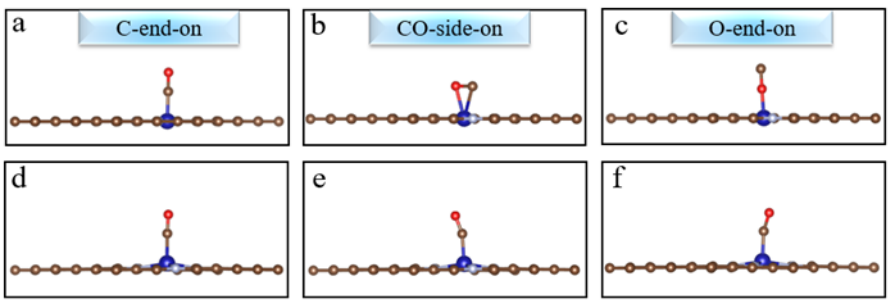

Figure S3. Geometry optimization for the CO adsorption on Co-doped graphene with different initial configurations. (a-c) are different initial orientations of the CO adsorption on CoN_4 via (a) C-end-on, (b) CO-side-on, and (c) O-end-on patterns. (d-f) are the final optimized structures correspondingly.

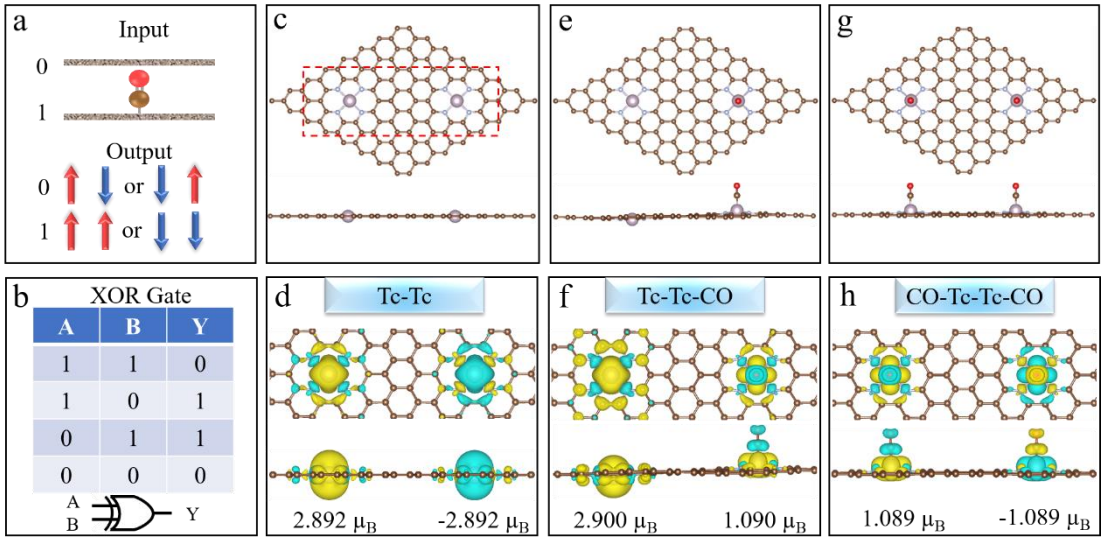

Figure S4. (a) The design of input and output. (b) Truth table and schematic representation of XOR gate. Input A and B are defined as the absence (logic 0) or presence (logic 1) of CO on the two Tc sites. (c), (e), and (g) are top and side views of optimized structures for Tc-Tc, Tc-Tc-CO, and CO-Tc-Tc-CO, respectively. (d), (f) and (h) are the net spin electron densities for Tc-Tc, Tc-Tc-CO, and CO-Tc-Tc-CO at an isosurface value of 0.001 eÅ^{-3}, respectively. The yellow and blue represent positive and negative signs of the spin densities, respectively. Tc-Tc, Tc-Tc-CO, and CO-Tc-Tc-CO represent TcN_4-TcN_4, TcN_4-TcN_4 with the presence of CO on the Tc site, and TcN_4-TcN_4 with the presence of COs on two Tc sites, respectively.

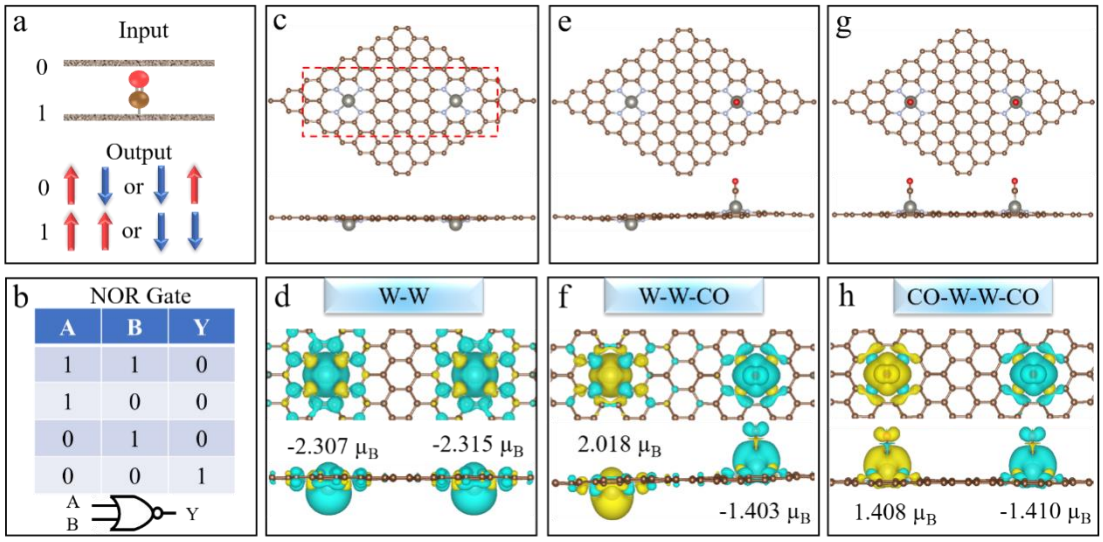

Figure S5. (a) The design of input and output. (b) Truth table and schematic representation of NOR gate. Input A and B are defined as the absence (logic 0) or presence (logic 1) of CO on the two W sites. (c), (e), and (g) are top and side views of optimized structures for W-W, W-W-CO, and CO-W-W-CO, respectively. (d), (f) and (h) are the net spin electron densities for W-W, W-W-CO, and CO-W-W-CO at an isosurface value of 0.001 eÅ^{-3}, respectively. The yellow and blue represent positive and negative signs of the spin densities, respectively. W-W, W-W-CO, and CO-W-W-CO represent WN_4-WN_4, WN_4-WN_4 with the presence of CO on the W site, and WN_4-WN_4 with the presence of COs on two W sites, respectively.

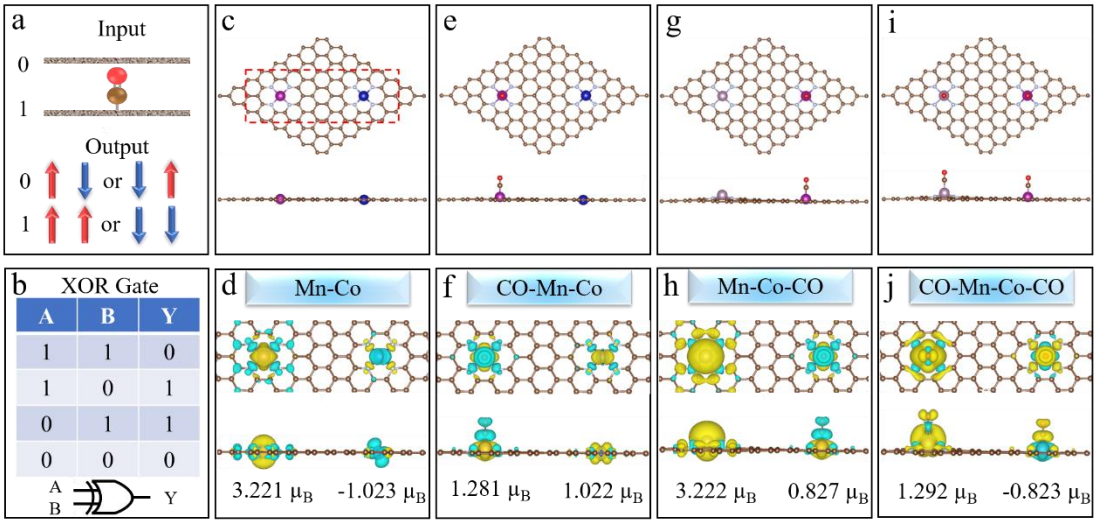

Figure S6. (a) The design of input and output. (b) Truth table and schematic representation of XOR gate. Input A and B are defined as the absence (logic 0) or presence (logic 1) of CO on the Mn and Co sites, respectively. (c), (e), (g), and (i) are top and side views for optimized structures of Mn-Co, CO-Mn-Co, Mn-Co-CO, and CO-Mn-Co-CO, respectively. (d), (f), (h) and (j) are the net spin electron densities for Mn-Co, CO-Mn-Co, Mn-Co-CO, and CO-Mn-Co-CO at an isosurface value of 0.001 eÅ^{-3}, respectively. The yellow and blue represent positive and negative signs of the spin densities, respectively. Mn-Co, CO-Mn-Co, Mn-Co-CO, and CO-Mn-Co-CO represent MnN_4-CoN_4, MnN_4-CoN_4 with the presence of CO on the Mn site, MnN_4-CoN_4 with the presence of CO on the Co site, and MnN_4-CoN_4 with the presence of COs on both Mn and Co sites, respectively.

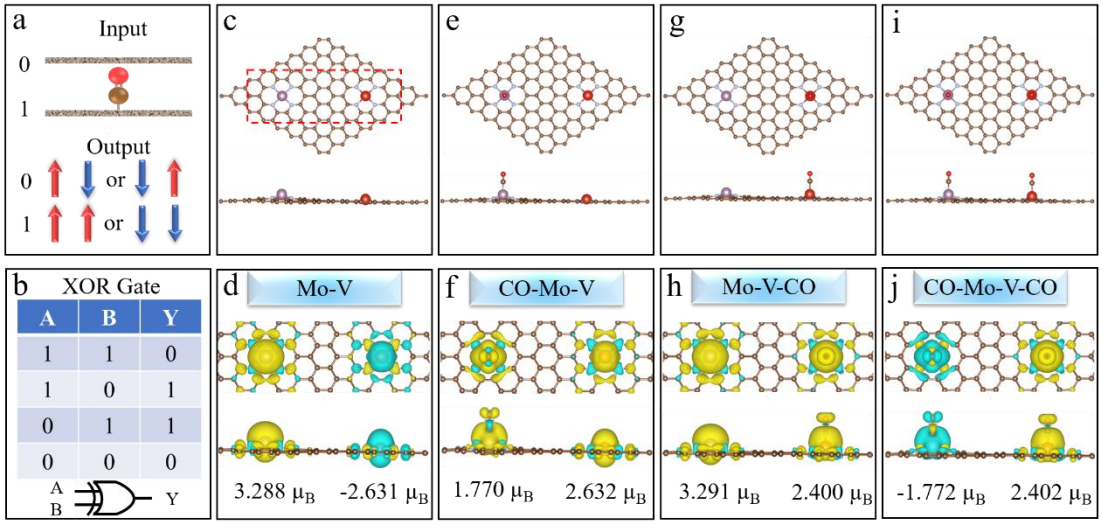

Figure S7. (a) The design of input and output. (b) Truth table and schematic representation of XOR gate. Input A and B are defined as the absence (logic 0) or presence (logic 1) of CO on the Mo and V sites, respectively. (c), (e), (g), and (i) are top and side views for optimized structures of Mo-V, CO-Mo-V, Mo-V-CO, and CO-Mo-V-CO, respectively. (d), (f), (h) and (j) are the net spin electron densities for Mo-V, CO-Mo-V, Mo-V-CO, and CO-Mo-V-CO at an isosurface value of 0.001 eÅ^{-3}, respectively. The yellow and blue represent positive and negative signs of the spin densities, respectively. Mo-V, CO-Mo-V, Mo-V-CO, and CO-Mo-V-CO represent MoN_4-VN_4, MoN_4-VN_4 with the presence of CO on the Mo site, MoN_4-VN_4 with the presence of CO on the V site, and MoN_4-VN_4 with the presence of COs on both Mo and V sites, respectively.

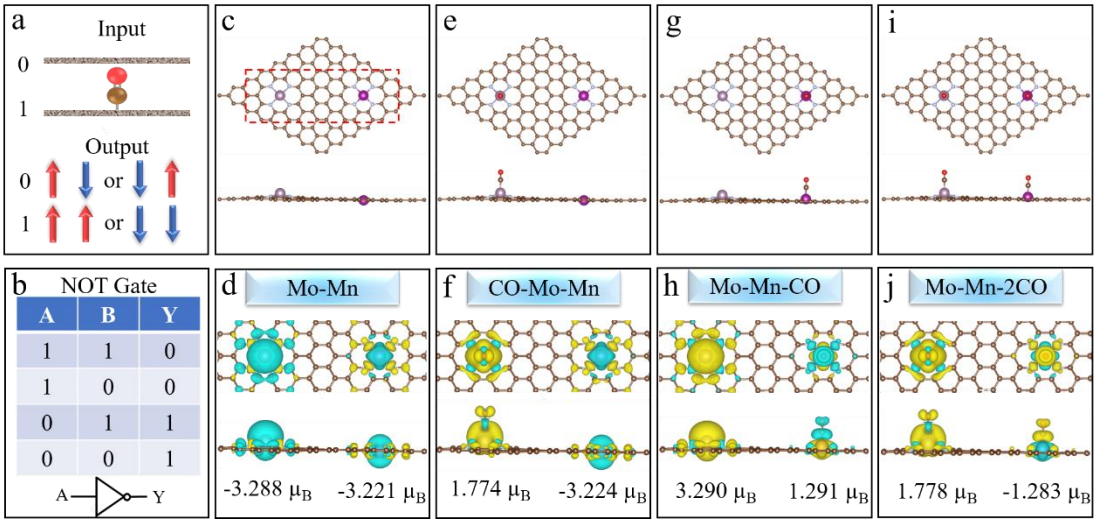

Figure S8. (a) The design of input and output. (b) Truth table and schematic representation of NOT gate. Input A and B are defined as the absence (logic 0) or presence (logic 1) of CO on the Mo and Mn sites, respectively. (c), (e), (g), and (i) are top and side views for optimized structures of Mo-Mn, CO-Mo-Mn, Mo-Mn-CO, and CO-Mo-Mn-CO, respectively. (d), (f), (h) and (j) are the net spin electron densities for Mo-Mn, CO-Mo-Mn, Mo-Mn-CO, and CO-Mo-Mn-CO at an isosurface value of 0.001 eÅ^{-3}, respectively. The yellow and blue represent positive and negative signs of the spin densities, respectively. Mo-Mn, CO-Mo-Mn, Mo-Mn-CO, and CO-Mo-Mn-CO represent MoN_4-MnN_4, MoN_4-MnN_4 with the presence of CO on the Mo site, MoN_4-MnN_4 with the presence of CO on the Mn site, and MoN_4-MnN_4 with the presence of COs on both Mo and Mn sites, respectively.

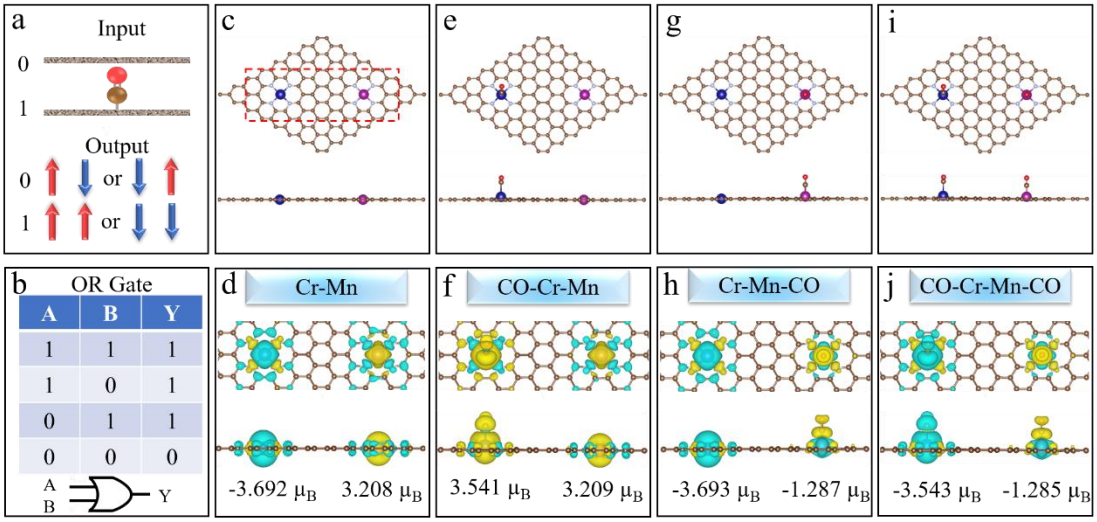

Figure S9. (a) The design of input and output. (b) Truth table and schematic representation of OR gate. Input A and B are defined as the absence (logic 0) or presence (logic 1) of CO on the Cr and Mn sites, respectively. (c), (e), (g), and (i) are top and side views for optimized structures of Cr-Mn, CO-Cr-Mn, Cr-Mn-CO, and CO-Cr-Mn-CO, respectively. (d), (f), (h) and (j) are the net spin electron densities for Cr-Mn, CO-Cr-Mn, Cr-Mn-CO, and CO-Cr-Mn-CO at an isosurface value of 0.001 eÅ^{-3}, respectively. The yellow and blue represent positive and negative signs of the spin densities, respectively. Cr-Mn, CO-Cr-Mn, Cr-Mn-CO, and CO-Cr-Mn-CO represent CrN_4-MnN_4, CrN_4-MnN_4 with the presence of CO on the Cr site, CrN_4-MnN_4 with the presence of CO on the Mn site, and CrN_4-MnN_4 with the presence of COs on both Cr and Mn sites, respectively.

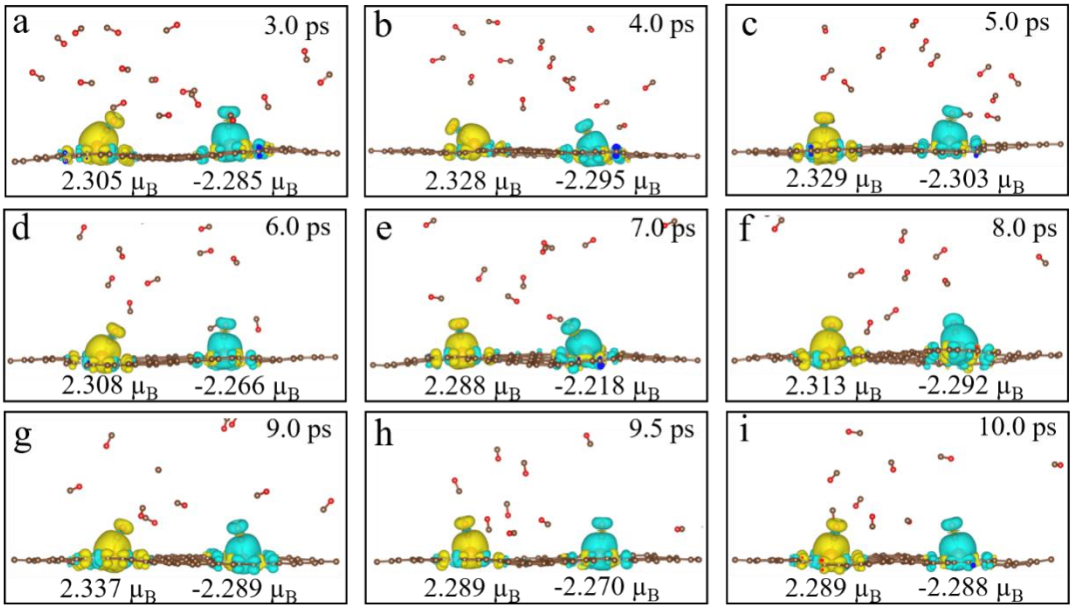

Figure S10. AIMD simulation of CO-V-V-CO in the CO environment at 300K. The spin electron densities at different times plotted at an isosurface value of 0.001 eÅ^{-3} are shown in (a-i). (a) t = 3.0 ps, (b) t = 4.0 ps, (c) t = 5.0 ps, (d) t = 6.0 ps, (e) t = 7.0 ps, (f) t = 8.0 ps, (g) t = 9.0 ps, (h) t = 9.5 ps, (i) t = 10.0 ps.

The studies of the spin-coupling effect and its distance dependence or space propagation in the main text are performed under vacuum condition. In general, the environment around the system under study can affect the properties of the material. In order to roughly understand the influence of the environment on the spin coupling of the materials, here take CO-V-V-CO as an example and carry out the AIMD simulation at room temperature (300K) under an environment full of COs. The results are shown in Figure S10, which show that the spin magnetic moment at a metal site does not change much, and most of the net spin density is distributed on V metals. The directions of the spin magnetic moments on both V sites do not change during simulation, which remain antiparallel. In addition, we also find that the addition of COs in environment can increase the energy difference between different spin states, which thus increases the discrimination of different spin states as compared to vacuum. Therefore, combining AIMD simulations can facilitate the search for the ground-state electronic structure.

Supplementary Tables

Table S1: Logic gates of the homobimetallic systems (TM_1N_4-TM_1N_4) and the corresponding truth tables.

system		Co-Co	V-V	Tc-Tc	W-W
1	1	1	0	0	0
1	0	1	1	1	0
0	1	1	1	1	0
0	0	0	0	0	1
logic gate		OR	XOR	XOR	NOR

Table S2: Logic gates of the heterobimetallic systems (TM_1N_4-TM_2N_4) and the corresponding truth tables.

system		Mo-Mn	Mo-Co	Mo-V	V-Co	Cr-Mn
1	1	0	0	0	0	1
1	0	0	1	1	1	1
0	1	1	1	1	0	1
0	0	1	0	0	0	0
logic gate		OR	NOT	XOR	XOR	INHIBIT

Table S3. The directions and magnitudes of the total spin magnetic moments and the spin magnetic moments on the two metals sites (TM_1 and TM_2, which can be either the same or different) in the absence and presence of CO. TM_1-TM_2, CO-TM_1-TM_2, TM_1-TM_2-CO, and CO-TM_1-TM_2-CO represent TM_1N_4-TM_2N_4, TM_1N_4-TM_2N_4 with the presence of CO on the TM_1 site, TM_1N_4-TM_2N_4 with the presence of CO on the TM_2 site, and TM_1N_4-TM_2N_4 with the presence of COs on both TM_1 and TM_2 sites, respectively. For homobimetallic systems, TM_1 and TM_2 are the same, so CO-TM_1-TM_2 and TM_1-TM_2-CO are equivalent. Here use TM-TM-CO to represent TMN_4-TMN_4 with the presence of CO on one TM site.

	Direction	**Spin magnetic moment (μ_B)**		
		total	**TM_1**	**TM_2**
Co-Co	antiparallel	0	-1.023	1.023
Co-Co-CO	parallel	1.7590	1.031	0.835
CO-Co-Co-CO	parallel	1.5682	0.838	0.834
Mn-Mn	antiparallel	0	3.215	-3.215
Mn-Mn-CO	antiparallel	-1.9956	-3.223	1.289
CO-Mn-Mn-CO	antiparallel	0.0001	1.282	-1.282
V-V	antiparallel	0	-2.633	2.634
V-V-CO	parallel	6.0187	2.637	2.403
CO-V-V-CO	antiparallel	0.0007	2.400	-2.400
Tc-Tc	antiparallel	0	2.892	-2.892
Tc-Tc-CO	parallel	4.0060	2.900	1.090
CO-Tc-Tc-CO	antiparallel	0	1.089	-1.089
Fe-Fe	antiparallel	0	2.020	-2.020

Fe-Fe-CO	no	2.0015	2.021	0
CO-Fe-Fe-CO	no	0	0	0
Ru-Ru	antiparallel	-0.0012	1.795	-1.795
Ru-Ru-CO	no	2.0056	1.800	0.002
CO-Ru-Ru-CO	no	0	0	0
Mo-Mo	antiparallel	-0.0038	3.280	-3.281
Mo-Mo-CO	antiparallel	-1.9574	-3.283	1.761
CO-Mo-Mo-CO	antiparallel	0	1.779	-1.779
Cr-Cr	antiparallel	-0.0003	-3.691	3.691
Cr-Cr-CO	antiparallel	-0.1174	-3.692	3.536
CO-Cr-Cr-CO	antiparallel	-0.0210	3.537	-3.542
W-W	parallel	-6.7907	-2.307	-2.315
W-W-CO	antiparallel	0.2545	2.018	-1.403
CO-W-W-CO	antiparallel	-0.0001	1.408	-1.410
Mn-Co	antiparallel	1.9980	3.211	-1.023
CO-Mn-Co	parallel	2	1.281	1.022
Mn-Co-CO	parallel	3.8130	3.222	0.827
CO-Mn-Co-CO	antiparallel	0.5000	1.292	-0.823
Mo-Mn	parallel	-6.9576	-3.288	-3.221
CO-Mo-Mn	antiparallel	-0.9989	1.774	-3.224
Mo-Mn-CO	parallel	4.9872	3.290	1.291
CO-Mo-Mn-CO	antiparallel	0.9988	1.778	-1.283
Mo-Co	antiparallel	2.9454	3.291	-1.021
CO-Mo-Co	parallel	-3.0036	-1.768	-1.024
Mo-Co-CO	antiparallel	3.2320	3.288	-0.824
CO-Mo-Co-CO	parallel	2.8080	1.774	0.832
Mo-V	antiparallel	1	3.288	-2.631
CO-Mo-V	parallel	4.9995	1.770	2.632
Mo-V-CO	parallel	6.9913	3.291	2.400
CO-Mo-V-CO	antiparallel	1.0036	-1.772	2.402
V-Co	antiparallel	1.9885	2.636	-1.022
CO-V-Co	parallel	-4.0210	-2.403	-1.023
V-Co-CO	antiparallel	2.2238	2.633	-0.830
CO-V-Co-CO	antiparallel	2.2968	2.406	-0.829
Tc-Co	parallel	4	2.896	1.022
CO-Tc-Co	parallel	-2.0052	-1.089	-1.022
Tc-Co-CO	parallel	-3.7497	-2.901	-0.827
CO-Tc-Co-CO	parallel	2	1.089	0.838
Cr-Co	antiparallel	-3.0188	-3.693	1.021
CO-Cr-Co	antiparallel	2.9396	3.546	-1.022
Cr-Co-CO	antiparallel	3.2861	3.692	-0.828

CO-Cr-Co-CO	antiparallel	3.2354	3.547	-0.829
Tc-V	parallel	6	2.894	2.587
CO-Tc-V	parallel	3.9908	1.091	2.636
Tc-V-CO	parallel	6	2.633	2.402
CO-Tc-V-CO	parallel	4	1.090	2.400
Cr-Mn	antiparallel	-1.0173	-3.692	3.208
CO-Cr-Mn	parallel	7	3.541	3.209
Cr-Mn-CO	parallel	-5.0368	-3.693	-1.287
CO-Cr-Mn-CO	parallel	-4.9768	-3.543	-1.285

Table S4. The directions and magnitudes of the total spin magnetic moments and the spin magnetic moments of the Cr and Mn sites with different distances in the Cr-Mn system. For different intermetallic distances, the Cr site is unchanged, while the Mn site is located at 1, 2, 3 and 4, respectively (Sites 1-4 are shown in Figure 3 of the main text). Cr-Mn, CO-Cr-Mn, Cr-Mn-CO, and CO-Cr-Mn-CO represent CrN_4-MnN_4, CrN_4-MnN_4 with the presence of CO on the Cr site, CrN_4-MnN_4 with the presence of CO on the Mn site, and CrN_4-MnN_4 with the presence of COs on both Cr and Mn sites, respectively.

		Direction	**Spin magnetic moment (μ_B)**		
			total	**Cr**	**Mn**
1	Cr-Mn	antiparallel	-1	-3.691	3.227
	CO-Cr-Mn	antiparallel	-1	-3.691	3.140
	Cr-Mn-CO	antiparallel	-3	-3.692	1.347
	CO-Cr-Mn-CO	parallel	5	3.563	1.347
2	Cr-Mn	antiparallel	-1	-3.692	3.223
	CO-Cr-Mn	antiparallel	-1	-3.692	3.138
	Cr-Mn-CO	antiparallel	-3	-3.693	1.350
	CO-Cr-Mn-CO	parallel	5	3.563	1.348
3	Cr-Mn	antiparallel	-1	-3.693	3.222
	CO-Cr-Mn	antiparallel	-1	-3.693	3.137
	Cr-Mn-CO	antiparallel	-3	-3.692	1.348
	CO-Cr-Mn-CO	parallel	5	3.559	1.347
4	Cr-Mn	antiparallel	-1	-3.691	3.223
	CO-Cr-Mn	antiparallel	-1	-3.691	3.135
	Cr-Mn-CO	antiparallel	-3	-3.693	1.343
	CO-Cr-Mn-CO	parallel	5	3.559	1.349

Table S5. The spin direction, the total spin moment and the spin moments of the two metals (TM_1 and TM_2, which can be either the same or different) located at different layers (2 and 3 refer to two and three layers, respectively). For Heterobimetallic systems, TM_1-TM_2, CO-TM_1-TM_2, TM_1-TM_2-CO, and CO-TM_1-TM_2-CO represent TM_1N_4-TM_2N_4, TM_1N_4-TM_2N_4 with the presence of CO on the TM_1 site, TM_1N_4-TM_2N_4 with the presence of CO on the TM_2 site, and TM_1N_4-TM_2N_4 with the

presence of COs on both TM_1 and TM_2 sites, respectively. For homobimetallic systems, TM_1 and TM_2 are the same, so CO-TM_1-TM_2 and TM_1-TM_2-CO are equivalent. Here, only use TM-TM-CO to represent TMN_4-TMN_4 with the presence of CO on the TM site.

		Direction	Spin magnetic moment (μ_B)		
			total	TM_1	TM_2
2	Tc-Tc	antiparallel	0	2.922	-2.922
	Tc-Tc-CO	parallel	3.9977	1.088	2.933
	CO-Tc-Tc-CO	antiparallel	0	-1.087	1.087
3	Tc-Tc	antiparallel	0	2.918	-2.918
	Tc-Tc-CO	parallel	3.9631	1.089	2.926
	CO-Tc-Tc-CO	antiparallel	0	-1.088	1.088
2	Cr-Cr	antiparallel	-0.0001	-3.683	3.683
	Cr-Cr-CO	antiparallel	0.0043	3.578	-3.685
	CO-Cr-Cr-CO	antiparallel	0.0012	3.582	-3.581
3	Cr-Cr	antiparallel	0.0039	-3.693	3.693
	Cr-Cr-CO	antiparallel	-0.1026	3.573	-3.694
	CO-Cr-Cr-CO	antiparallel	0.0147	-3.574	3.576
2	Co-Co	parallel	1.9976	1.026	1.026
	Co-Co-CO	parallel	1.6798	0.844	1.028
	CO-Co-Co-CO	parallel	-1.5684	-0.844	-0.842
3	Co-Co	parallel	2.0046	1.030	1.030
	Co-Co-CO	antiparallel	0.3990	-0.827	1.030
	CO-Co-Co-CO	antiparallel	0.0001	-0.827	0.828
2	Mn-Mn	antiparallel	0	3.287	-3.287
	Mn-Mn-CO	antiparallel	1.9972	-1.272	3.289
	CO-Mn-Mn-CO	antiparallel	0	1.273	-1.274
3	Mn-Mn	antiparallel	-0.0009	3.279	-3.280
	Mn-Mn-CO	antiparallel	-1.9346	1.280	-3.291
	CO-Mn-Mn-CO	antiparallel	-0.0018	-1.275	1.275
2	V-V	antiparallel	0.0003	2.503	-2.503
	V-V-CO	antiparallel	0.1848	2.391	-2.484
	CO-V-V-CO	antiparallel	-0.0001	2.402	-2.402
3	V-V	parallel	-5.5555	-2.570	-2.568
	V-V-CO	antiparallel	0.3345	2.405	-2.550
	CO-V-V-CO	parallel	-6.1755	-2.409	-2.409
2	Cr-Mn	antiparallel	0.9986	3.687	-3.277
	CO-Cr-Mn	antiparallel	0.9986	3.578	-3.284
	Cr-Mn-CO	parallel	5.0203	3.687	1.279
	CO-Cr-Mn-CO	parallel	-5.0259	-3.589	-1.278
3	Cr-Mn	antiparallel	1.0179	3.694	-3.280
	CO-Cr-Mn	antiparallel	0.9098	3.570	-3.288
	Cr-Mn-CO	antiparallel	2.9493	3.695	-1.283

	CO-Cr-Mn-CO	antiparallel	2.8914	3.578	-1.281

Table S6. The formation energies (ΔE) and TM-N bond lengths of TM_1N_4-TM_2N_4. The TM-N bond lengths are ordered by increasing m values (m = 1,2,3,4,5,6,7,8) provided in Figure S1. TM_1-TM_2, TM_1-TM_2-nlayer (n = 2,3) and Cr-Mn-n (n=1-4) represent TM_1N_4-TM_2N_4, TM_1N_4-TM_2N_4 from different layers (n is the number of layers), and CrN_4-MnN_4 with different distances between the Cr and Mn sites within the same graphite layer (the Cr site is unchanged, n represents the position of the Mn site, concretely shown in Figure 3 of the main text), respectively.

	ΔE (eV)	**TM-N Bond Length (Å)**
Co-Co	-1.662	1.900,1.900,1.901,1.901,1.901,1.901,1.900,1.900
Mn-Mn	-2.387	1.931,1.930,1.932,1.932,1.931,1.932,1.930,1.930
Tc-Tc	-3.936	1.992,1.992,1.991,1.991,1.991,1.991,1.992,1.992
V-V	-1.092	2.001,2.001,2.001,2.001,2.002,2.001,2.001,2.001
Fe-Fe	-0.858	1.917,1.917,1.918,1.918,1.918,1.918,1.917,1.917
Ru-Ru	-2.536	1.971,1.971,1.972,1.971,1.970,1.971,1.971,1.970
Mo-Mo	1.245	2.076,2.075,2.076,2.076,2.075,2.075,2.075,2.075
Cr-Cr	-2.200	1.968,1.969,1.969,1.969,1.969,1.969,1.968,1.969
W-W	2.687	2.044,2.044,2.040,2.041,2.041,2.041,2.045,2.044
Mn-Co	-2.025	1.932,1.932,1.933,1.933,1.899,1.899,1.898,1.899
Mo-Mn	-0.610	2.077,2.077,2.078,2.078,1.932,1.932,1.930,1.930
Mo-Co	-0.250	2.078,2.078,2.078,2.077,1.899,1.899,1.898,1.898
Mo-V	0.066	2.078,2.077,2.079,2.078,1.993,1.993,1.993,1.993
V-Co	-1.389	2.002,2.002,2.001,2.001,1.899,1.898,1.897,1.897
Tc-Co	-2.823	2.003,2.002,2.002,2.003,1.892,1.892,1.890,1.890
Cr-Co	-1.942	1.971,1.971,1.971,1.971,1.899,1.898,1.897,1.897
Tc-V	-2.520	1.994,1.994,1.993,1.994,2.000,2.000,2.000,2.000
Cr-Mn	-2.295	1.970,1.970,1.970,1.970,1.931,1.931,1.930,1.930
Tc-Tc-2layer	-4.590	1.998,1.998,1.996,1.996,1.996,1.996,1.998,1.998
Tc-Tc-3layer	-4.506	1.996,1.997,1.997,1.996,1.996,1.996,1.996,1.996
Cr-Cr-2layer	-2.538	1.976,1.977,1.975,1.975,1.976,1.975,1.977,1.976
Cr-Cr-3layer	-2.496	1.976,1.976,1.977,1.976,1.976,1.976,1.976,1.976
Co-Co-2layer	-1.934	1.912,1.912,1.911,1.911,1.911,1.911,1.912,1.912
Co-Co-3layer	-1.865	1.911,1.912,1.912,1.912,1.912,1.912,1.912,1.911
Mn-Mn-2layer	-2.809	1.938,1.939,1.937,1.937,1.937,1.937,1.939,1.939
Mn-Mn-3layer	-2.717	1.937,1.937,1.938,1.937,1.937,1.937,1.937,1.937
V-V-2layer	-1.899	2.034,2.035,2.044,2.044,2.044,2.044,2.034,2.034
V-V-3layer	-1.605	2.031,2.031,2.027,2.026,2.031,2.031,2.026,2.026
Cr-Mn-2layer	-2.665	1.977,1.976,1.974,1.974,1.937,1.937,1.938,1.938
Cr-Mn-3layer	-2.608	1.977,1.977,1.976,1.976,1.937,1.937,1.937,1.937
Cr-Mn-1	-1.188	1.981,1.981,1.980,1.980,1.935,1.935,1.935,1.935
Cr-Mn-2	-1.185	1.981,1.981,1.981,1.981,1.936,1.936,1.936,1.936

Cr-Mn-3	-1.179	1.980,1.981,1.981,1.980,1.936,1.936,1.936,1.936
Cr-Mn-4	-1.179	1.980,1.980,1.980,1.980,1.937,1.937,1.937,1.937

Table S7. CO adsorption energies, TM-C (in the presence CO) bond lengths and TM-N bond lengths of the homobimetallic systems. TM-TM-CO and CO-TM-TM-CO represent TMN_4-TMN_4 with the presence of CO on the TM site, and TMN_4-TMN_4 with the presence of COs on two TM sites, respectively. nlayer (n = 2,3) represent systems with different layers (n being the number of layers). ΔE of TM-TM-CO and CO-TM-TM-CO represent the adsorption energy of the first and the second CO, respectively. For CO-TM-TM-CO, the order of TM-C bond lengths are the first one for the left or top TM, while the second one for the right or down TM. The TM-N bond lengths are ordered by increasing m values (m = 1,2,3,4,5,6,7,8) shown in Figure S1.

	ΔE (eV)	**TM-C Bond Length (Å)**	**TM-N Bond Length (Å)**
Co-Co-CO	-0.600	1.859	1.932,1.931,1.933,1.932,1.906,1.907,1.905,1.904
CO-Co-Co-CO	-0.640	1.859,1.863	1.933,1.932,1.934,1.934,1.932,1.930,1.933,1.931
Mn-Mn-CO	-0.362	1.763	1.952,1.953,1.953,1.953,1.932,1.932,1.932,1.931
CO-Mn-Mn-CO	-0.338	1.763,1.762	1.954,1.954,1.953,1.954,1.952,1.952,1.952,1.952
V-V-CO	-1.259	2.018	2.043,2.043,2.044,2.044,2.004,2.005,2.005,2.005
CO-V-V-CO	-1.162	2.018,2.018	2.042,2.042,2.041,2.042,2.040,2.041,2.042,2.042
Tc-Tc-CO	-1.803	1.821	2.022,2.022,2.022,2.021,1.997,1.997,1.997,1.998
CO-Tc-Tc-CO	-1.692	1.820,1.820	2.019,2.019,2.019,2.019,2.019,2.019,2.019,2.019
Fe-Fe-CO	-0.722	1.721	1.930,1.930,1.930,1.930,1.918,1.918,1.918,1.918
CO-Fe-Fe-CO	-0.717	1.722,1.722	1.931,1.931,1.931,1.931,1.931,1.931,1.931,1.931
Ru-Ru-CO	-2.176	1.777	1.990,1.990,1.993,1.992,1.972,1.972,1.973,1.973
CO-Ru-Ru-CO	-2.126	1.778,1.778	1.992,1.992,1.994,1.993,1.991,1.990,1.990,1.990
Mo-Mo-CO	-1.498	1.973	2.070,2.069,2.066,2.066,2.072,2.073,2.072,2.073
CO-Mo-Mo-CO	-1.496	1.975,1.975	2.070,2.069,2.066,2.067,2.062,2.062,2.068,2.067
Cr-Cr-CO	-0.312	2.255	1.986,1.990,1.987,1.990,1.970,1.970,1.970,1.969
CO-Cr-Cr-CO	-0.301	2.253,2.268	1.988,1.991,1.988,1.992,1.984,1.987,1.983,1.986
W-W-CO	-2.393	1.968	2.061,2.061,2.066,2.066,2.034,2.034,2.033,2.033
CO-W-W-CO	-2.182	1.968,1.968	2.059,2.059,2.061,2.060,2.060,2.060,2.061,2.061
Tc-Tc-CO 2layer	-1.627	1.822	2.013,2.013,2.010,2.010,1.998,1.999,2.001,2.001
CO-Tc-Tc-CO 2layer	-1.548	1.823,1.823	2.012,2.012,2.007,2.007,2.007,2.007,2.012,2.012
Tc-Tc-CO 3layer	-1.625	1.821	2.011,2.012,2.012,2.012,1.998,1.997,1.997,1.997
CO-Tc-Tc-CO 3layer	-1.596	1.821,1.821	2.011,2.011,2.012,2.012,2.010,2.010,2.011,2.011
Cr-Cr-CO 2layer	-0.235	2.356	1.977,1.979,1.976,1.978,1.976,1.976,1.977,1.977
CO-Cr-Cr-CO	-0.231	2.361,2.366	1.977,1.978,1.976,1.978,1.975,1.977,1.976,1.978

2layer			
Cr-Cr-CO	-0.247	2.334	1.980,1.977,1.980,1.977,1.977,1.977,1.977,1.978
3layer			
CO-Cr-Cr-CO	-0.239	2.334,2.338	1.980,1.978,1.980,1.978,1.979,1.977,1.980,1.977
3layer			
Co-Co-CO	-0.533	1.871	1.933,1.933,1.935,1.936,1.911,1.911,1.911,1.911
2layer			
CO-Co-Co-CO	-0.555	1.875,1.876	1.931,1.932,1.935,1.935,1.935,1.933,1.934,1.931
2layer			
Co-Co-CO	-0.593	1.861	1.934,1.934,1.937,1.936,1.911,1.912,1.912,1.912
3layer			
CO-Co-Co-CO	-0.593	1.862,1.862	1.933,1.934,1.936,1.935,1.937,1.936,1.933,1.933
3layer			
Mn-Mn-CO	-0.234	1.764	1.954,1.954,1.951,1.951,1.938,1.937,1.939,1.939
2layer			
CO-Mn-Mn-CO	-0.222	1.764,1.765	1.953,1.954,1.951,1.951,1.952,1.952,1.954,1.953
2layer			
Mn-Mn-CO	-0.258	1.765	1.953,1.953,1.955,1.954,1.937,1.937,1.938,1.938
3layer			
CO-Mn-Mn-CO	-0.252	1.765,1.765	1.953,1.953,1.954,1.954,1.953,1.953,1.954,1.954
3layer			
V-V-CO	-0.882	2.021	2.030,2.032,2.033,2.034,2.060,2.061,2.047,2.047
2layer			
CO-V-V-CO	-0.786	2.020,2.020	2.035,2.036,2.034,2.034,2.034,2.034,2.035,2.035
2layer			
V-V-CO	-1.024	2.019	2.037,2.038,2.036,2.037,2.041,2.041,2.038,2.040
3layer			
CO-V-V-CO	-0.909	2.019,2.020	2.035,2.034,2.035,2.035,2.035,2.035,2.036,2.036
3layer			

Table S8. CO adsorption energies, TM-C bond lengths and TM-N bond lengths of the heterobimetallic systems. CO-TM_1-TM_2, TM_1-TM_2-CO, and CO-TM_1-TM_2-CO represent TM_1N_4-TM_2N_4, TM_1N_4- TM_2N_4 with the presence of CO on the TM_1 site, TM_1N_4-TM_2N_4 with the presence of CO on the TM_2 site, and TM_1N_4-TM_2N_4 with the presence of COs on both TM_1 and TM_2 sites, respectively. nlayer (n = 2,3) and n (n = 1-4) represent systems different layers (n being the number of layers) and different positions of Mn site within the same graphite layer (with the Cr site unchanged, concretely shown in Figure 3), respectively. Subscript a and b represent the first and the second adsorption sites, respectively. ΔE of CO-TM_1-TM_2 and TM_1-TM_2-CO represent the adsorption energies of the first CO, and ΔE of CO-TM_1-TM_2-CO represents the adsorption energy of the second CO. The order of TM-C bond lengths for CO-TM_1-TM_2-CO are the first one for TM_1 and the second one for TM_2. The TM-N bond lengths are ordered by increasing m values (m = 1,2,3,4,5,6,7,8) shown in Figure S1.

	ΔE (eV)	**TM-C Bond**	**TM-N Bond Length (Å)**

		Length (Å)	
CO-Mn-Co	-0.354	1.763	1.954,1.954,1.954,1.954,1.899,1.899,1.898,1.899
CO-Mn$_a$-Co$_b$-CO	-0.609	1.763,1.768	1.953,1.953,1.955,1.955,1.927,1.928,1.927,1.928
Mn-Co-CO	-0.615	1.857	1.932,1.932,1.933,1.933,1.931,1.931,1.931,1.930
CO-Mn$_b$-Co$_a$-CO	-0.348	1.763,1.768	1.953,1.953,1.955,1.955,1.927,1.928,1.927,1.928
CO-Mo-Mn	-1.518	1.975	2.070,2.069,2.070,2.069,1.932,1.932,1.932,1.931
CO-Mo$_a$-Mn$_b$-CO	-0.327	1.974,1.764	2.069,2.068,2.066,2.067,1.952,1.952,1.952,1.952
Mo-Mn-CO	-0.359	1.763	2.079,2.078,2.078,2.077,1.951,1.951,1.951,1.951
CO-Mo$_b$-Mn$_a$-CO	-1.486	1.974,1.764	2.069,2.068,2.066,2.067,1.952,1.952,1.952,1.952
CO-Mo-Co	-1.489	1.973	2.068,2.069,2.068,2.069,1.900,1.901,1.899,1.899
CO-Mo$_a$-Co$_b$-CO	-0.598	1.973,1.859	2.069,2.069,2.067,2.067,1.931,1.931,1.932,1.932
Mo-Co-CO	-0.613	1.855	2.077,2.076,2.077,2.077,1.931,1.930,1.931,1.931
CO-Mo$_b$-Co$_a$-CO	-1.475	1.973,1.859	2.069,2.069,2.067,2.067,1.931,1.931,1.932,1.932
CO-Mo-V	-1.499	1.974	2.070,2.070,2.070,2.070,1.994,1.995,1.996,1.995
CO-Mo$_a$-V$_b$-CO	-1.205	1.975,2.018	2.070,2.070,2.068,2.068,2.039,2.041,2.041,2.041
Mo-V-CO	-1.211	2.017	2.079,2.078,2.079,2.078,2.039,2.039,2.041,2.041
CO-Mo$_b$-V$_a$-CO	-1.493	1.975,2.018	2.070,2.070,2.068,2.068,2.039,2.041,2.041,2.041
CO-V-Co	-1.212	2.019	2.045,2.044,2.043,2.044,1.901,1.901,1.900,1.900
CO-V$_a$-Co$_b$-CO	-0.608	2.019,1.861	2.045,2.044,2.044,2.044,1.931,1.930,1.932,1.931
V-Co-CO	-0.618	1.856	2.000,2.000,2.000,2.001,1.931,1.931,1.930,1.931
V$_b$-Co$_a$-CO	-1.203	2.019,1.861	2.045,2.044,2.044,2.044,1.931,1.930,1.932,1.931
CO-Tc-Co	-2.016	1.821	2.022,2.022,2.022,2.022,2.006,2.006,2.006,2.006
CO-Tc$_a$-Co$_b$-CO	-0.615	1.821,2.017	2.023,2.023,2.022,2.022,2.039,2.039,2.039,2.039
Tc-Co-CO	-0.893	2.018	2.004,2.004,2.004,2.004,2.042,2.042,2.041,2.042
CO-Tc$_b$-Co$_a$-CO	-1.738	1.821,2.017	2.023,2.023,2.022,2.022,2.039,2.039,2.039,2.039
CO-Cr-Co	-0.303	2.271	1.987,1.990,1.987,1.990,1.899,1.899,1.898,1.898
CO-Cr$_a$-Co$_b$-CO	-0.621	2.271,1.856	1.988,1.991,1.988,1.992,1.931,1.932,1.931,1.930
Cr-Co-CO	-0.619	1.854	1.971,1.971,1.972,1.972,1.931,1.931,1.929,1.930
CO-Cr$_b$-Co$_a$-CO	-0.304	2.271,1.856	1.988,1.991,1.988,1.992,1.931,1.932,1.931,1.930
CO-Tc-V	-2.100	1.821	2.022,2.022,2.022,2.022,2.006,2.006,2.006,2.006
CO-Tc$_a$-V$_b$-CO	-1.149	1.821,2.017	2.023,2.023,2.022,2.022,2.039,2.039,2.039,2.039
Tc-V-CO	-1.169	2.018	1.995,1.995,1.996,1.995,2.042,2.042,2.040,2.040
CO-Tc$_b$-V$_a$-CO	-1.786	1.821,2.017	2.023,2.023,2.022,2.022,2.039,2.039,2.039,2.039
CO-Cr-Mn	-0.305	2.262	1.987,1.990,1.986,1.990,1.932,1.932,1.930,1.930
CO-Cr$_a$-Mn$_b$-CO	-0.352	2.262,1.762	1.989,1.992,1.988,1.992,1.952,1.952,1.951,1.951
Cr-Mn-CO	-0.358	1.762	1.971,1.971,1.971,1.971,1.951,1.951,1.951,1.951
CO-Cr$_b$-Mn$_a$-CO	-0.299	2.262,1.762	1.989,1.992,1.988,1.992,1.952,1.952,1.951,1.951
CO-Cr-Mn 2layer	-0.241	2.350	1.977,1.979,1.975,1.977,1.937,1.938,1.938,1.938
CO-Cr$_a$-Mn$_b$-CO 2layer	-0.232	2.385,1.765	1.975,1.977,1.974,1.976,1.952,1.953,1.954,1.953
Cr-Mn-CO	-0.246	1.765	1.978,1.978,1.977,1.977,1.952,1.952,1.954,1.954

2layer CO-Cr_b-Mn_a-CO	-0.228	2.385,1.765	1.975,1.977,1.974,1.976,1.952,1.953,1.954,1.953
2layer CO-Cr-Mn	-0.245	2.325	1.979,1.981,1.978,1.980,1.938,1.937,1.936,1.937
3layer CO-Cr_a-Mn_b-CO	-0.259	2.338,1.764	1.978,1.980,1.978,1.980,1.954,1.954,1.953,1.953
3layer Cr-Mn-CO	-0.265	1.764	1.977,1.977,1.977,1.977,1.953,1.953,1.954,1.954
3layer CO-Cr_b-Mn_a-CO	-0.240	2.338,1.764	1.978,1.980,1.978,1.980,1.954,1.954,1.953,1.953
3layer			
CO-Cr-Mn-1	-0.449	2.152	1.951,1.954,1.951,1.954,1.981,1.981,1.981,1.981
CO-Cr_a-Mn_b-CO-1	-0.377	2.300,1.765	1.998,1.994,1.997,1.994,1.951,1.951,1.952,1.952
Cr-Mn-CO-1	-0.530	1.765	1.982,1.981,1.981,1.981,1.950,1.950,1.951,1.952
CO-Cr_b-Mn_a-CO-1	-0.296	2.300,1.765	1.998,1.994,1.997,1.994,1.951,1.951,1.952,1.952
CO-Cr-Mn-2	-0.421	2.154	1.952,1.956,1.952,1.956,1.981,1.982,1.982,1.981
CO-Cr_a-Mn_b-CO-2	-0.384	2.301,1.765	1.998,1.995,1.998,1.995,1.952,1.952,1.952,1.952
Cr-Mn-CO-2	-0.506	1.766	1.982,1.982,1.982,1.982,1.953,1.952,1.952,1.952
CO-Cr_b-Mn_a-CO-2	-0.299	2.301,1.765	1.998,1.995,1.998,1.995,1.952,1.952,1.952,1.952
CO-Cr-Mn-3	-0.419	2.151	1.954,1.956,1.953,1.956,1.982,1.982,1.982,1.982
CO-Cr_a-Mn_b-CO-3	-0.400	2.292,1.765	1.998,1.996,1.999,1.995,1.952,1.952,1.953,1.952
Cr-Mn-CO-3	-0.511	1.765	1.981,1.982,1.981,1.982,1.952,1.951,1.952,1.952
CO-Cr_b-Mn_a-CO-3	-0.308	2.292,1.765	1.998,1.996,1.999,1.995,1.952,1.952,1.953,1.952
CO-Cr-Mn-4	-0.421	2.148	1.953,1.957,1.953,1.956,1.981,1.981,1.981,1.981
CO-Cr_a-Mn_b-CO-4	-0.391	2.294,1.765	1.998,1.995,1.998,1.995,1.953,1.953,1.953,1.953
Cr-Mn-CO-4	-0.520	1.764	1.982,1.982,1.981,1.982,1.951,1.950,1.950,1.950
CO-Cr_b-Mn_a-CO-4	-0.292	2.294,1.765	1.998,1.995,1.998,1.995,1.953,1.953,1.953,1.953

Table S9: Collection of calculated spin states. The initial spin moments on two metal sites, final total spin moments and total energies are provided. TM_1-TM_2, CO-TM_1-TM_2, TM_1-TM_2-CO and CO-TM_1-TM_2-CO represent TM_1N_4-TM_2N_4, TM_1N_4-TM_2N_4 with the presence of CO on the TM_1 site, TM_1N_4-TM_2N_4 with the presence of CO on the TM_2 site, and TM_1N_4-TM_2N_4 with the presence of COs on both TM_1 and TM_2 sites, respectively. For the homobimetallic systems, TM_1 and TM_2 are the same, so CO-TM_1-TM_2 and TM_1-TM_2-CO are equivalent. Here use TM-TM-CO to represent TMN_4-TMN_4 with the presence of CO on one TM site. nlayer (n = 2,3) and L-n (n = 1-4) represent systems with different layers (n being the number of layers) and different positions of Mn site within the same graphite layer (concretely shown in Figure 3), respectively. The spin moments with the lowest energy are in bold.

Initial spin (TM_1) (μ_B)	**Initial spin (TM_2) (μ_B)**	**Final total spin (μ_B)**	**Total energy (eV)**
0	0	0.9942	-1150.578350
0	1	0.9792	-1150.563718
0	-1	-0.0011	-1151.137407

Co-Co	1	1	-0.9940	-1150.578274
	1	-1	-0.0011	-1151.137321
	-1	1	-0.9942	-1150.578363
	1.5	1.5	2	-1151.137345
	-1.5	-1.5	0.0002	-1149.985972
	2	2	2.0001	-1151.126083
	-2	-2	-1.9976	-1151.123760
	-1	**-1**	**0**	**-1151.148766**
Co-Co-CO	0	0	-0.0338	-1165.801309
	1	0	-1.7580	-1166.523366
	-1	0	-1.0051	-1166.325903
	0	1	-1.7923	-1166.521044
	0	**-1**	**1.7590**	**-1166.523670**
	1	1	1.0074	-1166.319170
	-1	1	1.0074	-1166.319049
	1	-1	0.0006	-1165.788656
	-1.5	1	0	-1166.522355
	1.5	-1	0	-1166.522614
	-1	-1	0.0001	-1165.788246
CO-Co-Co-CO	0	0	0	-1181.455072
	0	1	0.9236	-1181.711819
	0	-1	0	-1181.454727
	1.5	1.5	-0.1030	-1181.918890
	1	1	-1.5643	-1181.937811
	-1	1	-1.5684	-1181.938623
	-1	-1	-0.9111	-1181.709745
	1	**-1**	**1.5682**	**-1181.938808**
Mn-Mn	1	1	1.9987	-1154.413259
	1	3	6.4572	-1155.226760
	1	-3	-4.0181	-1154.180907
	-1	3	2.0002	-1154.440667
	-1	-3	-1.9976	-1154.290648
	3	3	5.9993	-1155.555028
	3	-3	0.0468	-1155.218760
	-3	3	-0.0594	-1155.217258
	-3.5	3.5	0	-1155.556404
	4	**-4**	**0**	**-1155.556406**
	4	4	6.0768	-1155.216420
	-4	-4	-5.9993	-1155.555057
	3.5	-3.5	1.9886	-1155.296437
	-3	3	-4.0071	-1170.690779
	-1	**1**	**-1.9956**	**-1170.693349**

	3	3	4.0652	-1170.354783
Mn-Mn-CO	3	1	3.9599	-1169.605413
	3	-1	4.0070	-1170.690406
	3.5	3.5	1.9956	-1170.693246
	1	1	2.0195	-1185.805073
	1	**-1**	**0.0001**	**-1185.806909**
	3	3	0	-1185.805558
CO-Mn-Mn-CO	3	-3	-2.0196	-1185.803323
	-3	3	-1.1051	-1185.006046
	-3	-3	2.0196	-1185.803825
	3.5	3.5	0.0001	-1185.805662
	3.5	-3.5	2.0196	-1185.804028
	1	1	6.0067	-1154.265948
	1	-1	-0.0019	-1153.084754
	-1	-1	-5.9707	-1154.537012
	1	3	5.9697	-1154.536408
	2.5	-2.5	0	-1153.356919
V-V	-2.5	2.5	0	-1152.789698
	3	3	2.0001	-1153.115004
	-3.5	3.5	-2.0074	-1153.775550
	4	**-4**	**0**	**-1154.538355**
	-4	-4	-5.9696	-1154.537090
	3	-3	-1.9178	-1153.812161
	1	1	6.0182	-1170.572496
	-1	1	0.0426	-1170.570374
	-1	-1	-2.0007	-1169.271272
V-V-CO	3	1	2.0065	-1169.199973
	-3	1	0.0190	-1170.247352
	3	**3**	**6.0187**	**-1170.572679**
	-3	3	-1.9982	-1169.714200
	1	1	2.0094	-1185.271739
	1	-1	-0.0018	-1185.274327
	-1	-1	-2.0047	-1185.106491
CO-V-V-CO	2.5	2.5	5	-1186.359846
	-2.5	-2.5	-6.0419	-1186.509764
	1	3	4.0174	-1185.807059
	1	**-3**	**0.0007**	**-1186.510123**
	3	3	2.0047	-1185.106754
	3	-3	0.0008	-1186.509354
	1	1	6.0006	-1152.410790
	1	**-1**	**0**	**-1152.414264**
	1	3	2.9295	-1151.452757

Tc-Tc	1	-3	-1.9974	-1151.154474
	-1	3	4.0101	-1151.464120
	3	3	6.0006	-1152.410790
	3	-3	0	-1152.414264
Tc-Tc-CO	-3	2	2.0011	-1168.457076
	-1	1	1.0808	-1167.992555
	3	1	3.9996	-1168.448803
	-3	1	-2.0011	-1168.456688
	3	-1	-2.0083	-1168.368381
	-3	1.5	2.0076	-1168.360158
	3	-2	2	-1168.356090
	3	1.5	3.9997	-1168.454337
	3	**2**	**4.0060**	**-1168.992554**
	3	3	0.0075	-1168.358153
	-3.5	2	2.0077	-1168.360238
	-3	2	1.9220	-1168.170760
	3.5	-1.5	3.9997	-1168.454337
	3.5	-2	-2.0076	-1168.360149
	-3.5	1.5	2.0076	-1168.360155
	-3	3	2.0077	-1168.360008
CO-Tc-Tc-CO	1	1	2.0059	-1185.459544
	1	-1	0	-1185.459676
	1	3	2.0012	-1184.910739
	1	-3	-0.0006	-1184.910956
	-1	**3**	**0**	**-1185.460063**
	3	3	0	-1185.459869
	3	-3	2.0058	-1185.459490
W-W	3	3	6.7908	-1155.361640
	-3	3	1.1217	-1155.347108
	3	-3	-1.1274	-1155.347866
	-3	**-3**	**-6.7907**	**-1155.361644**
	4	-4	0	-1155.319811
W-W-CO	3	3	4.4776	-1172.522192
	-3	3	-0.2559	-1172.529987
	3	**-3**	**0.2545**	**-1172.530095**
	-3	-3	-4.4747	-1172.521880
	4	3	5	-1172.514720
CO-W-W-CO	2	2	4.0058	-1189.482517
	2	**-2**	**-0.0001**	**-1189.487674**
	-2	2	0.0001	-1189.487674
	-2	-2	-4.0057	-1189.482516
	0	**4**	**-0.0003**	**-1157.087232**

Cr-Cr	2	2	8.0473	-1157.086264
	2	-2	0.0003	-1157.087228
	-2	-2	-8.0473	-1157.086265
Cr-Cr-CO	2	0	7.9282	-1172.169468
	-2	0	-4.0139	-1171.440689
	4	0	6.0534	-1170.964212
	-4	0	-6.0386	-1171.978653
	0	-2	0.1136	-1172.173292
	-2	**2**	**-0.1174**	**-1172.173970**
	-2	-2	-7.9255	-1172.170343
	0	-4	-5.9199	-1170.857868
CO-Cr-Cr-CO	4	4	7.8178	-1187.249174
	4	**-4**	**-0.0210**	**-1187.249916**
	-4	4	0.0205	-1187.249914
	-4	-4	-7.8191	-1187.248600
Fe-Fe	0	0	0	-1152.282678
	0	2	0	-1153.445672
	0	4	2.0002	-1152.690098
	2	2	3.9976	-1152.559846
	2	**-2**	**0**	**-1153.445760**
	4	4	4.0032	-1153.444863
	4	-4	-2.0013	-1152.864206
	4.5	4.5	4.0032	-1153.444769
Fe-Fe-CO	0	0	0.0001	-1168.360415
	2	0	2.0015	-1168.942406
	4	**0**	**2.0015**	**-1168.942680**
	2	2	0.0661	-1168.583678
	4	4	-0.0001	-1168.360463
	-4	4	-2.0015	-1168.942650
CO-Fe-Fe-CO	0	0	-1.9674	-1184.081750
	0	2	-1.9731	-1184.084324
	0	**4**	**0**	**-1184.434930**
	2	2	-1.9703	-1184.082775
	2	-2	1.9676	-1184.082471
	4	4	0	-1184.434763
	4	-4	0	-1184.433908
Ru-Ru	0	0	-1.3807	-1150.348760
	0	2	-1.8735	-1150.457782
	0	4	-1.4928	-1150.273319
	2	2	0.0164	-1150.261645
	2	-2	-0.0908	-1150.737550
	4	4	3.9968	-1150.882611

	4	**-4**	**-0.0012**	**-1150.885542**
Ru-Ru-CO	0	0	0.0001	-1167.208560
	2	0	-2.0058	-1167.835086
	4	**0**	**2.0056**	**-1167.836398**
	2	2	-2.0058	-1167.835588
	-2	2	2.0058	-1167.835248
	4	4	2.0058	-1167.835884
	-4	4	-2.0058	-1167.834925
CO-Ru-Ru-CO	0	0	0	-1184.737287
	0	2	0	-1184.737321
	0	4	0	-1184.737290
	2	**2**	**0**	**-1184.737535**
	2	-2	0	-1184.737168
Mo-Mo	0	0	0.0010	-1151.289444
	0	2	3.9163	-1152.225853
	0	4	-0.0108	-1153.183617
	2	-2	0.0120	-1153.183514
	3.5	3.5	7.8053	-1153.178038
	3.5	**-3.5**	**-0.0038**	**-1153.186357**
	4	4	7.8107	-1153.174621
	4	-4	0.0073	-1153.182792
Mo-Mo-CO	2	0	-0.0104	-1168.065043
	4	0	-0.0102	-1168.065545
	2	2	-0.0076	-1168.243169
	-2	2	-0.0076	-1168.243423
	4	4	5.9780	-1169.458830
	-4	**4**	**-1.9574**	**-1169.459620**
CO-Mo-Mo-CO	0	0	0	-1185.188364
	0	2	0.0001	-1185.192093
	0	4	0	-1185.730255
	2	2	2.0009	-1185.460233
	2	-2	0	-1185.730635
	4	4	4.0017	-1185.728223
	4	**-4**	**0**	**-1185.730878**
Mn-Co	**3.5**	**1**	**1.9980**	**-1153.352506**
	3.5	-1	3.9983	-1153.340769
	-3.5	1	-3.0491	-1152.766370
	3.5	1.5	4	-1152.988152
	-3.5	-2	-2.970	-1152.764887
	4	2	3.722	-1152.807044
	3.5	1	-1.0213	-1167.878097
	3.5	-1	-1.0215	-1167.877996

	-3.5	1	1.0216	-1167.878003
	-3.5	-1	1.0216	-1167.878051
CO-Mn-Co	**1.5**	**1**	**2**	**-1168.482298**
	1.5	-1	0.5000	-1168.449354
	-1.5	1	-2.0100	-1168.470501
	2	-2	0.0120	-1168.471103
	-2	2	-1.0183	-1167.840477
	3.5	1	2.2565	-1168.420749
	3.5	**-1**	**3.8130**	**-1168.743126**
Mn-Co-CO	-3.5	1	-3.8120	-1168.743050
	-3.5	-1	-2.2451	-1168.730953
	4	-1	3.8313	-1168.743107
	-4	1	-2.2468	-1168.730808
	3.5	1	1.0286	-1183.671229
	3.5	-1	1.0291	-1183.670249
	-3.5	1	-1.0293	-1183.671252
	-3.5	-1	-1.0293	-1183.671252
CO-Mn-Co-CO	1.5	1	2	-1183.865765
	1.5	**-1**	**0.5000**	**-1183.866282**
	-1.5	1	-0.3303	-1183.866073
	2	2	-1.0287	-1183.671313
	2	-2	0.6287	-1183.047878
	-2	2	1.029	-1183.671114
	4	3.5	0.9941	-1155.001173
	4	-3.5	0.9674	-1155.989764
	-4	**3.5**	**-1.0173**	**-1156.323699**
Cr-Mn	4	4	7	-1156.321960
	-4	-4	-0.9937	-1155.074507
	-4.5	-4	1.0182	-1156.323684
	-4	-3.5	-2.9996	-1154.570850
	4	3.5	-0.9512	-1171.402261
	4	-3.5	0.9512	-1171.402259
	-4	3.5	-0.9538	-1171.402831
CO-Cr-Mn	**4**	**4**	**7**	**-1171.404395**
	-4	-4	0.9534	-1171.402867
	4.5	4	-0.9535	-1171.402865
	-4.5	-4	0.9535	-1171.402866
	-4	-3.5	0.9514	-1171.402385
	4	3.5	4.0179	-1170.682577
	4	-3.5	2.9876	-1171.455090
	4.5	-3.5	2.9877	-1171.454994
Cr-Mn-CO	4	-3	5.0369	-1171.456990

	-4	3	-2.9876	-1171.454887
	-4	1.5	2.9353	-1170.940179
	4	-2	2.9354	-1170.939882
	-4	3.5	-5.0369	-1171.456699
	-4	**-3.5**	**-5.0368**	**-1171.457115**
	4	3.5	3.8651	-1185.762092
CO-Cr-Mn-CO	4	-3.5	2.9158	-1186.528923
	-4	**3.5**	**-4.9768**	**-1186.531645**
	-4	-3.5	-4.9776	-1186.531171
	4	1	3.0084	-1152.865081
	4	1.5	5.0106	-1154.118284
	4	-1	3.0091	-1152.765153
Cr-Co	-4	1	-5.0172	-1154.128493
	4.5	2	5.0107	-1154.118574
	4	-2	5.0106	-1154.118366
	-4	**-1**	**-3.0188**	**-1154.128960**
	4	1	3.9552	-1168.665236
CO-Cr-Co	**4**	**-1**	**2.9396**	**-1169.206850**
	-4	1	-4.9346	-1169.206066
	-4	-1	-2.9502	-1169.195961
	4	1	4.7163	-1169.516824
Cr-Co-CO	**4**	**-1**	**3.2861**	**-1169.523575**
	-4	1	-3.2852	-1169.523500
	-4	-1	-4.7163	-1169.515914
	4	1	4.6590	-1184.600282
CO-Cr-Co-CO	**4**	**-1**	**3.2354**	**-1184.602893**
	-4	1	-3.2362	-1184.602620
	-4	-1	-4.6578	-1184.599731
	3	1	3.9877	-1152.854747
V-Co	**3**	**-1**	**1.9885**	**-1152.855313**
	-3	1	-3.9869	-1152.854656
	-3	-1	-3.9870	-1152.854802
	3	1	3.0203	-1168.269339
	3	-1	4.0210	-1168.842270
	-3	1	-0.0058	-1168.246239
	-3	-1	-3.0204	-1168.269367
CO-V-Co	2.5	-1	1.5000	-1167.982597
	-2.5	**1.5**	**-4.0210**	**-1168.842479**
	3	-1.5	4.0211	-1168.842425
	-2.5	1	0.0081	-1168.297720
	4	-2	2	-1168.830395
	-4	2	-3.0216	-1168.269233

	-2.5	1	0.0081	-1168.297720
V-Co-CO	3	1	0.2013	-1167.486352
	3	**-1**	**2.2238**	**-1168.248200**
	-3	1	-3.7162	-1168.239760
	-3	-1	-0.2846	-1167.525876
CO-V-Co-CO	3	1	3.8117	-1184.219554
	3	-1	0.2740	-1183.674874
	-3	1	-2.9719	-1184.019771
	-3	-1	-0.2948	-1183.683241
	-2.5	1	-2.2968	-1184.226064
	2.5	**-1**	**2.2968**	**-1184.226065**
Mo-Mn	3.5	3.5	6.5000	-1154.392654
	3.5	-3.5	0	-1154.334834
	-3.5	-3.5	-6.9792	-1154.078110
	-3.5	3.5	0	-1154.334727
	4	4	2.9903	-1153.460907
	-4	**-4**	**-6.9576**	**-1154.410266**
CO-Mo-Mn	2	3.5	5	-1170.683298
	2	-3.5	-3	-1170.413168
	-2	3.5	1.5000	-1170.631434
	-2	-3.5	-5.0013	-1170.683261
	2	4	5.0015	-1170.683317
	-2	4	0.9992	-1170.685478
	2	**-4**	**-0.9989**	**-1170.685481**
Mo-Mn-CO	3.5	1.5	5	-1169.526418
	3.5	-1.5	2	-1169.437810
	-3.5	1.5	-4.9874	-1169.526491
	4	**2**	**4.9872**	**-1169.526518**
	4	-2	-1.0087	-1168.525103
	-4	2	2.9309	-1169.520565
CO-Mo-Mn-CO	2	1.5	3	-1185.786167
	2	-1.5	0.5000	-1185.460335
	-2	1.5	3.0069	-1185.785847
	2	-2	-0.9985	-1185.787276
	-2	**2**	**0.9988**	**-1185.787302**
	-2	-1.5	0.9988	-1185.787294
Mo-Co	3.5	1	4.9487	-1152.196419
	3.5	**-1**	**2.9454**	**-1152.208392**
	-3.5	1	-2.9357	-1152.194518
CO-Mo-Co	2	1	1.0026	-1168.469770
	2	-1	1.0025	-1168.469979
	-2	**1**	**-3.0036**	**-1168.472527**

	3.5	1	4	-1167.548853
	3.5	-1	-0.9190	-1166.576133
Mo-Co-CO	**4**	**1.5**	**3.2320**	**-1167.596134**
	4	-1.5	1.2141	-1166.704483
	4	-2	-4.6342	-1167.590276
	2	**1**	**2.8080**	**-1183.846065**
CO-Mo-Co-CO	2	-1	1.2828	-1183.840799
	-2	1	-1.2828	-1183.842950
	3.5	3	6.9229	-1153.869638
	3.5	-3	-3.0093	-1152.867802
Mo-V	-4	3	-0.9416	-1153.872026
	4	**-3**	**1**	**-1153.872467**
	-3.5	-3	-6.9210	-1153.870077
	2	**3**	**4.9995**	**-1170.146541**
CO-Mo-V	2	-3	-0.9887	-1170.145369
	-2	3	0.9891	-1170.145256
	-2	-3	-4.9997	-1170.146379
	3.5	**2.5**	**6.9913**	**-1169.858776**
Mo-V-CO	3.5	-2.5	0.9131	-1169.858348
	-3.5	2.5	-0.9137	-1169.856397
	-3.5	-2.5	-4.9777	-1169.316566
	2	2.5	5.0128	-1186.123930
CO-Mo-V-CO	2	-2.5	-1.0035	-1186.125627
	-2	**2.5**	**1.0036**	**-1186.126519**
	-2	-2.5	-5.0128	-1186.124745
	3	1	-1.9983	-1151.164690
	3	-1	2.0007	-1151.118358
	-3	1	1.9982	-1151.164615
	-3	-1	1.9997	-1151.174070
	3.5	1	4	-1151.353874
	3.5	-1	2	-1151.528391
Tc-Co	-3.5	1	1.0526	-1150.564336
	-3.5	-1	1.0528	-1150.564831
	3.5	1.5	-0.9689	-1150.581756
	-3.5	-1.5	0.9655	-1150.592622
	4	1	-0.9793	-1150.583004
	-4	-1	-0.0003	-1151.161199
	4	**2**	**4**	**-1151.806006**
	-4	-2	-2.9668	-1151.227435
	4	1.5	2.9953	-1151.228814
	-4	-1.5	-0.9943	-1150.605862
	3	**1**	**-2.0052**	**-1168.319707**

	3	-1	1.0111	-1167.736313
	-3	1	-1.0063	-1167.725075
	-3	-1	-1.0063	-1167.725123
	1	1	2	-1168.309243
	1	-1	0	-1167.605685
	-1	1	0	-1167.579720
CO-Tc-Co	1.5	1	2	-1167.565183
	1.5	-1	0	-1167.063588
	1.5	1.5	-1.0064	-1167.724477
	1.5	-1.5	1.0063	-1167.724764
	-1.5	1.5	-1.0102	-1167.735985
	2	2	1.0062	-1167.724861
	2	-2	-1.0063	-1167.724986
	2.5	-2.5	0	-1168.309659
	-2.5	2.5	0	-1168.319574
	-2	2	1.0063	-1167.725367
	3	1	-0.2552	-1166.494427
	3	-1	-2.0942	-1166.419676
	-3	1	3.7490	-1167.196370
	-3	-1	0.2530	-1166.494246
	3.5	**1**	**-3.7497**	**-1167.196762**
Tc-Co-CO	3.5	-1	2	-1166.516352
	-3.5	1	2	-1166.864863
	4	-1	-0.2568	-1166.54605
	-4	1	0.2566	-1166.546123
	4	-1.5	-3.7497	-1167.196758
	4	-2	2	-1167.191339
	-4	2	1.7405	-1166.547428
	-4	1.5	3.7496	-1167.196722
	3	1	1.0108	-1183.527119
	1	**1**	**2**	**-1183.709548**
CO-Tc-Co-CO	1	-1	0	-1183.708786
	-1	1	0	-1183.707130
	-1	-1	1.7168	-1183.708857
	3	3	4.1049	-1152.821334
	3	-3	-4.2960	-1152.688399
	-3	3	3.9890	-1152.875540
	-3	-3	-3.9838	-1152.803385
	3.5	3	6	-1153.188628
Tc-V	3.5	-3	0	-1152.080370
	-3.5	3	0	-1152.425949
	4	4	1.9828	-1152.851158

	4	-4	0.2100	-1152.333751
	-4	**4**	**5.9787**	**-1153.482078**
	-4	-4	-1.9867	-1152.835609
	-3.5	-3	-1.9822	-1152.851374
	3	**3**	**3.9908**	**-1170.063499**
CO-Tc-V	3	-3	-1.9777	-1170.062145
	-3	3	3.9908	-1170.062973
	-3	-3	-2.0541	-1169.336007
	3	3	4.0269	-1168.809359
	3	-3	-4.0173	-1168.846113
	-3	3	4.0178	-1168.848823
	3	2.5	6	-1169.208662
Tc-V-CO	-3	2.5	0	-1168.378467
	4	4	2.0155	-1168.845561
	4	-4	0.5310	-1168.106855
	-4	4	4.0213	-1168.847959
	-4	**-4**	**5.3320**	**-1169.426175**
	-3	-2.5	-2.0216	-1168.847782
	2	**2.5**	**4**	**-1185.987889**
	2	-2.5	-4.0210	-1185.985555
CO-Tc-V-CO	-1	2.5	1.5	-1185.946651
	1.5	-2.5	-4.0211	-1185.987492
	2	-3	-2.0137	-1185.987550
	-2	3	2.0137	-1185.987550
		n-layer		
	3	3	6	-895.6121007
	3	**-3**	**0**	**-895.6268769**
Tc-Tc	1	1	0.0001	-895.6265081
2layer	1	-1	0.0001	-895.6260195
	1	3	6	-895.6123609
	1	-3	-0.0001	-895.6258701
	-1	3	0.0002	-895.6203083
	2	3	4	-912.0284619
	1	3	4	-912.0284977
	1	-3	-1.9947	-912.0285739
Tc-Tc-CO	-1	3	1.9945	-912.0282449
2layer	1.5	3	4	-912.0284978
	1.5	**-3**	**3.9977**	**-912.0289443**
	1.5	3.5	4	-912.0284978
	-2	3	1	-911.2065307
	2	**-2**	**0**	**-928.3518415**
	1	1	2	-928.3516860

CO-Tc-Tc-CO	-1	-1	1.0714	-927.6092389
2layer	1	-1	0	-928.3518205
	-1	1	0	-928.3518123
	2	2	-2.0031	-928.3516559
	3	3	6	-1362.151811
	1	1	1.9830	-1361.495489
Tc-Tc	1	-1	1.9893	-1361.510485
3layer	-1	1	-1.9893	-1361.510361
	3	-3	0	-1362.172040
	-3	**3**	**0**	**-1362.172642**
	1	3	4	-1377.436963
	1	-3	2	-1377.888935
	1	-3	0.1438	-1377.898672
	2	3	1.9141	-1377.900442
	3	3	4	-1377.482568
Tc-Tc-CO	1	3.5	4	-1377.435526
3layer	**1**	**-3.5**	**3.9631**	**-1378.572942**
	2	3.5	4	-1377.437715
	3.5	3.5	5	-1378.464838
	-1	4	2.0002	-1377.893473
	1	-4	2.1375	-1377.930645
	-2	4	2	-1377.893432
	-4	4	-2.1293	-1377.930537
	4	-4	2.1274	-1377.930800
	3	3.5	6	-1378.113747
	1	1	2	-1394.944361
	1	-1	0	-1394.944349
Tc-Tc-CO	**-1**	**1**	**0**	**-1394.944610**
3layer	-1	-1	2.0359	-1394.944453
	2	2	-2.0360	-1394.944438
	2	-2	-0.0004	-1394.944376
	3.6	2.5	3.9884	-898.2542539
	3.7	3.7	5.9954	-898.6709116
Cr-Cr	4	4	7.9866	-899.9699414
2layer	4	-4	0.0001	-899.9835608
	-4	**4**	**-0.0001**	**-899.9840675**
	-4	-4	-7.9864	-899.9698363
	4.5	4.5	7.9865	-899.9698507
	3	2.1	-0.0043	-914.9945790
	2.5	2	3.9918	-914.2546656
	3	2	6.0334	-914.8068455
	2	3.6	7.9867	-914.9882781

	2.5	3.6	-0.0043	-914.9941991
Cr-Cr-CO	3	3.6	7.9868	-914.9883318
2layer	3.7	3.7	7.9866	-914.9882507
	4	4	-0.0038	-914.9934445
	-4	4	-1.9652	-914.7964836
	4	-4	1.9641	-914.7983284
	-4	**-4**	**0.0043**	**-914.9946076**
	4	4	-4.0009	-929.2546568
	4	-4	0	-928.4992473
CO-Cr-Cr-CO	-4	4	-4.0013	-929.2564811
2layer	-4	-4	4.0008	-929.2553971
	4.5	4.5	7.9934	-929.9985889
	4.5	**-4.5**	**0.0012**	**-930.0007764**
	4	4	8.0359	-1366.569041
Cr-Cr	4	-4	-0.005	-1366.571863
3layer	**-4**	**4**	**0.0039**	**-1366.571970**
	-4	-4	-8.0402	-1366.568700
	4	4	7.9547	-1381.592246
Cr-Cr-CO	**-4**	**4**	**-0.1026**	**-1381.593757**
3layer	4	-4	0.1042	-1381.593707
	-4	-4	-7.9589	-1381.592177
	4	4	3.8814	-1395.853433
CO-Cr-Cr-CO	4	-4	-0.0151	-1396.608243
3layer	**-4**	**4**	**0.0147**	**-1396.608277**
	-4	-4	-7.8532	-1396.608262
	1.1	-1.1	0.9985	-893.3641402
	1.5	-1.5	0.0111	-892.7175691
Co-Co	1	-1	0	-893.9793511
2layer	-1	1	2.0002	-893.8999816
	-1	**-1**	**1.9976**	**-893.9798359**
	1	1	1.6763	-909.2876567
Co-Co-CO	1	-1	-1.6774	-909.2879696
2layer	**-1**	**1**	**1.6798**	**-909.2881226**
	-1	-1	-0.9404	-908.6947625
	1	**1**	**-1.5684**	**-924.6178576**
CO-Co-Co-CO	1	-1	0	-924.5998886
2layer	-1	1	0.0129	-924.6011992
	-1	-1	1.5680	-924.6172661
	1	1	-0.9680	-1359.841443
	0	-1	-1.9878	-1360.476545
Co-Co	**1**	**-1**	**2.0046**	**-1360.540163**
3layer	1.2	-1.2	1.0361	-1359.915254

	-1	1	-1.9877	-1360.476531
	-1	-1	0.0878	-1359.307490
	1	1	0.0001	-1375.027983
Co-Co-CO	-1	1	0.3991	-1375.908317
3layer	1	-1	-0.9782	-1375.593745
	-1	**-1**	**0.3990**	**-1375.908785**
	1	1.5	1.8000	-1375.156497
	1	1	1.3993	-1391.262351
CO-Co-Co-CO	1	-1	-1.3886	-1391.259226
3layer	-1	1	0	-1390.730129
	-1	**-1**	**0.0001**	**-1391.277037**
	3	3	6.0160	-898.5339520
Mn-Mn	3.5	3.5	5.9879	-897.7734636
2layer	3	-3	0.0023	-896.2499750
	3.5	**-3.5**	**0**	**-898.5370012**
Mn-Mn-CO	3.5	3.5	4.0022	-913.5459042
2layer	3.5	-3.5	-1.9964	-913.5460834
	-1.5	**3.5**	**1.9972**	**-913.5463341**
	3.5	-3.5	2.0197	-928.5425653
CO-Mn-Mn-CO	3.5	3.5	-1.1178	-927.7330674
2layer	-3.5	-3.5	2.0198	-928.5425353
	3	3	0	-928.5439699
	3	**-3**	**0**	**-928.5440266**
	3.5	3.5	6.0289	-1365.072813
Mn-Mn	**3.5**	**-3.5**	**-0.0009**	**-1365.075321**
3layer	3	3	6.0287	-1365.073846
	-3.5	-3.5	-6.0284	-1365.074350
	3.5	3.5	2.0840	-1378.984596
Mn-Mn-CO	-3.5	3.5	4.0632	-1380.106858
3layer	**3.5**	**-3.5**	**-1.9346**	**-1380.108248**
	-3.5	-3.5	-4.0624	-1380.107831
CO-Mn-Mn-CO	3.5	3.5	-2.1122	-1395.133659
3layer	3.5	-3.5	-0.0027	-1395.134337
	3	**3**	**-0.0018**	**-1395.135813**
	3	3	5.7521	-897.8650413
V-V	**3**	**-3**	**0.0003**	**-897.9045924**
2layer	-3	3	-0.0012	-897.9038882
	-3	-3	-5.7506	-897.8650338
	3	3	5.7275	-913.5199510
V-V-CO	**3**	**-3**	**0.1848**	**-913.5622867**
2layer	2.5	3	5.7242	-913.5199065

	-2.5	3	-0.1901	-913.5621289
	-2.5	-3	-3.9743	-913.0553224
	3	3	4.0154	-928.4896404
CO-V-V-CO	**3**	**-3**	**-0.0001**	**-929.1230387**
2layer	2.5	2.5	4.0303	-928.6110261
	-3	-3	-6.0464	-929.1226994
	-2.5	2.5	2.0036	-928.6098769
	3	3	5.5556	-1364.240068
V-V	3	-3	3.5512	-1363.503288
3layer	-3	3	-0.0001	-1364.227110
	-3	**-3**	**-5.5555**	**-1364.240228**
	3	3	5.7434	-1380.037894
V-V-CO	-3	3	-0.3331	-1380.039555
3layer	**3**	**-3**	**0.3345**	**-1380.039862**
	-3	-3	-3.7019	-1379.523333
	3	3	6.1743	-1395.723809
CO-V-V-CO	3	-3	0.0043	-1395.724166
3layer	-3	3	-2.0856	-1395.208593
	-3	**-3**	**-6.1755**	**-1395.724503**
	4	3.5	3.0032	-897.5354466
Cr-Mn	**4**	**-3.5**	**0.9986**	**-899.2517859**
2layer	-4	3.5	-0.9973	-898.8829665
	-4	-3.5	0.9987	-899.2516553
	4	3.5	-0.9987	-914.2683799
CO-Cr-Mn	**4**	**-3.5**	**0.9986**	**-914.2684388**
2layer	-4	3.5	-0.9986	-914.2683724
	-4	-3.5	0.9986	-914.2685358
	4	3.5	5.0211	-914.2726398
	4	-3.5	5.0205	-914.2727316
	4	-2	2.9662	-914.2702436
Cr-Mn-CO	**4**	**2**	**5.0203**	**-914.2729830**
2layer	4.5	-4	5.0202	-914.2729059
	-4	3.5	-5.0212	-914.2726342
	4	-1.5	2.9665	-914.2701955
	3.5	1.5	2.9678	-914.2699039
	-4	-3.5	-2.9659	-914.2701560
	4	3.5	5.0258	-929.2754949
CO-Cr-Mn-CO	4	-3.5	5.0259	-929.2756977
2layer	-4	3.5	-2.9815	-929.2736816
	-4	**-3.5**	**-5.0259**	**-929.2757286**
	4	3.5	0.9538	-1362.907122
Cr-Mn	4	-3.5	-3.0636	-1364.073182

3layer	-4	3.5	3.0402	-1364.073289
	-4	**-3.5**	**1.0179**	**-1365.825386**
	4	3.5	-0.9344	-1380.845281
CO-Cr-Mn	**4**	**-3**	**0.9098**	**-1380.845711**
3layer	4	-3.5	0.9319	-1380.845211
	-4	-3.5	-0.9161	-1380.630067
	4	**3.5**	**2.9493**	**-1380.865164**
Cr-Mn-CO	4	-3.5	5.1271	-1380.864056
3layer	-4	3.5	-5.1266	-1380.864043
	-4	-3.5	-2.9488	-1380.864751
	4	**3.5**	**2.8914**	**-1395.880137**
	3.6	1.3	5.0540	-1395.878833
CO-Cr-Mn-CO	4	2	-5.0549	-1395.877839
3layer	4	2.5	5.0524	-1395.877812
	4	-3.5	5.0582	-1395.879061
	-4	3.5	-5.0598	-1395.879072
	-4	-3.5	-2.8864	-1395.878870
		L		
	4	3.5	3	-1684.797769
Cr-Mn	4	-3.5	1	-1686.568992
L-1	**-4**	**3.5**	**-1**	**-1686.569152**
	-4	-3.5	-7	-1686.569129
	4	3.5	1	-1700.525122
	4	-3.5	-1	-1701.793222
CO-Cr-Mn	-4	3.5	1	-1701.794142
L-1	4.5	3.5	7	-1701.794166
	4.5	**-3.5**	**-1**	**-1701.794179**
	-4	-3.5	-1	-1700.526522
	4	3.5	5	-1701.335615
Cr-Mn-CO	4	-1.5	3	-1701.874357
L-1	-4	3.5	-3	-1701.872237
	-4	**3**	**-3**	**-1701.874540**
	-4	2	-3	-1701.873893
	4	**3.5**	**5**	**-1716.945804**
CO-Cr-Mn-CO	4	-3.5	3	-1716.943032
L-1	-4	3.5	-3	-1716.945588
	4	**3.5**	**-1**	**-1686.580506**
	4	-3.5	1	-1686.580503
Cr-Mn	-4	3.5	-1	-1686.580451
L-2	4	4	7.0029	-1686.578666
	-4	4	-0.9996	-1686.580425
	-4	-3.5	-1	-1685.312626

	4	3.5	-1	-1701.776098
CO-Cr-Mn	**4**	**-3.5**	**-1**	**-1701.776754**
L-2	-4	3.5	1	-1701.776710
	-4	-3.5	-7	-1701.775969
	4	3.5	5	-1701.861177
	4	-3.5	3	-1701.861703
Cr-Mn-CO	**-4**	**3.5**	**-3**	**-1701.862228**
L-2	4	1.5	5.0007	-1701.862211
	4	-1.5	2.9998	-1701.862195
	-4	1.5	-3	-1701.862225
	4	3.5	3	-1716.934786
	4	**3**	**5**	**-1716.935961**
CO-Cr-Mn-CO	4	2	1	-1716.273966
L-2	4	-2	3	-1716.935922
	-4	-3.5	-5	-1716.933323
	4	3.5	-1	-1686.221284
	4	-3.5	1	-1686.572657
	-4	2	-1	-1686.572886
Cr-Mn	-4	3	1	-1685.304558
L-3	-4	3.5	-1	-1686.572238
	4	4	7.0007	-1686.572795
	-4	**4**	**-1**	**-1686.572914**
	-4	-4	-5	-1685.295296
	-4	-3.5	-3	-1684.799441
	4	**3.5**	**-1**	**-1701.766826**
	4	-3.5	-1	-1701.763828
	-4	3.5	1	-1701.763913
CO-Cr-Mn	4	4	7	-1701.766812
L-3	-4	4	1.0001	-1701.766818
	-4	-4	-7.0006	-1701.766644
	-4	-3.5	-5	-1700.495381
	4	3	5	-1701.855709
Cr-Mn-CO	4	-3	3	-1701.858934
L-3	4	-3.5	3	-1701.858958
	-4	3	-3	-1701.858748
	-4	**3.5**	**-3**	**-1701.859126**
	4	**3.5**	**5**	**-1716.941999**
CO-Cr-Mn-CO	4	-3.5	1	-1716.851402
L-3	-4	-3.5	-3	-1716.940988
	-4	-3.5	-3	-1716.940984
	4	3.5	-1	-1686.571430
	4	-3.5	1	-1686.571532

Cr-Mn	-4	3.5	-1	-1686.571534
L-4	**-4**	**4**	**-1**	**-1686.571558**
	-4	-4	-7.0007	-1686.571511
	-4	-3.5	-1	-1685.304777
	4	**3.5**	**-1**	**-1701.767414**
	4	-3.5	-1	-1701.765517
CO-Cr-Mn	-4	3.5	1	-1701.767413
L-4	4	4	7	-1701.767400
	-4	4	0.9999	-1701.767406
	-4	-3.5	-2.9679	-1699.638179
Cr-Mn-CO	4	3.5	5	-1701.867018
L-4	4	-3.5	3	-1701.866482
	-4	**3.5**	**-3**	**-1701.867108**
	4	**3.5**	**5**	**-1716.933879**
CO-Cr-Mn-CO	4	-3.5	3	-1716.933188
L-4	-4	3.5	-3	-1716.933161
	-4	-3.5	-5	-1716.933183
Mn-Mn	3.5	3.5	6	-1685.798602
L-1	**3.5**	**-3.5**	**0**	**-1685.798855**
	-3.5	-3.5	-6	-1685.798491
	3.5	3.5	2	-1701.091961
Mn-Mn-CO	**3.5**	**-3.5**	**2**	**-1701.093001**
L-1	3.5	1.5	4	-1700.765545
	-3.5	1.5	-2	-1701.091957
	3.5	2	4.5	-1700.948193
	-3.5	-1.5	-2	-1701.091956
	3.5	**3.5**	**2**	**-1716.354479**
CO-Mn-Mn-CO	2	-2	0	-1715.812488
L-1	-2	2	0	-1715.270127
	1.5	-1.5	0	-1716.354438
	-1.5	1.5	-2	-1715.700775
Mn-Mn	3.5	3.5	6	-1685.801870
L-2	3.5	-3.5	0	-1685.142473
	-3.5	**3.5**	**0**	**-1685.802048**
	3.5	**3.5**	**2**	**-1701.076015**
Mn-Mn-CO	3.5	-3.5	2	-1701.074991
L-2	-3.5	3.5	-2	-1701.075061
	-3.5	-3.5	-3.5097	-1700.276397
	3.5	**3.5**	**2**	**-1716.340367**
CO-Mn-Mn-CO	3.5	-3.5	-2	-1716.262848
L-2	1.5	-1.5	0	-1716.340358

	-1.5	1.5	0	-1715.798728
In the environment full of CO				
	3	3	5.9998	-1626.962264
V-V-2CO	**3**	**-3**	**-0.0001**	**-1626.970263**
t=3.0 ps	-3	3	0.0001	-1626.970263
	-3	-3	-5.9999	-1626.962264
	3	3	4.0001	-1625.468617
t=4.0 ps	**3**	**-3**	**0.0001**	**-1625.665164**
	-3	-3	-5.9998	-1625.662652
t=5.0 ps	3	3	5.9998	-1628.005521
	3	**-3**	**-0.0002**	**-1628.008728**
t=6.0 ps	3	3	5.9997	-1627.687626
	3	**-3**	**-0.0001**	**-1627.695955**
	3	3	6	-1626.007678
t=7.0 ps	**3**	**-3**	**-0.0009**	**-1626.025676**
	-3	-3	-4.0001	-1625.780788
t=8.0 ps	3	3	5.9998	-1626.470227
	3	**-3**	**-0.0001**	**-1626.474790**
t=9.0 ps	3	3	5.9998	-1627.761818
	3	**-3**	**-0.0001**	**-1627.768244**
t=9.5 ps	3	3	5.9998	-1626.846927
	3	**-3**	**-0.0002**	**-1626.855003**
t=10.0 ps	3	3	5.9999	-1627.281730
	3	**-3**	**-0.0004**	**-1627.285193**