Gold coated transition metal anion $[\text{Mn}_{13}@\text{Au}_{20}]^-$ with ultra high magnetic moment

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Supporting information

Table S1. The total energy (E_t), the HOMO-LUMO gap (Δ), the binding energy per atom (BE/atom), the relative energy (ΔE) of the Mn_{13}^- cluster in different spin states (S_z). The boldfaced value highlights the lowest-energy state. The negative HOMO-LUMO gap for some isomers is an artifact of the imposed spin moment.

S_z (μ_B)	E_t (Hartree)	Δ (eV)	BE/atom (eV)	ΔE (eV)
2	-15061.5884536	0.315	2.463	0
4	-15061.5771752	-0.059	2.439	0.307
6	-15061.5727636	0.115	2.430	0.427
8	-15061.5636073	-0.044	2.411	0.676
10	-15061.5386813	-0.028	2.359	1.354
12	-15061.5260212	-0.155	2.332	1.699
14	-15061.5422929	0.200	2.366	1.256
16	-15061.5400542	-0.143	2.362	1.317
18	-15061.5325715	0.075	2.346	1.521
20	-15061.5085743	0.123	2.296	2.174
22	-15061.5368237	0.109	2.355	1.405
24	-15061.5109238	0.347	2.301	2.110
26	-15061.5012523	0.138	2.280	2.373
28	-15061.5015734	-0.057	2.281	2.364
30	-15061.5120549	0.061	2.303	2.079
32	-15061.4779447	0.149	2.232	3.007
34	-15061.4966243	0.226	2.271	2.499
36	-15061.5428100	0.112	2.367	1.242
38	-15061.4966141	0.157	2.213	2.499
40	-15061.5251748	-0.159	2.330	1.722
42	-15061.5024343	0.166	2.283	2.341
44	-15061.5076120	-0.032	2.123	2.200
46	-15061.5222907	0.152	2.324	1.800
48	-15061.5106358	-0.245	2.300	2.117
50	-15061.4956152	0.021	2.176	2.526
52	-15061.4789435	0.088	2.189	2.980
54	-15061.4639186	0.223	2.202	3.389
56	-15061.4752222	0.060	2.226	3.081
58	-15061.4754826	0.081	2.226	3.074
60	-15061.4248943	0.134	2.121	4.451
62	-15061.3789212	0.181	2.024	5.702
64	-15061.3373997	-0.020	1.937	6.831

Table S2. The total energy (E_t), the HOMO-LUMO gap (Δ), the binding energy per atom (BE/atom), the relative energy (ΔE) of the Co_{13}^- cluster in different spin states (S_z). The boldfaced value highlights the lowest-energy states.

S_z (μ_B)	E_t (Hartree)	Δ (eV)	BE/atom (eV)	ΔE (eV)
2	-18064.1490643	0.173	3.379	5.338
4	-18064.1593887	-0.011	3.401	5.058
6	-18064.1630647	-0.075	3.408	4.957
8	-18064.1731025	-0.266	3.429	4.684
10	-18064.1890915	-0.209	3.463	4.249
12	-18064.2011065	0.253	3.488	3.922
14	-18064.2258970	-0.347	3.540	3.248
16	-18064.2346463	0.046	3.558	3.010
18	-18064.2646503	-0.122	3.621	2.193
20	-18064.2938453	-0.032	3.682	1.399
22	-18064.2968241	0.206	3.688	1.318
24	-18064.3032450	0.192	3.702	1.143
26	-18064.3204417	0.150	3.738	0.675
28	-18064.1504496	0.443	3.382	5.301
30	-18064.3452469	0.025	3.790	0
32	-18064.3442200	0.035	3.787	0.028
34	-18064.2722249	-2.526	3.637	1.987
36	-18064.1750822	-1.994	3.433	4.630
38	-18064.0768252	-2.257	3.228	7.304

Table S3. The total energy (E_t), the HOMO-LUMO gap (Δ), the binding energy per atom (BE/atom), the relative energy (ΔE) of the $[\text{Mn}_{13}@\text{Au}_{20}]^-$ cluster in different spin states (S_z). The boldfaced value highlights the lowest-lying states.

S_z (μ_B)	E_t (Hartree)	Δ (eV)	BE/atom (eV)	ΔE (eV)
2	-383022.4468568	0.146	3.225	0.071
4	-383022.4237694	0.040	3.206	0.699
6	-383022.4188119	0.016	3.202	0.834
8	-383022.4072275	-0.084	3.193	1.149
10	-383022.4023458	0.036	3.189	1.282
12	-383022.43536930	0.004	3.216	0.383
14	-383022.4315085	0.071	3.213	0.488
16	-383022.4128619	0.104	3.197	0.996
18	-383022.4208768	0.045	3.204	0.778
20	-383022.4316481	0.009	3.213	0.484
22	-383022.4254339	-0.063	3.208	0.654
24	-383022.4039870	0.117	3.190	1.237
26	-383022.4169887	0.064	3.201	0.883
28	-383022.4200488	0.103	3.203	0.8
30	-383022.3894880	0.064	3.178	1.632
32	-383022.4356843	-0.072	3.216	0.375
34	-383022.4067400	0.097	3.192	1.162
36	-383022.4445555	0.116	3.223	0.133
38	-383022.4327489	-0.061	3.214	0.455
40	-383022.4280841	0.014	3.210	0.581
42	-383022.4427599	-0.053	3.222	0.182
44	-383022.4494518	0.248	3.227	0
46	-383022.4013271	0.213	3.188	1.31
48	-383022.4191853	0.120	3.203	0.824
50	-383022.4272085	0.128	3.209	0.605
52	-383022.4401454	0.112	3.220	0.253
54	-383022.4392740	0.103	3.219	0.277
56	-383022.4085255	0.206	3.194	1.114
58	-383022.3823446	0.292	3.172	1.826
60	-383022.3492700	0.167	3.145	2.726
62	-383022.3197644	0.301	3.121	3.529
64	-383022.3076446	0.395	3.111	3.859

Table S4. The total energy (E_t), the HOMO-LUMO gap (Δ), the binding energy per atom (BE/atom), the relative energy (ΔE) of the $[\text{Co}_{13}@\text{Au}_{20}]^-$ cluster in different spin states (S_z). The boldfaced value highlights the lowest-energy state.

S_z (μ_B)	E_t (Hartree)	Δ (eV)	BE/atom (eV)	ΔE (eV)
2	-386024.9009278	0.019	3.535	4.956
4	-386024.9193596	0.106	3.550	4.454
6	-386024.9119254	-0.331	3.544	4.656
8	-386024.9270641	-0.402	3.557	4.244
10	-386024.9479822	-0.230	3.574	3.675
12	-386024.9645822	-0.584	3.587	3.223
14	-386024.9879713	-0.469	3.607	2.587
16	-386025.0156301	-0.261	3.630	1.834
18	-386025.0473372	-0.346	3.656	0.972
20	-386025.0830398	0.338	3.685	0
22	-386025.0700188	0.338	3.674	0.354
24	-386025.0561343	0.327	3.663	0.732
26	-386025.0484902	0.307	3.657	0.940
28	-386025.0341421	0.291	3.645	1.331
30	-386024.9973158	-0.473	3.614	2.333
32	-386024.9783778	-0.406	3.599	2.848
34	-386024.9383916	-0.199	3.566	3.936
36	-386024.8979161	-0.321	3.532	5.038
38	-386024.8882441	-0.031	3.525	5.301

Complete Reference 3:

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