Stability Trends of Near- and Equiatomic ($n \simeq m$) Co$_n$Mo$_m$ and Mo$_n$Co$_m$ ($n + m = 2 - 15$) Subnanoalloys From DFT and *K*-Means Clustering[†]

Olga Gabriela Santos de Araújo, Amanda Souza Alves, Maíra dos Santos

Costa, and Karla Furtado Andriani[*]

Departament of Exact Sciences, State University of Santa Cruz, P.O. Box 45662-900, Ilhéus, BA,

Brazil

E-mail: kfandriani@uesc.br

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1 Mathematical Background

1.1 Relative Total Energy

A crucial aspect of our investigation involves the use of several energetic properties; however, their mathematical definitions are not explicitly outlined in the main manuscript. Therefore, we provide these definitions here to ensure clarity and completeness. We define the relative total energy (ΔE_{tot}^i) as follows:

$$\Delta E_{\text{tot}}^i = E_{\text{tot}}^i - E_{\text{tot}}^{\text{lowest}}, \tag{1}$$

where E_{tot}^i denotes the total energy of configuration i under consideration, and $E_{\text{tot}}^{\text{lowest}}$ denotes the total energy of the lowest-energy configuration. Accordingly, ΔE_{tot}^i quantifies the relative stability of each configuration and provides a normalized metric that facilitates direct comparison among different isomers.

1.2 Second Order Energy

To evaluate the relative stability of the clusters as a function of size, we calculate the second-order difference in total energy, $\Delta_2 E$, which we define as:

$$\Delta^2 E(N) = E_{\text{tot}}(N-1) + E_{\text{tot}}(N+1) - 2E_{\text{tot}}(N), \tag{2}$$

where $E_{\text{tot}}(N)$ represents the total energy of the lowest-energy isomer of size N. In this

analysis, positive values (peaks) in $\Delta^2 E$ indicate cluster sizes that exhibit enhanced stability relative to their neighbors ($N-1$ and $N+1$).

1.3 Binding Energy

To obtain the binding energy, E_b, we employed the following equation:

$$E_b = \frac{1}{(n+m)}\left(E_{tot}^{Mo_nCo_m} - nE_{tot}^{Mo,free-atom} - mE_{tot}^{Co,free-atom}\right),\qquad(3)$$

where $E_{tot}^{Mo_nCo_m}$ is the total energy of the Mo_nCo_m cluster, while $E_{tot}^{Mo free-atom}$ and $E_{tot}^{Co free-atom}$ are the total energies of the free-atoms Mo and Co, respectively.

1.4 Excess Energy

The excess energy, E_{exc}, is one of the most important parameters to evaluate the relative energetic stability of a given specific binary composition with respect to their parent unary clusters. The E_{exc} is defined as follows,

$$E_{exc} = \frac{1}{(n+m)}\left(E_{tot}^{Mo_nCo_m} - \frac{n}{(n+m)}E_{tot}^{Mo_{(n+m)}} - \frac{m}{(n+m)}E_{tot}^{Co_{(m+n)}}\right),\qquad(4)$$

where $E_{tot}^{Mo_nCo_m}$ is the total energy of the binary Mo_nCo_m cluster. $E_{tot}^{Mo_{(n+m)}}$ and $E_{tot}^{Co_{(m+n)}}$ are the total energies of the $Mo_{(n+m)}$ and $Co_{(m+n)}$ unary clusters, respectively, in their lowest energy configuration. From its definition, $E_{exc} = 0\,\text{meV}$ for $Mo_{(n+m)}$ and $Co_{(m+n)}$ clusters, where a negative value of E_{exc} indicates a favorable energetic mixing, whereas positive values imply that the binary clusters are less stable than their parent unary ones.

1.5 Stabilization Energy

The stabilization energy, E_{stab}, quantifies the tendency to form a specific binary composition relative to its corresponding gas-phase unary clusters.

$$E_{stab} = \frac{1}{(n+m)}\left(E_{tot}^{Mo_nCo_m} - E_{tot}^{Mo_n} - Etot^{Co_m}\right),\qquad(5)$$

where $Etot^{Mo_nCo_m}$ denotes the total energy of the binary $MonCom$ cluster. E_{tot}^{Mon} and $Etot^{Com}$ denote the total energies of the Mon and Co_m unary clusters, respectively, in their lowest-energy configurations.

1.6   Structural Parameters

Following the approach adopted in several previous studies[1,2], we evaluated the most relevant structural properties using the effective coordination concept[3,4]. As a result, we obtained the weighted bond length (d_{av}) and the effective coordination number (ECN^i) for each atom i within the cluster. In this framework, the weighted quantities are calculated using an exponential function to determine the d_{av}^i values, as described below:

$$d_{av}^{i,new} = \frac{\sum_j d_{ij} \exp\left[1 - \left(\frac{d_{ij}}{d_{av}^{i,old}}\right)^6\right]}{\sum_j \exp\left[1 - \left(\frac{d_{ij}}{d_{av}^{i,old}}\right)^6\right]} , \tag{6}$$

where d_{av}^i is determined using a self-consistent procedure.

In our implementation, the initial value of $d_{av}^{i,old}$ is set equal to the shortest distance between atoms i and j. Convergence is achieved when the condition $| d_{av}^{i,new} - d_{av}^{i,old} | < 10^{-4}$ Å is satisfied for every atom i in the molecular system. Convergence typically occurs in fewer than 10 iterations for complex systems with reduced symmetry. Furthermore, once the d_{av}^i values are determined, the ECN^i values are obtained using the following equation:

$$ECN^i = \sum_j \exp\left[1 - \left(\frac{d_{ij}}{d_{av}^i}\right)^6\right] . \tag{7}$$

Thus, the average values of ECN^i and d_{av}^i, hereafter denoted as $ECNav$ and dav, respectively, are obtained as follows:

$$ECNav = \frac{1}{N} \sum i ECNi , \tag{8}$$

and

$$dav = \frac{1}{N} \sum_i d_{av}^i , \tag{9}$$

where N denotes the total number of atoms in the system.

1.7 average chemical order parameter and Number of Chemical Bonds

To characterize the formation of bonds among the A and B atoms, we calculated the average chemical order parameter, σ_{av}, as follows:

$$\sigma_{av} = \frac{N_{Mo-Mo} + N_{Co-Co} - N_{Mo-Co}}{N_{Mo-Mo} + N_{Co-Co} + N_{Mo-Co}} , \tag{10}$$

where N_{Mo-Mo}, N_{Co-Co}, N_{Mo-Co} are the numbers of $Mo-Mo$, $Co-Co$ and $Mo-Co$ bonds, respectively. Therefore, from its definition σ can assume values ranging from -1 to 1. A value of $\sigma \approx -1$ indicates a homogeneous distribution of Mo and Co (mixing), whereas $\sigma \approx 1$ implies the complete segregation of Mo and Co, leading to the formation of homogeneous regions within the $Mo_n Co_m$ alloys.

1.8 Self-Consistency Computational Parameters

Table SI1: Self-consistency computational parameters employed to control the self-consistency process, namely sc_accuracy_etot (total energy), sc_accuracy_rho (electron density), sc_accuracy_eev (sum of the eigenvalues), sc_accuracy_forces (atomic forces) and relax_geometry trm (geometric optimization).

Flags	Values
sc_accuracy_etot	1.0×10^{-6} eV
sc_accuracy_force	1.0×10^{-4} eV $\mathring{A}^{-1}$
sc_accuracy_rho	1.0×10^{-5} e
sc_accuracy_eev	1.0×10^{-3} eV
relax_geometry trm	1.0×10^{-3} eV $\mathring{A}^{-1}$

2   Gas-phase Co$_n$ Clusters

Table SI2: Structural, energetic and electronic properties for Co$_n$ clusters with $n = 2 - 5$, as follows: configuration number (i), relative DFT total energy (ΔE_{tot}^{DFT}, in meV), binding energy (E_b, in eV), total magnetic moment (M_{tot}, in μ_B, HOMO energy (ε_{HOMO}, in eV), LUMO energy (ε_{LUMO}, in eV), HOMO-LUMO energy difference, (E_{gap}, in eV), total number of bonds (N_b), average bond length (d_{av}, in Å), average chemical order parameter (σ_{av}), average effective coordination number (ECN_{av}, NNN), and average radius (R_{av}, in Å).

Co$_n$	i	ΔE_{tot}^{DFT}	E_b	M_{tot}	ε_{HOMO}	ε_{LUMO}	E_{gap}	ECN_{av}	d_{av}	N_b	σ_{av}	R_{av}
Co$_2$	1	0	−1.27	4	−3.75	−3.09	0.66	1	1.96	1	1.00	0.98
Co$_3$	2	0	−1.68	7	−3.65	−3.53	0.11	1	2.11	3	1.00	1.30
Co$_3$	1	0	−1.68	7	−3.65	−3.53	0.12	1	2.11	3	1.00	1.30
Co$_4$	1	68	−2.15	10	−4.19	−3.83	0.35	2	2.15	5	1.00	1.67
Co$_4$	3	68	−2.15	10	−4.19	−3.83	0.35	2	2.15	5	1.00	1.67
Co$_4$	4	68	−2.15	10	−4.19	−3.83	0.35	2	2.15	5	1.00	1.67
Co$_4$	2	0	−2.17	10	−4.16	−3.65	0.51	2	2.14	6	1.00	1.40
Co$_5$	1	1399	−2.19	11	−3.77	−3.54	0.22	1	2.12	5	1.00	1.91
Co$_5$	3	687	−2.33	11	−3.98	−3.53	0.45	2	2.22	7	1.00	2.23
Co$_5$	8	687	−2.33	11	−3.98	−3.53	0.45	2	2.22	7	1.00	2.23
Co$_5$	7	524	−2.36	11	−3.86	−3.32	0.53	2	2.21	8	1.00	2.06
Co$_5$	5	152	−2.44	13	−4.04	−3.90	0.14	3	2.24	8	1.00	1.55
Co$_5$	6	152	−2.44	13	−4.04	−3.90	0.14	3	2.24	8	1.00	1.55
Co$_5$	2	152	−2.44	13	−4.04	−3.90	0.14	3	2.24	8	1.00	1.55
Co$_5$	4	0	−2.47	13	−4.20	−3.71	0.49	2	2.22	9	1.00	1.56

Table SI3: Structural, energetic and electronic properties for Co$_6$ cluster, as follows: configuration number (i), relative DFT total energy (ΔE_{tot}^{DFT}, in meV), binding energy (E_b, in eV), total magnetic moment (M_{tot}, in μ_B, HOMO energy (ε_{HOMO}, in eV), LUMO energy (ε_{LUMO}, in eV), HOMO-LUMO energy difference, (E_{gap}, in eV), total number of bonds (N_b), average bond length (d_{av}, in Å), average chemical order parameter (σ_{av}), average effective coordination number (ECN_{av}, NNN), and average radius (R_{av}, in Å).

i	ΔE_{tot}^{DFT}	E_b	M_{tot}	ε_{HOMO}	ε_{LUMO}	E_{gap}	ECN_{av}	d_{av}	N_b	σ_{av}	R_{av}
4	3223	−2.28	14	−4.07	−3.77	0.30	2	2.21	8	1.00	3.01
5	2218	−2.45	12	−3.93	−3.61	0.32	2	2.22	9	1.00	2.40
1	1783	−2.52	14	−3.72	−3.63	0.08	2	2.21	10	1.00	1.90
6	1626	−2.55	12	−3.48	−3.15	0.33	3	2.23	10	1.00	1.95
2	1102	−2.64	14	−3.95	−3.58	0.36	2	2.21	9.	1.00	1.72
0	1045	−2.65	14	−3.81	−3.57	0.23	3	2.24	11	1.00	1.89
9	1	−2.82	14	−3.98	−3.45	0.53	4	2.27	12	1.00	1.60
7	0	−2.82	14	−3.98	−3.45	0.53	4	2.27	12	1.00	1.60
3	0	−2.82	14	−3.98	−3.45	0.53	4	2.27	12	1.00	1.60

Table SI4: Structural, energetic and electronic properties for Co_7 cluster, as follows: configuration number (i), relative DFT total energy (ΔE_{tot}^{DFT}, in meV), binding energy (E_b, in eV), total magnetic moment (M_{tot}, in μ_B, HOMO energy (ε_{HOMO}, in eV), LUMO energy (ε_{LUMO}, in eV), HOMO-LUMO energy difference, (E_{gap}, in eV), total number of bonds (N_b), average bond length (d_{av}, in Å), average chemical order parameter (σ_{av}), average effective coordination number (ECN_{av}, NNN), and average radius (R_{av}, in Å).

i	ΔE_{tot}^{DFT}	E_b	M_{tot}	ε_{HOMO}	ε_{LUMO}	E_{gap}	ECN_{av}	d_{av}	N_b	σ_{av}	R_{av}
5	2620	−2.50	15	−3.88	−3.73	0.15	3	2.23	11	1.00	2.98
11	1103	−2.72	15	−3.86	−3.58	0.27	3	2.24	12	1.00	2.31
7	891	−2.75	15	−3.75	−3.42	0.33	3	2.27	14	1.00	2.30
3	890	−2.75	15	−3.75	−3.42	0.33	3	2.27	14	1.00	2.30
14	890	−2.75	15	−3.75	−3.42	0.33	3	2.27	14	1.00	2.30
2	800	−2.76	15	−3.66	−3.39	0.27	3	2.24	13	1.00	2.09
8	659	−2.78	15	−3.67	−3.47	0.19	4	2.30	15	1.00	2.29
10	461	−2.81	15	−3.64	−3.64	0.00	4	2.29	15	1.00	2.01
9	377	−2.82	15	−3.64	−3.33	0.30	3	2.24	13	1.00	1.93
12	327	−2.83	15	−3.61	−3.41	0.19	3	2.23	13	1.00	1.78
1	238	−2.84	15	−3.62	−3.39	0.23	3	2.25	13	1.00	1.95
13	224	−2.84	15	−3.73	−3.49	0.24	4	2.30	16	1.00	1.95
4	184	−2.85	15	−3.61	−3.37	0.23	3	2.27	15	1.00	2.06
16	184	−2.85	15	−3.61	−3.37	0.23	3	2.27	15	1.00	2.06
6	145	−2.85	15	−3.59	−3.40	0.18	4	2.29	16	1.00	1.89
15	0	−2.88	15	−3.72	−3.38	0.33	4	2.29	15	1.00	2.21

Table SI5: Structural, energetic and electronic properties for Co$_8$ cluster, as follows: configuration number (i), relative DFT total energy (ΔE_{tot}^{DFT}, in meV), binding energy (E_b, in eV), total magnetic moment (M_{tot}, in μ_B, HOMO energy (ε_{HOMO}, in eV), LUMO energy (ε_{LUMO}, in eV), HOMO-LUMO energy difference, (E_{gap}, in eV), total number of bonds (N_b), average bond length (d_{av}, in Å), average chemical order parameter (σ_{av}), average effective coordination number (ECN_{av}, NNN), and average radius (R_{av}, in Å).

i	ΔE_{tot}^{DFT}	E_b	M_{tot}	ε_{HOMO}	ε_{LUMO}	E_{gap}	ECN_{av}	d_{av}	N_b	σ_{av}	R_{av}
15	3018	−2.61	16	−3.86	−3.65	0.20	3	2.22	13	1.00	2.88
3	1404	−2.81	16	−3.70	−3.40	0.29	3	2.27	16	1.00	2.51
11	1401	−2.81	16	−3.70	−3.40	0.29	3	2.27	16	1.00	2.52
2	956	−2.86	16	−3.53	−3.31	0.21	4	2.30	18	1.00	2.41
5	894	−2.87	16	−3.53	−3.28	0.25	3	2.22	14	1.00	2.17
4	868	−2.87	16	−3.61	−3.20	0.41	3	2.20	18	1.00	1.98
14	759	−2.89	16	−3.68	−3.39	0.29	4	2.28	19	1.00	2.36
6	681	−2.90	18	−3.88	−3.67	0.20	4	2.32	18	1.00	2.81
18	672	−2.90	16	−3.68	−3.37	0.31	4	2.30	18	1.00	2.41
8	670	−2.90	16	−3.68	−3.37	0.31	4	2.30	18	1.00	2.41
19	452	−2.93	16	−3.56	−3.35	0.20	4	2.30	18	1.00	2.43
17	423	−2.93	16	−3.57	−3.34	0.23	4	2.32	19	1.00	2.39
16	370	−2.94	16	−3.66	−3.48	0.17	4	2.29	18	1.00	2.12
13	335	−2.94	16	−3.60	−3.30	0.29	4	2.30	18	1.00	2.17
10	156	−2.96	16	−3.62	−3.23	0.39	4	2.30	19	1.00	2.17
1	100	−2.97	16	−3.56	−3.19	0.36	4	2.28	17	1.00	2.12
9	100	−2.97	16	−3.56	−3.19	0.36	4	2.28	17	1.00	2.12
7	0	−2.98	16	−3.56	−3.25	0.30	4	2.30	20	1.00	2.10
12	0	−2.98	16	−3.56	−3.26	0.30	4	2.30	20	1.00	2.10

Table SI6: Structural, energetic and electronic properties for Co_9 cluster, as follows: configuration number (i), relative DFT total energy (ΔE_{tot}^{DFT}, in meV), binding energy (E_b, in eV), total magnetic moment (M_{tot}, in μ_B, HOMO energy (ε_{HOMO}, in eV), LUMO energy (ε_{LUMO}, in eV), HOMO-LUMO energy difference, (E_{gap}, in eV), total number of bonds (N_b), average bond length (d_{av}, in Å), average chemical order parameter (σ_{av}), average effective coordination number (ECN_{av}, NNN), and average radius (R_{av}, in Å).

i	ΔE_{tot}^{DFT}	E_b	M_{tot}	ε_{HOMO}	ε_{LUMO}	E_{gap}	ECN_{av}	d_{av}	N_b	σ_{av}	R_{av}
16	3179	−2.70	19	−3.90	−3.59	0.31	3	2.25	16	1.00	3.03
13	1281	−2.91	19	−3.79	−3.54	0.24	4	2.31	21	1.00	3.01
2	1208	−2.92	19	−3.73	−3.48	0.24	4	2.29	21	1.00	3.03
7	1057	−2.94	17	−3.42	−3.20	0.22	4	2.30	21	1.00	2.52
6	687	−2.98	19	−3.76	−3.54	0.22	4	2.32	22	1.00	2.93
20	652	−2.98	19	−3.80	−3.53	0.26	4	2.32	22	1.00	2.86
21	651	−2.98	19	−3.80	−3.53	0.26	4	2.32	22	1.00	2.86
10	626	−2.99	17	−3.42	−3.24	0.18	4	2.32	22	1.00	2.44
4	610	−2.99	19	−3.78	−3.54	0.23	4	2.32	22	1.00	2.92
15	586	−2.99	17	−3.58	−3.35	0.22	4	2.30	21	1.00	2.47
5	520	−3.00	17	−3.42	−3.23	0.18	4	2.29	20	1.00	2.37
14	506	−3.00	17	−3.55	−3.30	0.25	4	2.32	22	1.00	2.47
17	445	−3.01	17	−3.47	−3.20	0.26	4	2.30	21	1.00	2.26
9	435	−3.01	17	−3.42	−3.20	0.22	5	2.33	23	1.00	2.32
11	430	−3.01	19	−3.71	−3.46	0.24	4	2.31	22	1.00	2.78
8	395	−3.01	19	−3.74	−3.53	0.20	4	2.31	23	1.00	2.87
19	342	−3.02	17	−3.66	−3.39	0.26	4	2.31	22	1.00	2.40
1	301	−3.02	17	−3.45	−3.24	0.20	4	2.30	23	1.00	2.38
12	299	−3.02	17	−3.45	−3.24	0.20	4	2.30	23	1.00	2.38
3	0	−3.06	17	−3.48	−3.31	0.17	4	2.30	21	1.00	2.21
18	0	−3.06	17	−3.48	−3.31	0.17	4	2.30	21	1.00	2.21

Table SI7: Structural, energetic and electronic properties for Co_{10} cluster, as follows: configuration number (i), relative DFT total energy (ΔE_{tot}^{DFT}, in meV), binding energy (E_b, in eV), total magnetic moment (M_{tot}, in μ_B, HOMO energy (ε_{HOMO}, in eV), LUMO energy (ε_{LUMO}, in eV), HOMO-LUMO energy difference, (E_{gap}, in eV), total number of bonds (N_b), average bond length (d_{av}, in Å), average chemical order parameter (σ_{av}), average effective coordination number (ECN_{av}, NNN), and average radius (R_{av}, in Å).

i	ΔE_{tot}^{DFT}	E_b	M_{tot}	ε_{HOMO}	ε_{LUMO}	E_{gap}	ECN_{av}	d_{av}	N_b	σ_{av}	R_{av}
14	784	−3.04	18	−3.41	−3.20	0.20	5	2.33	26	1.00	2.51
20	757	−3.05	20	−3.66	−3.44	0.22	4	2.32	25	1.00	2.84
17	755	−3.05	20	−3.66	−3.43	0.23	4	2.31	24	1.00	3.14
25	734	−3.05	18	−3.59	−3.33	0.25	4	2.31	24	1.00	2.57
10	723	−3.05	20	−3.64	−3.42	0.21	4	2.32	26	1.00	3.12
16	721	−3.05	20	−3.64	−3.42	0.21	4	2.32	26	1.00	3.11
15	721	−3.05	20	−3.65	−3.45	0.20	4	2.32	26	1.00	2.82
26	668	−3.06	20	−3.49	−3.41	0.08	4	2.31	26	1.00	2.42
18	587	−3.06	20	−3.60	−3.44	0.15	5	2.33	26	1.00	2.98
21	553	−3.07	18	−3.41	−3.19	0.22	5	2.34	27	1.00	2.37
22	546	−3.07	20	−3.70	−3.50	0.19	5	2.33	26	1.00	2.90
24	545	−3.07	20	−3.70	−3.50	0.19	5	2.33	26	1.00	2.90
11	544	−3.07	20	−3.63	−3.46	0.16	4	2.31	26	1.00	2.96
2	542	−3.07	20	−3.49	−3.41	0.07	4	2.32	25	1.00	2.41
19	517	−3.07	22	−3.90	−3.72	0.17	4	2.31	25	1.00	2.76
5	485	−3.07	18	−3.42	−3.26	0.15	4	2.31	27	1.00	2.43
03	458	−3.08	18	−3.45	−3.16	0.29	5	2.33	26	1.00	2.48
9	415	−3.08	18	−3.46	−3.23	0.23	4	2.31	25	1.00	2.34
12	414	−3.08	20	−3.65	−3.50	0.14	4	2.31	24	1.00	2.79
1	380	−3.09	20	−3.57	−3.44	0.13	4	2.32	26	1.00	2.69
6	379	−3.09	20	−3.62	−3.49	0.13	4	2.31	24	1.00	2.74
23	287	−3.09	20	−3.72	−3.40	0.31	4	2.31	24	1.00	2.87
8	243	−3.10	20	−3.73	−3.45	0.28	5	2.33	26	1.00	2.82
7	238	−3.10	18	−3.44	−3.23	0.21	4	2.31	24	1.00	2.40
4	0	−3.12	20	−3.67	−3.46	0.20	4	2.31	25	1.00	2.63

Table SI8: Structural, energetic and electronic properties for Co_{11} cluster, as follows: configuration number (i), relative DFT total energy (ΔE_{tot}^{DFT}, in meV), binding energy (E_b, in eV), total magnetic moment (M_{tot}, in μ_B, HOMO energy (ε_{HOMO}, in eV), LUMO energy (ε_{LUMO}, in eV), HOMO-LUMO energy difference, (E_{gap}, in eV), total number of bonds (N_b), average bond length (d_{av}, in Å), average chemical order parameter (σ_{av}), average effective coordination number (ECN_{av}, NNN), and average radius (R_{av}, in Å).

i	ΔE_{tot}^{DFT}	E_b	M_{tot}	ε_{HOMO}	ε_{LUMO}	E_{gap}	ECN_{av}	d_{av}	N_b	σ_{av}	R_{av}
25	949	−3.07	23	−3.84	−3.63	0.20	4	2.32	28	1.00	3.18
19	899	−3.08	23	−3.77	−3.58	0.19	4	2.32	28	1.00	3.04
22	870	−3.08	21	−3.51	−3.36	0.14	5	2.33	29	1.00	2.54
16	867	−3.08	21	−3.51	−3.36	0.15	5	2.33	29	1.00	2.54
12	747	−3.09	21	−3.64	−3.41	0.23	4	2.31	28	1.00	3.34
13	552	−3.11	23	−3.85	−3.68	0.17	4	2.32	29	1.00	3.21
20	467	−3.12	23	−3.74	−3.63	0.10	5	2.33	29	1.00	2.89
14	463	−3.12	21	−3.63	−3.49	0.13	4	2.32	28	1.00	2.81
21	431	−3.12	23	−3.67	−3.55	0.12	5	2.36	31	1.00	2.49
6	395	−3.12	21	−3.61	−3.38	0.23	5	2.32	28	1.00	2.97
17	387	−3.12	19	−3.31	−3.08	0.22	5	2.34	30	1.00	2.45
30	368	−3.12	21	−3.58	−3.41	0.17	4	2.31	27	1.00	2.88
36	367	−3.12	21	−3.70	−3.48	0.21	4	2.31	29	1.00	2.90
4	353	−3.13	23	−3.80	−3.60	0.19	4	2.33	30	1.00	3.08
34	349	−3.13	21	−3.60	−3.46	0.13	5	2.32	29	1.00	3.07
10	334	−3.13	23	−3.81	−3.68	0.13	4	2.32	27	1.00	2.89
24	331	−3.13	19	−3.42	−3.21	0.21	4	2.31	31	1.00	2.40
9	322	−3.13	21	−3.61	−3.45	0.16	4	2.32	27	1.00	3.12
31	318	−3.13	21	−3.61	−3.45	0.16	4	2.32	27	1.00	3.12
3	317	−3.13	23	−3.74	−3.52	0.22	4	2.32	27	1.00	3.18
2	282	−3.13	23	−3.78	−3.55	0.23	4	2.32	27	1.00	3.02
33	270	−3.13	21	−3.57	−3.44	0.13	5	2.34	30	1.00	2.92
35	248	−3.14	21	−3.62	−3.39	0.22	5	2.34	30	1.00	3.03
23	246	−3.14	21	−3.62	−3.39	0.22	5	2.34	30	1.00	3.03
32	190	−3.14	23	−3.91	−3.64	0.27	4	2.32	30	1.00	2.86
1	190	−3.14	23	−3.70	−3.59	0.11	5	2.33	30	1.00	2.74
27	190	−3.14	23	−3.71	−3.59	0.11	5	2.33	30	1.00	2.74
15	190	−3.14	23	−3.70	−3.59	0.11	5	2.33	31	1.00	2.74
11	158	−3.14	21	−3.61	−3.47	0.14	5	2.32	28	1.00	2.73
18	143	−3.15	23	−3.83	−3.61	0.21	5	2.35	30	1.00	2.94
5	131	−3.15	21	−3.61	−3.38	0.22	5	2.33	30	1.00	2.76
7	72	−3.15	23	−3.82	−3.65	0.17	5	2.33	28	1.00	2.93
28	26	−3.16	23	−3.66	−3.56	0.09	5	2.32	29	1.00	2.70
8	22	−3.16	19	−3.43	−3.21	0.21	5	2.32	29	1.00	2.45
29	16	−3.16	23	−3.89	−3.66	0.22	5	2.33	30	1.00	3.02
26	0	−3.16	23	−3.81	−3.58	0.22	5	2.33	29	1.00	3.06

Table SI9: Structural, energetic and electronic properties for Co_{12} cluster, as follows: configuration number (i), relative DFT total energy (ΔE_{tot}^{DFT}, in meV), binding energy (E_b, in eV), total magnetic moment (M_{tot}, in μ_B, HOMO energy (ε_{HOMO}, in eV), LUMO energy (ε_{LUMO}, in eV), HOMO-LUMO energy difference, (E_{gap}, in eV), total number of bonds (N_b), average bond length (d_{av}, in Å), average chemical order parameter (σ_{av}), average effective coordination number (ECN_{av}, NNN), and average radius (R_{av}, in Å).

i	ΔE_{tot}^{DFT}	E_b	M_{tot}	ε_{HOMO}	ε_{LUMO}	E_{gap}	ECN_{av}	d_{av}	N_b	σ_{av}	R_{av}
11	1424	−3.11	30	−4.02	−3.90	0.12	5	2.36	30	1.00	2.25
30	844	−3.16	24	−3.84	−3.58	0.25	4	2.30	30	1.00	2.80
24	831	−3.16	24	−3.80	−3.58	0.22	4	2.32	30	1.00	2.98
29	780	−3.16	24	−3.78	−3.60	0.17	5	2.33	33	1.00	3.23
26	760	−3.16	24	−3.74	−3.56	0.17	4	2.32	30	1.00	3.14
22	754	−3.16	24	−3.77	−3.54	0.22	5	2.33	33	1.00	3.50
1	708	−3.17	24	−3.79	−3.54	0.24	5	2.32	32	1.00	3.36
18	692	−3.17	24	−3.74	−3.55	0.18	5	2.33	32	1.00	3.22
9	573	−3.18	24	−3.69	−3.49	0.19	5	2.35	34	1.00	3.19
4	565	−3.18	24	−3.76	−3.53	0.23	5	2.32	32	1.00	3.12
17	557	−3.18	24	−3.71	−3.49	0.22	5	2.32	32	1.00	2.97
3	537	−3.18	26	−3.79	−3.66	0.13	4	2.33	30	1.00	2.57
8	500	−3.19	24	−3.60	−3.41	0.18	5	2.38	36	1.00	2.39
12	499	−3.19	24	−3.71	−3.57	0.14	5	2.33	33	1.00	3.17
16	448	−3.19	24	−3.69	−3.45	0.24	4	2.32	32	1.00	3.08
23	377	−3.20	22	−3.51	−3.30	0.20	5	2.35	34	1.00	2.84
14	376	−3.20	24	−3.72	−3.52	0.19	5	2.34	33	1.00	3.06
28	357	−3.20	24	−3.80	−3.47	0.33	5	2.34	33	1.00	3.01
25	357	−3.20	24	−3.80	−3.47	0.33	5	2.34	33	1.00	3.01
31	345	−3.20	22	−3.55	−3.35	0.20	5	2.30	31	1.00	2.69
21	328	−3.20	24	−3.70	−3.47	0.22	5	2.33	31	1.00	3.27
2	271	−3.20	24	−3.68	−3.58	0.10	5	2.32	33	1.00	3.17
10	256	−3.21	24	−3.66	−3.46	0.19	5	2.33	35	1.00	2.68
27	251	−3.21	24	−3.79	−3.54	0.24	5	2.33	34	1.00	3.08
5	251	−3.21	24	−3.79	−3.54	0.24	5	2.33	33	1.00	3.08
6	203	−3.21	24	−3.70	−3.56	0.14	5	2.35	34	1.00	2.99
13	198	−3.21	24	−3.72	−3.52	0.20	5	2.36	34	1.00	2.82
19	156	−3.21	24	−3.65	−3.52	0.12	5	2.34	35	1.00	2.88
7	147	−3.21	24	−3.69	−3.49	0.19	5	2.34	35	1.00	2.99
15	110	−3.22	24	−3.73	−3.60	0.12	5	2.32	31	1.00	3.07
20	0	−3.23	24	−3.69	−3.49	0.20	5	2.33	33	1.00	2.76

Table SI10: Structural, energetic and electronic properties for Co_{13} cluster, as follows: configuration number (i), relative DFT total energy (ΔE_{tot}^{DFT}, in meV), binding energy (E_b, in eV), total magnetic moment (M_{tot}, in μ_B, HOMO energy (ε_{HOMO}, in eV), LUMO energy (ε_{LUMO}, in eV), HOMO-LUMO energy difference, (E_{gap}, in eV), total number of bonds (N_b), average bond length (d_{av}, in Å), average chemical order parameter (σ_{av}), average effective coordination number (ECN_{av}, NNN), and average radius (R_{av}, in Å).

i	ΔE_{tot}^{DFT}	E_b	M_{tot}	ε_{HOMO}	ε_{LUMO}	E_{gap}	ECN_{av}	d_{av}	N_b	σ_{av}	R_{av}
40	1548	−3.21	25	−3.72	−3.50	0.21	4	2.32	33	1.00	3.18
19	1547	−3.21	25	−3.66	−3.51	0.15	5	2.33	35	1.00	3.45
37	1488	−3.21	25	−3.79	−3.59	0.19	5	2.32	35	1.00	3.23
23	1403	−3.22	27	−3.91	−3.72	0.19	4	2.32	33	1.00	3.25
11	1352	−3.22	25	−3.64	−3.48	0.15	5	2.32	34	1.00	3.52
6	1285	−3.23	27	−3.92	−3.73	0.18	4	2.32	33	1.00	3.13
22	1252	−3.23	25	−3.66	−3.45	0.20	5	2.32	36	1.00	3.25
9	1247	−3.23	25	−3.63	−3.49	0.14	5	2.32	34	1.00	3.20
32	1222	−3.23	25	−3.63	−3.48	0.15	5	2.35	37	1.00	3.16
36	1219	−3.23	25	−3.53	−3.40	0.13	5	2.36	39	1.00	3.20
39	1217	−3.23	25	−3.70	−3.53	0.16	5	2.33	37	1.00	3.24
29	1193	−3.23	25	−3.67	−3.50	0.16	5	2.33	37	1.00	3.11
1	1162	−3.24	25	−3.59	−3.47	0.12	5	2.33	37	1.00	3.44
35	1154	−3.24	25	−3.66	−3.51	0.15	5	2.35	37	1.00	3.05
34	1045	−3.24	25	−3.62	−3.41	0.21	5	2.36	39	1.00	3.11
27	1030	−3.25	25	−3.65	−3.46	0.19	5	2.35	37	1.00	3.50
7	998	−3.25	25	−3.71	−3.52	0.18	5	2.33	34	1.00	3.20
26	991	−3.25	25	−3.62	−3.48	0.13	5	2.35	38	1.00	3.16
14	987	−3.25	27	−3.87	−3.68	0.18	5	2.32	33	1.00	3.19
20	985	−3.25	25	−3.72	−3.52	0.20	5	2.33	37	1.00	3.35
24	936	−3.25	25	−3.73	−3.52	0.21	5	2.33	36	1.00	3.08
15	899	−3.26	27	−3.76	−3.62	0.13	5	2.34	37	1.00	3.15
38	875	−3.26	25	−3.74	−3.42	0.31	5	2.33	36	1.00	2.84
8	860	−3.26	27	−3.83	−3.64	0.19	5	2.33	37	1.00	3.12
2	840	−3.26	25	−3.62	−3.50	0.12	5	2.35	38	1.00	3.00
28	791	−3.26	25	−3.67	−3.52	0.15	5	2.33	36	1.00	3.26
31	782	−3.26	27	−3.86	−3.68	0.17	5	2.34	38	1.00	3.12
18	772	−3.27	27	−3.78	−3.70	0.08	5	2.36	38	1.00	2.96
5	763	−3.27	25	−3.62	−3.50	0.12	5	2.35	36	1.00	2.97
13	740	−3.27	27	−3.80	−3.65	0.15	5	2.34	38	1.00	2.76
3	738	−3.27	27	−3.90	−3.63	0.27	5	2.35	36	1.00	2.63
10	717	−3.27	25	−3.61	−3.45	0.16	5	2.36	38	1.00	3.00
30	701	−3.27	25	−3.66	−3.52	0.13	5	2.33	37	1.00	3.21
12	661	−3.27	27	−3.78	−3.59	0.18	5	2.34	39	1.00	2.97
16	661	−3.27	27	−3.78	−3.59	0.18	5	2.34	39	1.00	2.97
21	586	−3.28	25	−3.60	−3.43	0.17	5	2.35	38	1.00	3.03
33	585	−3.28	27	−3.78	−3.65	0.13	5	2.34	39	1.00	3.15
4	585	−3.28	27	−3.79	−3.65	0.13	5	2.34	39	1.00	3.15
25	584	−3.28	27	−3.79	−3.65	0.13	5	2.34	39	1.00	3.16
17	0	−3.33	27	−3.89	−3.57	0.31	5	2.33	36	1.00	2.76

Table SI11: Structural, energetic and electronic properties for Co_{14} cluster, as follows: configuration number (i), relative DFT total energy (ΔE_{tot}^{DFT}, in meV), binding energy (E_b, in eV), total magnetic moment (M_{tot}, in μ_B, HOMO energy (ε_{HOMO}, in eV), LUMO energy (ε_{LUMO}, in eV), HOMO-LUMO energy difference, (E_{gap}, in eV), total number of bonds (N_b), average bond length (d_{av}, in Å), average chemical order parameter (σ_{av}), average effective coordination number (ECN_{av}, NNN), and average radius (R_{av}, in Å).

i	ΔE_{tot}^{DFT}	E_b	M_{tot}	ε_{HOMO}	ε_{LUMO}	E_{gap}	ECN_{av}	d_{av}	N_b	σ_{av}	R_{av}
29	1266	−3.26	28	−3.73	−3.62	0.11	5	2.33	38	1.00	3.40
1	1171	−3.27	28	−3.69	−3.52	0.17	5	2.33	38	1.00	3.35
18	1158	−3.27	28	−3.69	−3.54	0.14	5	2.34	39	1.00	3.45
32	957	−3.28	28	−3.69	−3.52	0.17	5	2.33	40	1.00	3.24
23	954	−3.28	28	−3.65	−3.49	0.15	5	2.34	38	1.00	3.42
5	939	−3.28	28	−3.85	−3.69	0.16	5	2.33	37	1.00	3.26
25	887	−3.29	28	−3.86	−3.67	0.18	5	2.33	37	1.00	3.28
21	805	−3.29	28	−3.86	−3.71	0.15	5	2.34	41	1.00	3.28
03	797	−3.29	28	−3.76	−3.54	0.21	5	2.35	41	1.00	2.82
17	795	−3.29	28	−3.75	−3.63	0.12	5	2.36	41	1.00	3.58
15	677	−3.30	30	−3.79	−3.69	0.09	6	2.40	45	1.00	3.13
20	667	−3.30	28	−3.73	−3.59	0.13	5	2.33	38	1.00	3.40
4	649	−3.30	28	−3.79	−3.66	0.13	5	2.35	39	1.00	3.31
7	638	−3.31	28	−3.63	−3.50	0.13	5	2.37	43	1.00	3.14
27	606	−3.31	28	−3.72	−3.59	0.12	5	2.34	43	1.00	2.59
33	570	−3.31	28	−3.79	−3.67	0.11	5	2.34	38	1.00	3.20
35	545	−3.31	28	−3.72	−3.55	0.17	5	2.35	41	1.00	3.06
19	514	−3.31	28	−3.74	−3.55	0.18	5	2.34	42	1.00	3.19
24	480	−3.32	27	−3.62	−3.62	0.00	5	2.36	42	1.00	3.04
30	460	−3.32	28	−3.74	−3.61	0.13	5	2.36	42	1.00	3.05
14	449	−3.32	28	−3.75	−3.61	0.13	5	2.34	43	1.00	3.22
31	448	−3.32	28	−3.75	−3.61	0.13	5	2.34	43	1.00	3.22
28	382	−3.32	26	−3.59	−3.42	0.17	5	2.36	42	1.00	3.43
9	370	−3.32	30	−3.90	−3.72	0.17	5	2.34	39	1.00	2.81
6	350	−3.33	28	−3.74	−3.60	0.13	5	2.34	40	1.00	3.29
13	324	−3.33	28	−3.74	−3.55	0.19	5	2.34	40	1.00	2.77
12	316	−3.33	28	−3.75	−3.62	0.12	5	2.34	39	1.00	3.10
16	316	−3.33	28	−3.78	−3.59	0.18	5	2.36	42	1.00	2.97
2	287	−3.33	28	−3.74	−3.58	0.15	5	2.34	39	1.00	3.48
22	248	−3.33	28	−3.78	−3.65	0.12	5	2.35	41	1.00	3.11
34	232	−3.33	26	−3.58	−3.37	0.20	5	2.36	42	1.00	3.07
26	205	−3.34	28	−3.84	−3.68	0.16	5	2.34	41	1.00	3.08
8	185	−3.34	28	−3.77	−3.65	0.12	5	2.36	42	1.00	3.07
11	120	−3.34	28	−3.76	−3.60	0.16	5	2.33	39	1.00	2.95
10	0	−3.35	28	−3.71	−3.56	0.15	5	2.33	39	1.00	3.22

*Co_{14} configuration 24 was excluded from the set.

Table SI12: Structural, energetic and electronic properties for Co_{15} cluster, as follows: configuration number (i), relative DFT total energy (ΔE_{tot}^{DFT}, in meV), binding energy (E_b, in eV), total magnetic moment (M_{tot}, in μ_B, HOMO energy (ε_{HOMO}, in eV), LUMO energy (ε_{LUMO}, in eV), HOMO-LUMO energy difference, (E_{gap}, in eV), total number of bonds (N_b), average bond length (d_{av}, in Å), average chemical order parameter (σ_{av}), average effective coordination number (ECN_{av}, NNN), and average radius (R_{av}, in Å).

i	ΔE_{tot}^{DFT}	E_b	M_{tot}	ε_{HOMO}	ε_{LUMO}	E_{gap}	ECN_{av}	d_{av}	N_b	σ_{av}	R_{av}
12	2011	−3.26	29	−3.71	−3.55	0.16	5	2.32	42	1.00	3.71
28	1899	−3.27	31	−3.87	−3.72	0.14	5	2.34	43	1.00	3.66
13	1597	−3.29	29	−3.73	−3.58	0.15	5	2.34	42	1.00	3.83
37	1465	−3.30	29	−3.72	−3.55	0.17	5	2.36	45	1.00	3.84
36	1373	−3.31	29	−3.60	−3.48	0.11	5	2.34	44	1.00	3.57
27	1271	−3.31	31	−3.90	−3.73	0.16	5	2.34	44	1.00	3.43
32	1244	−3.31	29	−3.69	−3.56	0.13	5	2.34	44	1.00	3.13
11	929	−3.34	29	−3.69	−3.54	0.14	5	2.36	45	1.00	3.53
22	918	−3.34	31	−3.85	−3.75	0.09	5	2.35	43	1.00	3.36
30	908	−3.34	31	−3.85	−3.73	0.11	5	2.35	43	1.00	3.35
26	875	−3.34	33	−3.97	−3.90	0.07	5	2.34	44	1.00	3.43
31	833	−3.34	29	−3.69	−3.56	0.13	5	2.34	45	1.00	3.32
38	788	−3.34	29	−3.68	−3.56	0.11	6	2.39	48	1.00	3.49
16	700	−3.35	29	−3.71	−3.56	0.14	5	2.34	42	1.00	3.38
1	629	−3.36	29	−3.75	−3.62	0.12	5	2.34	45	1.00	3.32
40	599	−3.36	33	−3.95	−3.81	0.14	5	2.36	46	1.00	2.98
6	574	−3.36	29	−3.68	−3.50	0.18	5	2.34	43	1.00	3.29
21	510	−3.36	31	−3.82	−3.64	0.18	5	2.36	45	1.00	3.02
25	476	−3.37	31	−3.79	−3.75	0.04	5	2.36	46	1.00	3.12
7	468	−3.37	29	−3.73	−3.62	0.11	5	2.35	43	1.00	3.23
23	454	−3.37	29	−3.73	−3.58	0.14	5	2.34	42	1.00	3.39
24	454	−3.37	31	−3.86	−3.73	0.12	5	2.35	42	1.00	3.21
39	452	−3.37	29	−3.64	−3.51	0.13	6	2.39	49	1.00	3.08
33	443	−3.37	33	−3.93	−3.74	0.18	5	2.38	48	1.00	3.05
10	415	−3.37	31	−3.86	−3.69	0.16	5	2.37	47	1.00	2.97
18	408	−3.37	29	−3.84	−3.65	0.18	5	2.34	41	1.00	3.29
34	387	−3.37	29	−3.64	−3.47	0.16	5	2.36	46	1.00	3.17
35	367	−3.37	31	−3.88	−3.72	0.15	5	2.35	48	1.00	3.09
17	354	−3.37	29	−3.74	−3.61	0.13	5	2.34	45	1.00	3.17
19	348	−3.37	31	−3.79	−3.66	0.12	5	2.36	47	1.00	2.83
4	320	−3.38	33	−3.93	−3.75	0.18	5	2.37	48	1.00	2.98
3	319	−3.38	33	−3.93	−3.75	0.18	5	2.37	49	1.00	2.97
09	315	−3.38	31	−3.87	−3.74	0.12	5	2.36	44	1.00	2.90
20	310	−3.38	27	−3.50	−3.38	0.12	5	2.36	46	1.00	3.45
14	306	−3.38	29	−3.66	−3.52	0.14	5	2.34	43	1.00	3.25
5	200	−3.38	31	−3.81	−3.71	0.09	5	2.35	43	1.00	3.06
2	172	−3.39	29	−3.73	−3.58	0.14	5	2.35	44	1.00	3.24
29	113	−3.39	29	−3.72	−3.53	0.18	5	2.36	46	1.00	3.08
8	0	−3.40	29	−3.68	−3.55	0.13	5	2.34	43	1.00	3.21

Table SI13: Lowest energy configurations for Co_n clusters with $n = 2 - 15$.

Co_2

Co_3

Co_4

Co_5

Co_6

Co_7

Co_8

Co_9

Co_{10}

Co_{11}

Co_{12}

Co_{13}

Co_{14}

Co_{15}
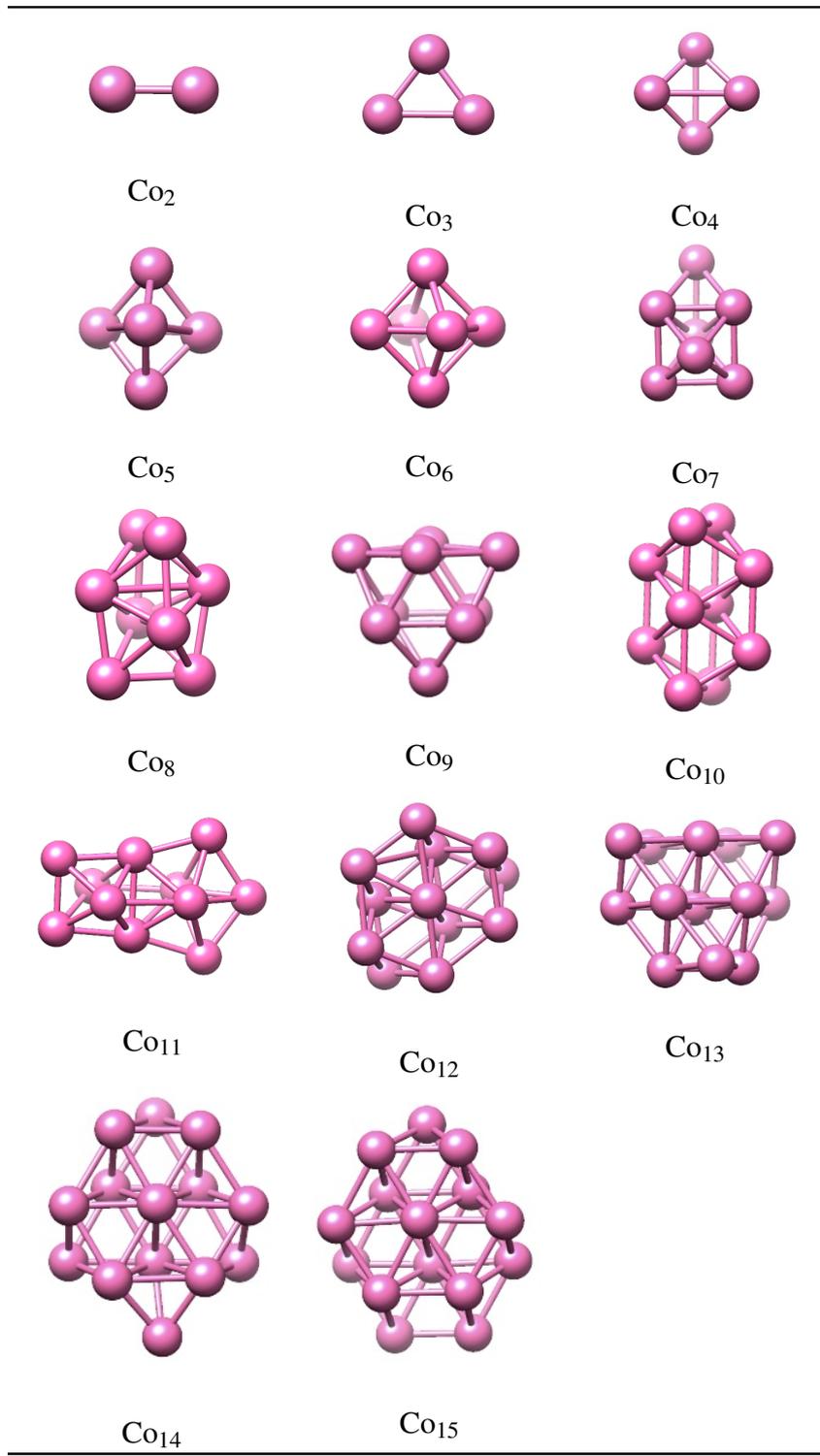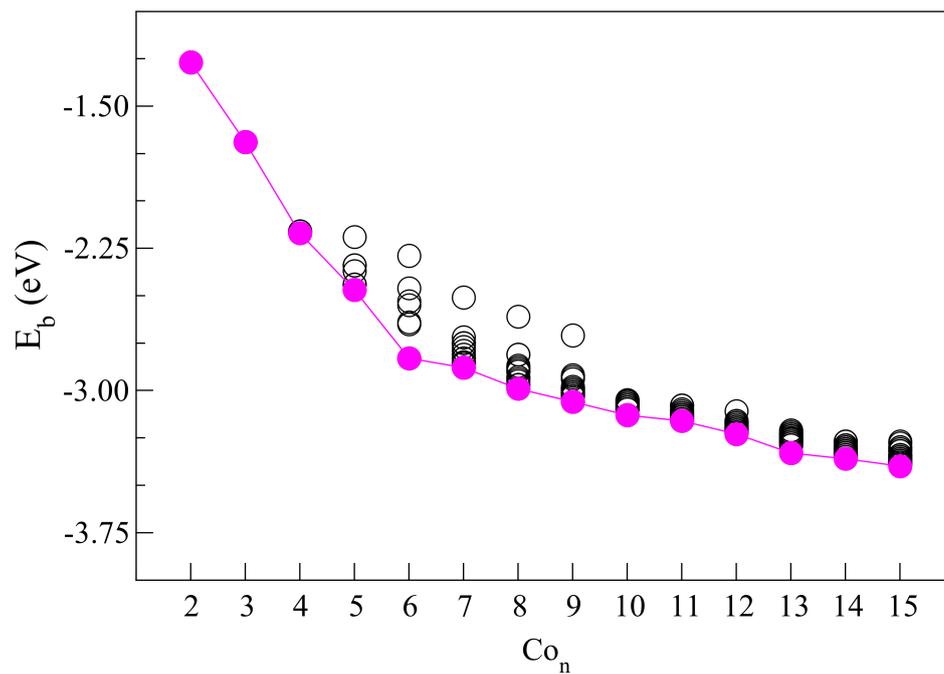
Figure SI1: Binding energy (E_b) for Co_n clusters with $n = 2 - 15$.
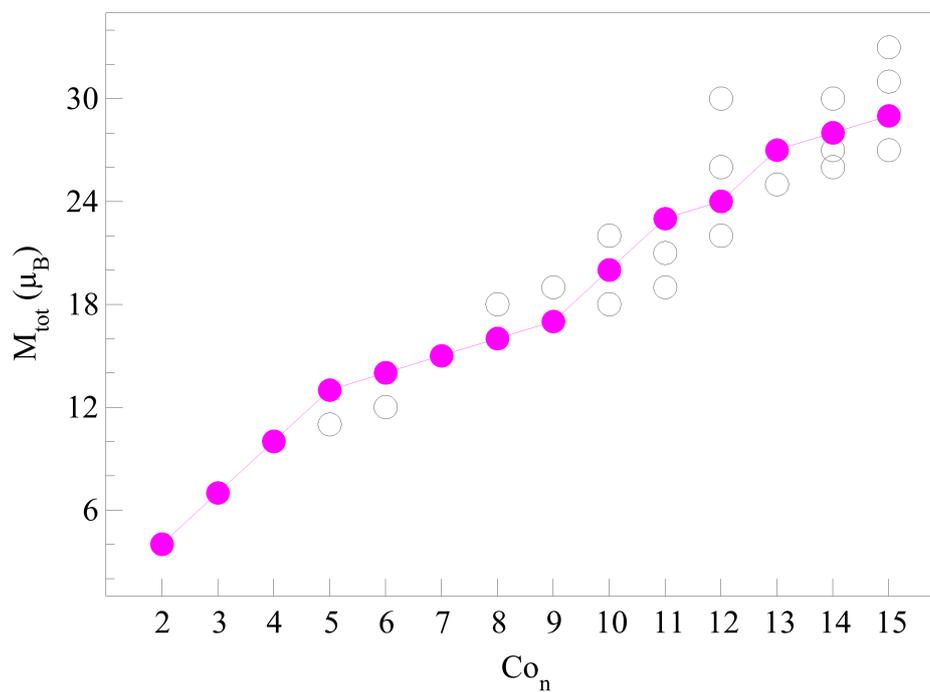
Figure SI2: Total magnetic moment (M_{tot}) for Co_n clusters with $n = 2 - 15$.
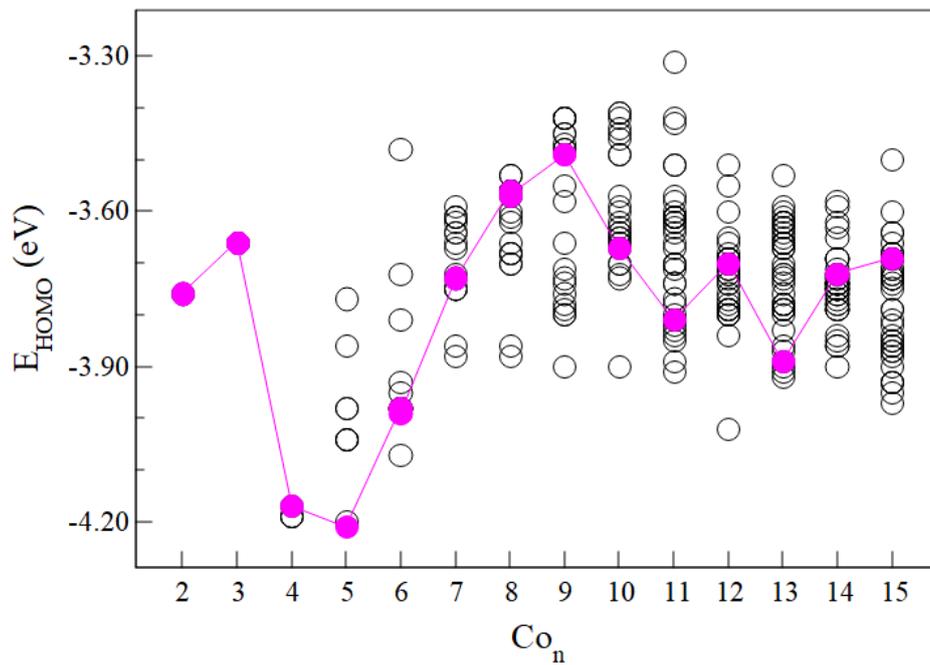
Figure SI3: HOMO energy (E_{HOMO}) for Co_n clusters with $n = 2 - 15$.
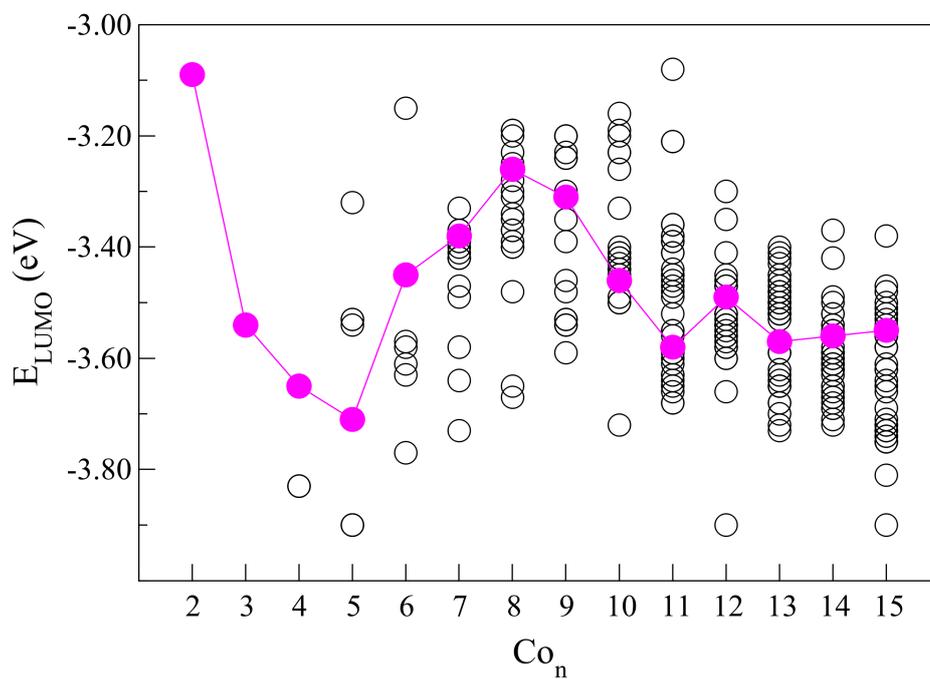
Figure SI4: LUMO energy (E_{LUMO}) for Co_n clusters with $n = 2 - 15$.
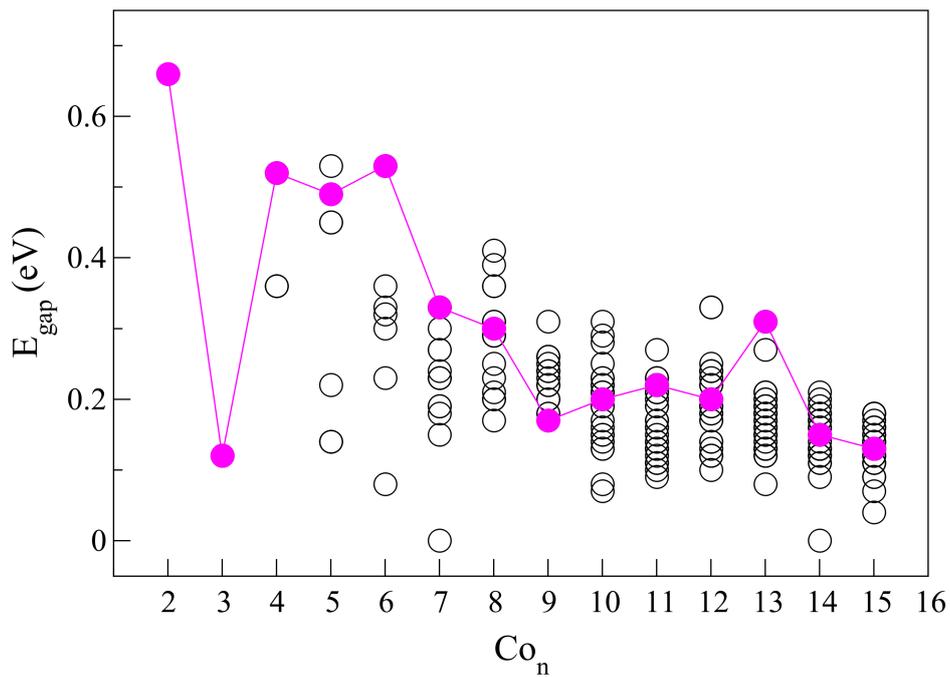
Figure SI5: HOMO-LUMO energy gap (E_{gap}) for Co_n clusters with $n = 2 - 15$.
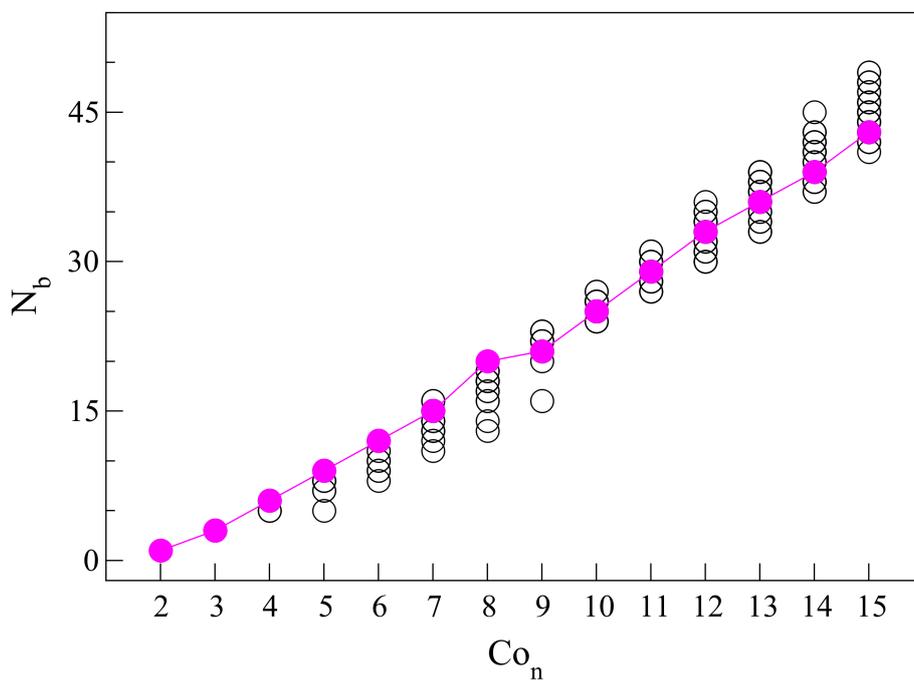
Figure SI6: Total number of bonds (N_b) for Co_n clusters with $n = 2 - 15$.

Figure SI7: Average chemical order parameter (σ_{av}) for Co$_n$ clusters with $n = 2 - 15$.

Figure SI8: Average bond length (d_{av}) for Co$_n$ clusters with $n = 2 - 15$.

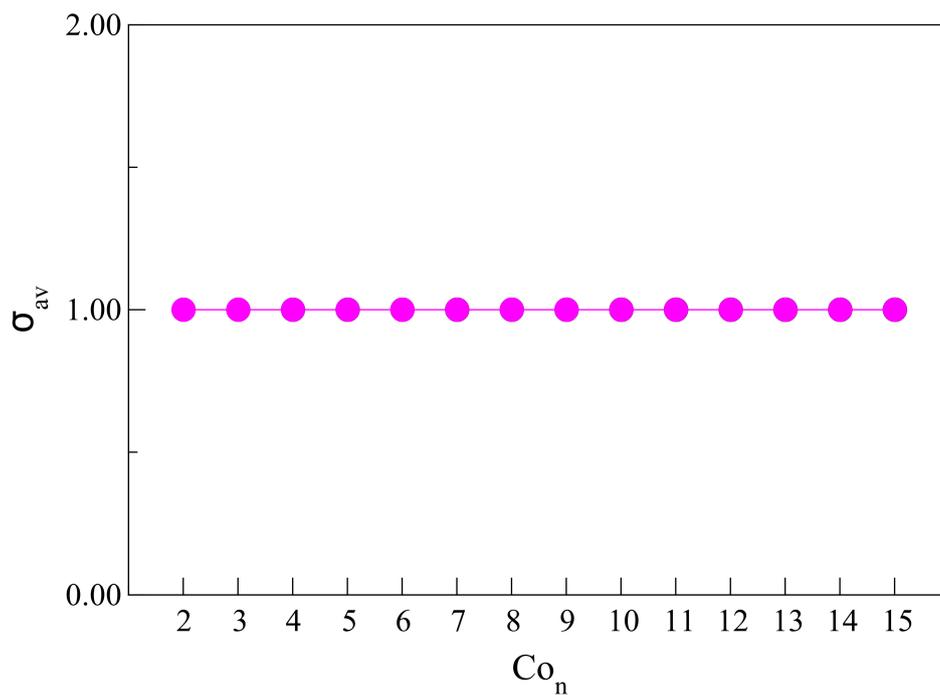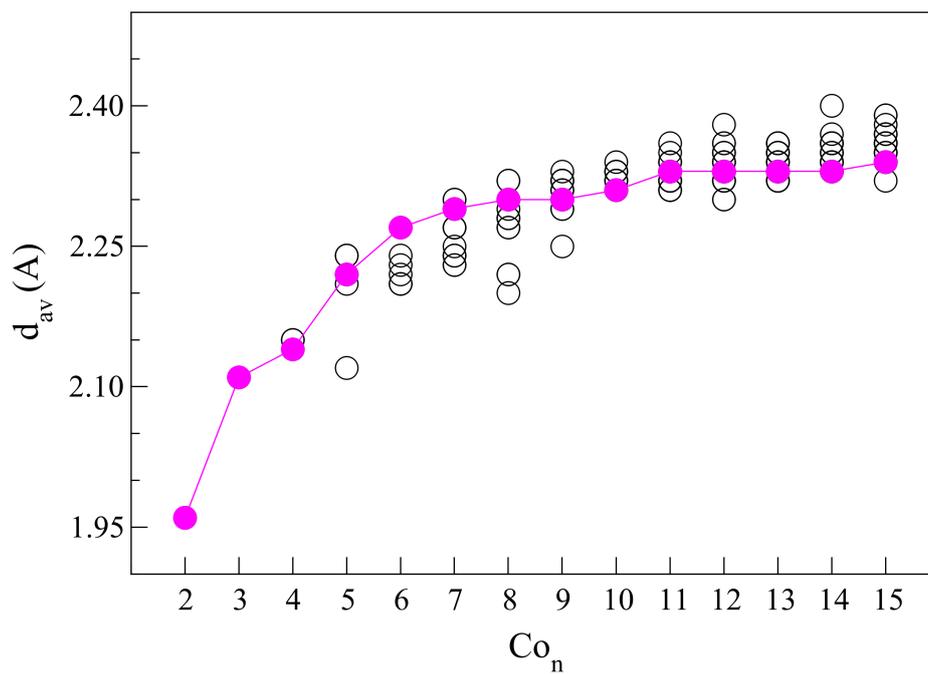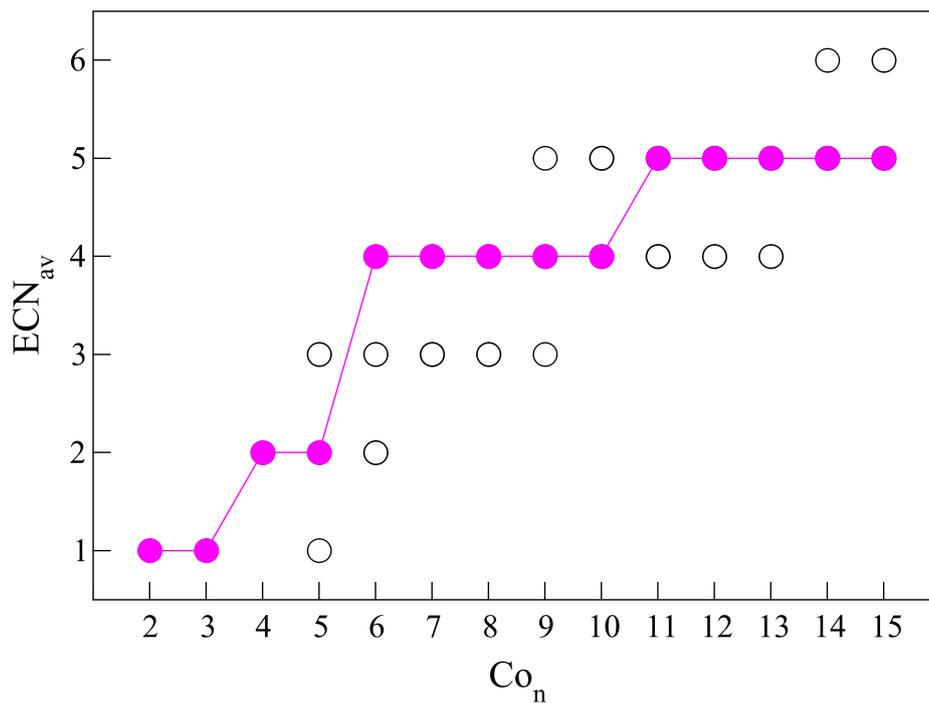Figure SI9: Average effective coordination number (ECN_{av}) for Co_n clusters with $n = 2 - 15$.
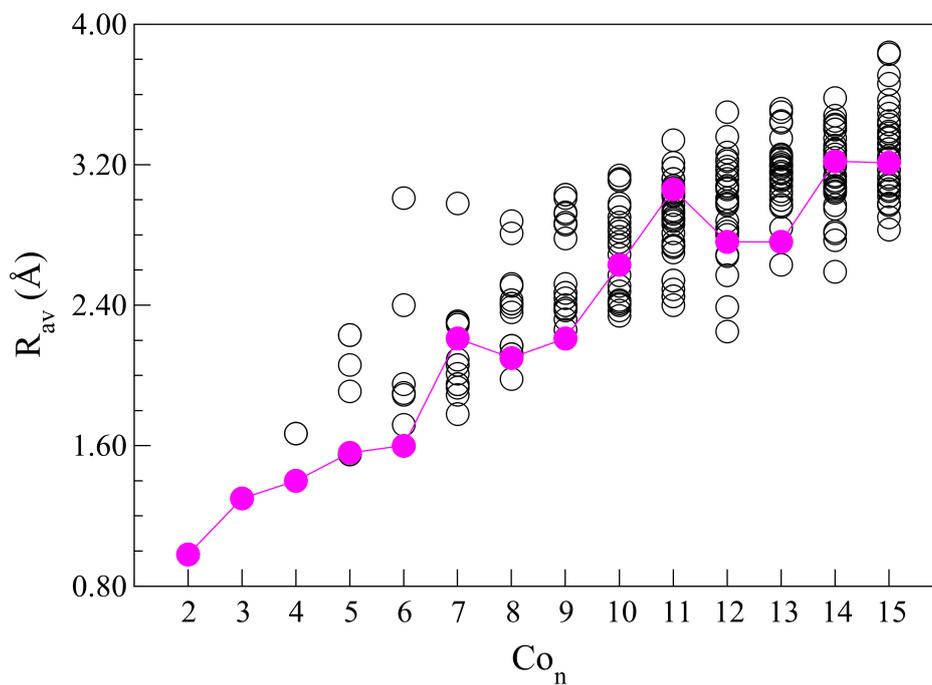
Figure SI10: Average radius R_{av} (in Å) for Co_n clusters ($n = 2$–15).

3 Gas-phase Mo$_n$ Clusters

Table SI14: Structural, energetic and electronic properties for Mo$_n$ cluster with $n = 1 - 5$, as follows: configuration number (i), relative DFT total energy (ΔE_{tot}^{DFT}, in meV), binding energy (E_b, in eV), total magnetic moment (M_{tot}, in μ_B), HOMO energy (ε_{HOMO}, in eV), LUMO energy (ε_{LUMO}, in eV), HOMO-LUMO energy difference, (E_{gap}, in eV), total number of bonds (N_b), average bond length (d_{av}, in Å), average chemical order parameter (σ_{av}), average effective coordination number (ECN_{av}, NNN), and average radius (R_{av}, in Å).

Mon	i	ΔE_{tot}^{DFT}	E_b	M_{tot}	ε_{HOMO}	ε_{LUMO}	E_{gap}	ECN_{av}	d_{av}	N_b	σ_{av}	R_{av}
Mo$_2$	1	0	−2.03	0	−4.18	−2.30	1.87	1	1.91	1.00	1.00	0.95
Mo$_3$	2	3265	−1.10	10	−3.19	−2.84	0.35	1	2.33	2.00	1.00	2.49
Mo$_3$	2	3265	−1.10	10	−3.19	−2.84	0.35	1	2.33	2.00	1.00	2.49
Mo$_3$	1	135	−2.14	2	−3.15	−2.80	0.34	2	2.21	3.00	1.00	1.19
Mo$_3$	3	0	−2.18	2	−2.91	−2.34	0.56	1	2.21	3.00	1.00	1.27
Mo$_4$	5	172	−2.66	0	−3.30	−2.67	0.63	2	2.26	5.00	1.00	1.72
Mo$_4$	6	170	−2.66	0	−3.31	−2.68	0.63	2	2.26	5.00	1.00	1.72
Mo$_4$	7	25	−2.70	0	−2.83	−2.14	0.68	1	2.09	6.00	1.00	1.42
Mo$_4$	3	2	−2.71	0	−3.30	−2.38	0.91	2	2.21	4.00	1.00	1.51
Mo$_4$	2	2	−2.71	0	−3.30	−2.38	0.91	2	2.21	4.00	1.00	1.51
Mo$_4$	1	2	−2.71	0	−3.30	−2.38	0.91	2	2.21	4.00	1.00	1.51
Mo$_4$	4	0	−2.71	0	−3.30	−2.39	0.91	2	2.21	4.00	1.00	1.51
Mo$_5$	1	1574	−2.71	0	−3.60	−3.01	0.58	1	2.19	5.00	1.00	2.00
Mo$_5$	4	1146	−2.80	0	−3.46	−2.78	0.67	1	2.16	6.00	1.00	2.27
Mo$_5$	8	899	−2.85	0	−3.24	−2.66	0.57	2	2.22	8.00	1.00	2.22
Mo$_5$	6	267	−2.97	0	−3.10	−2.58	0.52	2	2.35	9.00	1.00	1.65
Mo$_5$	9	4	−3.03	0	−2.88	−2.33	0.55	2	2.33	9.00	1.00	1.81
Mo$_5$	3	2	−3.03	0	−2.88	−2.33	0.55	2	2.33	9.00	1.00	1.81
Mo$_5$	2	0	−3.03	0	−2.88	−2.33	0.55	2	2.33	9.00	1.00	1.81
Mo$_5$	5	0	−3.03	0	−2.88	−2.33	0.55	2	2.33	9.00	1.00	1.81
Mo$_5$	7	0	−3.03	0	−2.88	−2.33	0.55	2	2.33	9.00	1.00	1.81

Table SI15: Structural, energetic and electronic properties for Mo_6 cluster, as follows: configuration number (i), relative DFT total energy (ΔE_{tot}^{DFT}, in meV), binding energy (E_b, in eV), total magnetic moment (M_{tot}, in μ_B), HOMO energy (ε_{HOMO}, in eV), LUMO energy (ε_{LUMO}, in eV), HOMO-LUMO energy difference, (E_{gap}, in eV), total number of bonds (N_b), average bond length (d_{av}, in Å), average chemical order parameter (σ_{av}), average effective coordination number (ECN_{av}, NNN), and average radius (R_{av}, in Å).

i	ΔE_{tot}^{DFT}	E_b	M_{tot}	ε_{HOMO}	ε_{LUMO}	E_{gap}	ECN_{av}	d_{av}	N_b	σ_{av}	R_{av}
4	3839	−2.72	0	−3.92	−3.16	0.75	1	1.95	3.00	1.00	2.50
10	1235	−3.16	0	−3.40	−2.59	0.80	2	2.27	11.00	1.00	2.47
8	1124	−3.17	0	−3.15	−2.61	0.53	3	2.42	12.00	1.00	2.02
2	1064	−3.18	2	−2.96	−2.65	0.31	3	2.42	12.00	1.00	2.05
11	1027	−3.19	0	−3.11	−2.47	0.63	2	2.28	9.00	1.00	2.05
9	1027	−3.19	0	−3.11	−2.47	0.63	2	2.28	9.00	1.00	2.05
5	1027	−3.19	0	−3.11	−2.48	0.63	2	2.28	9.00	1.00	2.05
6	1	−3.36	0	−2.98	−2.25	0.72	3	2.38	12.00	1.00	1.76
3	1	−3.36	0	−2.98	−2.25	0.72	3	2.38	12.00	1.00	1.76
12	1	−3.36	0	−2.98	−2.25	0.72	3	2.38	12.00	1.00	1.76
7	1	−3.36	0	−2.98	−2.25	0.72	3	2.38	12.00	1.00	1.76
1	0	−3.36	0	−2.98	−2.25	0.72	3	2.38	12.00	1.00	1.76

Table SI16: Structural, energetic and electronic properties for Mo$_7$ cluster, as follows: configuration number (i), relative DFT total energy (ΔE_{tot}^{DFT}, in meV), binding energy (E_b, in eV), total magnetic moment (M_{tot}, in μ_B), HOMO energy (ε_{HOMO}, in eV), LUMO energy (ε_{LUMO}, in eV), HOMO-LUMO energy difference, (E_{gap}, in eV), total number of bonds (N_b), average bond length (d_{av}, in Å), average chemical order parameter (σ_{av}), average effective coordination number (ECN_{av}, NNN), and average radius (R_{av}, in Å).

i	ΔE_{tot}^{DFT}	E_b	M_{tot}	ε_{HOMO}	ε_{LUMO}	E_{gap}	ECN_{av}	d_{av}	N_b	σ_{av}	R_{av}
8	1948	−3.22	0	−3.30	−2.59	0.70	2	2.19	11.00	1.00	2.51
0	1947	−3.22	0	−3.30	−2.59	0.71	2	2.19	11.00	1.00	2.51
5	1713	−3.25	0	−3.25	−2.71	0.54	2	2.31	15.00	1.00	2.48
3	1713	−3.25	0	−3.25	−2.71	0.54	2	2.31	15.00	1.00	2.48
7	1250	−3.32	0	−3.05	−2.70	0.34	2	2.30	14.00	1.00	2.73
4	973	−3.36	0	−3.22	−2.81	0.41	2	2.34	15.00	1.00	2.62
2	758	−3.39	0	−3.07	−2.73	0.34	3	2.41	15.00	1.00	2.31
3	499	−3.43	0	−2.94	−2.69	0.24	3	2.45	16.00	1.00	2.18
6	482	−3.43	0	−3.05	−2.61	0.44	3	2.39	14.00	1.00	2.42
5	202	−3.47	0	−2.94	−2.29	0.64	3	2.44	16.00	1.00	2.06
8	10	−3.50	0	−2.99	−2.39	0.60	3	2.38	16.00	1.00	2.33
0	10	−3.50	0	−3.00	−2.39	0.60	3	2.38	16.00	1.00	2.33
9	9	−3.50	0	−2.99	−2.39	0.60	3	2.38	16.00	1.00	2.33
4	6	−3.50	0	−2.82	−2.42	0.39	3	2.41	15.00	1.00	2.16
9	6	−3.50	0	−2.82	−2.42	0.39	3	2.41	15.00	1.00	2.16
1	2	−3.50	0	−2.83	−2.38	0.45	3	2.43	14.00	1.00	1.98
7	2	−3.50	0	−2.83	−2.38	0.44	3	2.43	15.00	1.00	1.98
6	2	−3.50	0	−2.83	−2.38	0.45	3	2.43	15.00	1.00	1.98
2	0	−3.50	0	−2.83	−2.38	0.44	3	2.43	14.00	1.00	1.98

Table SI17: Structural, energetic and electronic properties for Mo$_8$ cluster, as follows: configuration number (i), relative DFT total energy (ΔE_{tot}^{DFT}, in meV), binding energy (E_b, in eV), total magnetic moment (M_{tot}, in μ_B), HOMO energy (ε_{HOMO}, in eV), LUMO energy (ε_{LUMO}, in eV), HOMO-LUMO energy difference, (E_{gap}, in eV), total number of bonds (N_b), average bond length (d_{av}, in Å), average chemical order parameter (σ_{av}), average effective coordination number (ECN_{av}, NNN), and average radius (R_{av}, in Å).

i	ΔE_{tot}^{DFT}	E_b	M_{tot}	ε_{HOMO}	ε_{LUMO}	E_{gap}	ECN_{av}	d_{av}	N_b	σ_{av}	R_{av}
9	1918	−3.42	0	3.35	−3.07	0.28	3	2.38	18.00	1.00	2.53
15	1437	−3.48	0	3.17	−2.84	0.32	3	2.43	18.00	1.00	2.41
14	1024	−3.54	0	3.07	−2.63	0.43	3	2.41	18.00	1.00	2.60
10	743	−3.57	0	3.07	−2.64	0.43	3	2.41	19.00	1.00	2.74
19	693	−3.58	0	3.32	−2.70	0.61	3	2.42	19.00	1.00	2.81
16	693	−3.58	0	3.32	−2.70	0.61	3	2.42	19.00	1.00	2.81
7	475	−3.60	4	3.19	−2.85	0.33	3	2.45	18.00	1.00	2.61
6	474	−3.60	4	3.19	−2.85	0.33	3	2.45	18.00	1.00	2.61
8	472	−3.60	4	3.19	−2.85	0.33	3	2.45	18.00	1.00	2.61
3	180	−3.64	0	2.91	−2.67	0.23	3	2.44	18.00	1.00	2.47
13	177	−3.64	0	2.91	−2.67	0.24	3	2.44	18.00	1.00	2.47
18	177	−3.64	0	2.91	−2.67	0.24	3	2.44	18.00	1.00	2.47
11	161	−3.64	0	2.95	−2.75	0.19	3	2.45	19.00	1.00	2.44
5	134	−3.65	0	3.47	−2.64	0.83	3	2.45	18.00	1.00	2.19
17	125	−3.65	0	3.13	−2.33	0.80	3	2.46	16.00	1.00	1.97
4	123	−3.65	0	3.13	−2.33	0.80	3	2.46	16.00	1.00	1.97
2	121	−3.65	0	3.13	−2.33	0.79	3	2.46	16.00	1.00	1.97
12	95	−3.65	4	3.04	−2.68	0.35	3	2.43	18.00	1.00	2.11
1	0	−3.66	0	3.01	−2.43	0.58	3	2.42	18.00	1.00	2.36

Table SI18: Structural, energetic and electronic properties for Mo$_9$ cluster, as follows: configuration number (i), relative DFT total energy (ΔE_{tot}^{DFT}, in meV), binding energy (E_b, in eV), total magnetic moment (M_{tot}, in μ_B), HOMO energy (ε_{HOMO}, in eV), LUMO energy (ε_{LUMO}, in eV), HOMO-LUMO energy difference, (E_{gap}, in eV), total number of bonds (N_b), average bond length (d_{av}, in Å), average chemical order parameter (σ_{av}), average effective coordination number (ECN_{av}, NNN), and average radius (R_{av}, in Å).

i	ΔE_{tot}^{DFT}	E_b	M_{tot}	ε_{HOMO}	ε_{LUMO}	E_{gap}	ECN_{av}	d_{av}	N_b	σ_{av}	R_{av}
23	2566	−3.51	0	−3.44	−2.95	0.48	2	2.28	18.00	1.00	2.97
5	2107	−3.56	0	−3.38	−2.89	0.48	3	2.40	21.00	1.00	3.26
21	1701	−3.61	0	−3.21	−2.88	0.32	3	2.39	22.00	1.00	3.36
30	1499	−3.63	0	−3.08	−2.78	0.30	3	2.45	21.00	1.00	2.97
18	1473	−3.63	0	−3.06	−2.75	0.31	3	2.41	22.00	1.00	2.79
27	1470	−3.63	0	−3.06	−2.75	0.31	3	2.41	22.00	1.00	2.79
28	1431	−3.64	0	−3.11	−2.73	0.38	3	2.41	22.00	1.00	3.19
19	1137	−3.67	0	−3.14	−2.58	0.55	3	2.42	21.00	1.00	3.09
01	979	−3.69	0	−2.89	−2.67	0.22	3	2.45	21.00	1.00	2.51
14	941	−3.69	0	−3.20	−2.79	0.41	3	2.45	22.00	1.00	3.00
4	896	−3.69	0	−3.06	−2.70	0.36	3	2.42	21.00	1.00	2.80
10	895	−3.69	0	−3.06	−2.69	0.36	3	2.42	21.00	1.00	2.80
26	859	−3.70	0	−2.84	−2.55	0.28	3	2.44	21.00	1.00	2.59
8	830	−3.70	0	−3.01	−2.73	0.27	3	2.46	21.00	1.00	2.61
13	804	−3.70	0	−3.14	−2.88	0.26	3	2.45	23.00	1.00	2.85
06	738	−3.71	0	−2.96	−2.57	0.38	3	2.41	21.00	1.00	2.79
16	736	−3.71	0	−2.96	−2.57	0.38	3	2.41	21.00	1.00	2.79
2	587	−3.73	4	−3.06	−2.90	0.15	4	2.49	21.00	1.00	2.49
3	573	−3.73	0	−3.11	−2.72	0.39	4	2.47	23.00	1.00	2.47
15	572	−3.73	0	−3.11	−2.72	0.39	4	2.47	23.00	1.00	2.47
22	567	−3.73	0	−2.93	−2.61	0.31	3	2.45	21.00	1.00	2.54
29	496	−3.74	0	−3.10	−2.66	0.43	3	2.43	21.00	1.00	2.71
11	496	−3.74	0	−3.09	−2.66	0.43	3	2.43	22.00	1.00	2.71
12	495	−3.74	0	−3.09	−2.66	0.42	3	2.43	22.00	1.00	2.70
20	494	−3.74	0	−2.96	−2.66	0.30	3	2.44	22.00	1.00	2.55
25	91	−3.78	0	−3.06	−2.53	0.52	3	2.45	21.00	1.00	2.51
7	90	−3.78	0	−3.06	−2.53	0.53	3	2.45	21.00	1.00	2.51
17	90	−3.78	0	−3.06	−2.53	0.53	3	2.45	21.00	1.00	2.51
24	2	−3.79	0	−2.64	−2.59	0.04	4	2.47	21.00	1.00	2.10
9	0	−3.79	0	−2.64	−2.59	0.04	4	2.47	21.00	1.00	2.10

Table SI19: Structural, energetic and electronic properties for Mo_{10} cluster, as follows: configuration number (i), relative DFT total energy (ΔE_{tot}^{DFT}, in meV), binding energy (E_b, in eV), total magnetic moment (M_{tot}, in μ_B), HOMO energy (ε_{HOMO}, in eV), LUMO energy (ε_{LUMO}, in eV), HOMO-LUMO energy difference, (E_{gap}, in eV), total number of bonds (N_b), average bond length (d_{av}, in Å), average chemical order parameter (σ_{av}), average effective coordination number (ECN_{av}, NNN), and average radius (R_{av}, in Å).

i	ΔE_{tot}^{DFT}	E_b	M_{tot}	ε_{HOMO}	ε_{LUMO}	E_{gap}	ECN_{av}	d_{av}	N_b	σ_{av}	R_{av}
17	2129	−3.67	0	−2.94	−2.56	0.37	2	2.36	20.00	1.00	2.30
12	1944	−3.69	0	−2.98	−2.86	0.12	4	2.49	23.00	1.00	3.23
15	1055	−3.78	0	−3.17	−2.87	0.29	4	2.48	25.00	1.00	3.33
1	1045	−3.78	0	−3.00	−2.74	0.25	3	2.43	24.00	1.00	3.15
10	987	−3.79	0	−3.17	−2.72	0.44	4	2.48	26.00	1.00	2.65
18	951	−3.79	0	−3.09	−2.63	0.45	4	2.48	26.00	1.00	2.94
14	861	−3.80	0	−2.97	−2.79	0.18	3	2.47	24.00	1.00	2.89
3	847	−3.80	0	−2.98	−2.74	0.23	4	2.48	25.00	1.00	2.71
11	846	−3.80	0	−2.97	−2.74	0.23	4	2.48	25.00	1.00	2.71
13	772	−3.81	0	−2.99	−2.63	0.35	3	2.45	24.00	1.00	3.10
2	732	−3.81	0	−3.01	−2.64	0.37	3	2.46	26.00	1.00	2.61
4	683	−3.82	0	−3.02	−2.80	0.21	3	2.46	24.00	1.00	2.65
9	667	−3.82	0	−3.16	−2.73	0.43	4	2.44	26.00	1.00	3.40
16	624	−3.82	0	−3.04	−2.63	0.40	4	2.46	25.00	1.00	3.05
7	378	−3.85	0	−3.00	−2.82	0.18	3	2.47	25.00	1.00	2.56
6	254	−3.86	0	−3.03	−2.35	0.68	3	2.43	23.00	1.00	2.91
5	0	−3.89	0	−2.98	−2.76	0.22	3	2.47	24.00	1.00	2.64

Table SI20: Structural, energetic and electronic properties for Mo_{11} cluster, as follows: configuration number (i), relative DFT total energy (ΔE_{tot}^{DFT}, in meV), binding energy (E_b, in eV), total magnetic moment (M_{tot}, in μ_B), HOMO energy (ε_{HOMO}, in eV), LUMO energy (ε_{LUMO}, in eV), HOMO-LUMO energy difference, (E_{gap}, in eV), total number of bonds (N_b), average bond length (d_{av}, in Å), average chemical order parameter (σ_{av}), average effective coordination number (ECN_{av}, NNN), and average radius (R_{av}, in Å).

i	ΔE_{tot}^{DFT}	E_b	M_{tot}	ε_{HOMO}	ε_{LUMO}	E_{gap}	ECN_{av}	d_{av}	N_b	σ_{av}	R_{av}
28	2654	−3.72	0	−3.33	−3.19	0.13	4	2.47	28.00	1.00	3.28
32	1830	−3.80	0	−3.24	−3.06	0.18	3	2.42	27.00	1.00	3.20
24	1669	−3.81	0	−3.13	−2.92	0.21	4	2.47	28.00	1.00	3.18
30	1585	−3.82	0	−3.05	−2.97	0.07	3	2.48	27.00	1.00	2.67
9	1363	−3.84	0	−3.06	−2.91	0.15	3	2.47	27.00	1.00	2.78
19	1296	−3.84	0	−2.98	−2.80	0.17	3	2.48	27.00	1.00	2.82
11	1294	−3.84	0	−2.97	−2.80	0.17	3	2.48	27.00	1.00	2.82
23	1197	−3.85	0	−3.21	−2.86	0.35	3	2.41	28.00	1.00	3.44
4	1139	−3.86	0	−3.16	−2.92	0.24	4	2.46	28.00	1.00	3.16
25	1113	−3.86	0	−3.15	−2.76	0.38	3	2.45	31.00	1.00	2.85
07	996	−3.87	0	−3.12	−2.87	0.24	4	2.49	28.00	1.00	3.08
15	798	−3.89	0	−3.12	−2.90	0.21	4	2.48	27.00	1.00	2.85
1	789	−3.89	0	−3.06	−2.81	0.25	4	2.47	27.00	1.00	3.07
6	755	−3.89	0	−2.88	−2.68	0.19	4	2.48	29.00	1.00	3.01
18	746	−3.89	0	−2.83	−2.70	0.13	3	2.46	29.00	1.00	3.05
16	732	−3.90	0	−3.06	−2.87	0.19	4	2.49	29.00	1.00	2.81
14	656	−3.90	0	−3.03	−2.83	0.20	4	2.48	27.00	1.00	2.69
10	646	−3.90	0	−3.09	−2.85	0.23	4	2.48	27.00	1.00	3.07
27	645	−3.90	0	−3.08	−2.85	0.23	4	2.48	27.00	1.00	3.06
26	633	−3.90	0	−3.03	−2.79	0.24	4	2.48	28.00	1.00	2.90
2	631	−3.90	0	−3.03	−2.79	0.24	4	2.48	28.00	1.00	2.90
29	631	−3.90	0	−3.04	−2.79	0.24	4	2.48	28.00	1.00	2.90
8	602	−3.91	0	−3.05	−2.83	0.22	3	2.47	28.00	1.00	3.00
13	191	−3.94	0	−2.97	−2.56	0.40	3	2.44	30.00	1.00	2.87
31	155	−3.95	0	−2.90	−2.57	0.33	4	2.46	27.00	1.00	3.08
21	154	−3.95	0	−2.90	−2.57	0.33	4	2.46	27.00	1.00	3.08
17	71	−3.96	0	−3.25	−2.98	0.27	4	2.49	28.00	1.00	2.66
22	0	−3.96	0	−3.02	−2.62	0.39	4	2.46	27.00	1.00	3.04

Table SI21: Structural, energetic and electronic properties for Mo_{12} cluster, as follows: configuration number (i), relative DFT total energy (ΔE_{tot}^{DFT}, in meV), binding energy (E_b, in eV), total magnetic moment (M_{tot}, in μ_B), HOMO energy (ε_{HOMO}, in eV), LUMO energy (ε_{LUMO}, in eV), HOMO-LUMO energy difference, (E_{gap}, in eV), total number of bonds (N_b), average bond length (d_{av}, in Å), average chemical order parameter (σ_{av}), average effective coordination number (ECN_{av}, NNN), and average radius (R_{av}, in Å).

i	ΔE_{tot}^{DFT}	E_b	M_{tot}	ε_{HOMO}	ε_{LUMO}	E_{gap}	ECN_{av}	d_{av}	N_b	σ_{av}	R_{av}
35	2333	−3.87	0	−3.22	−2.90	0.31	3	2.41	32.00	1.00	4.14
2	2172	−3.88	0	−3.07	−2.77	0.30	4	2.47	32.00	1.00	3.57
36	2084	−3.89	0	−3.39	−3.09	0.29	3	2.44	33.00	1.00	3.54
9	1867	−3.91	0	−3.23	−3.00	0.23	4	2.48	31.00	1.00	3.32
37	1842	−3.91	0	−3.26	−3.05	0.21	3	2.42	32.00	1.00	3.42
22	1755	−3.92	0	−3.18	−3.04	0.14	3	2.44	32.00	1.00	3.47
20	1736	−3.92	0	−3.26	−2.92	0.34	3	2.42	32.00	1.00	3.35
29	1634	−3.93	0	−2.99	−2.96	0.02	4	2.49	32.00	1.00	3.71
3	1623	−3.93	0	−3.09	−2.81	0.27	3	2.44	33.00	1.00	3.32
6	1608	−3.93	0	−2.89	−2.65	0.24	3	2.46	30.00	1.00	3.48
34	1589	−3.93	0	−3.13	−2.95	0.18	4	2.49	30.00	1.00	3.16
32	1563	−3.93	0	−3.27	−2.96	0.31	3	2.40	30.00	1.00	3.44
4	1455	−3.94	0	−3.08	−2.82	0.25	4	2.47	33.00	1.00	3.26
10	1452	−3.94	0	−3.09	−2.83	0.25	4	2.47	33.00	1.00	3.26
17	1449	−3.94	0	−3.19	−2.87	0.32	4	2.46	32.00	1.00	3.75
24	1401	−3.94	0	−3.30	−2.98	0.31	4	2.47	33.00	1.00	3.17
23	1395	−3.95	0	−3.07	−2.63	0.43	4	2.45	29.00	1.00	3.16
18	1314	−3.95	0	−3.14	−2.84	0.30	4	2.45	32.00	1.00	3.03
21	1290	−3.95	0	−3.03	−2.81	0.22	4	2.51	31.00	1.00	3.22
38	1221	−3.96	0	−2.95	−2.79	0.15	3	2.44	30.00	1.00	2.79
1	1165	−3.96	0	−3.09	−2.86	0.22	4	2.49	32.00	1.00	3.52
15	1133	−3.97	0	−2.89	−2.70	0.18	3	2.45	30.00	1.00	2.67
27	1118	−3.97	0	−3.07	−2.77	0.30	4	2.48	32.00	1.00	3.15
28	1118	−3.97	0	−3.03	−2.74	0.28	4	2.47	30.00	1.00	3.45
30	1052	−3.97	0	−3.14	−2.68	0.45	3	2.42	29.00	1.00	3.17
33	983	−3.98	0	−3.14	−2.78	0.36	4	2.48	31.00	1.00	3.09
14	976	−3.98	0	−3.03	−2.81	0.21	4	2.48	33.00	1.00	3.44
31	919	−3.98	0	−3.13	−2.95	0.17	4	2.46	32.00	1.00	3.05
13	888	−3.99	0	−3.18	−2.86	0.32	4	2.47	32.00	1.00	3.03
19	885	−3.99	0	−3.00	−2.69	0.31	4	2.47	32.00	1.00	3.19
8	841	−3.99	0	−3.03	−2.63	0.39	4	2.49	31.00	1.00	3.25
26	827	−3.99	0	−3.23	−2.72	0.51	4	2.45	32.00	1.00	2.87
25	776	−4.00	0	−3.19	−2.92	0.27	4	2.48	32.00	1.00	3.35
5	693	−4.00	0	−3.05	−2.80	0.24	4	2.47	31.00	1.00	3.23
11	677	−4.00	0	−2.93	−2.65	0.28	4	2.48	34.00	1.00	3.12
16	676	−4.00	0	−2.93	−2.64	0.28	4	2.48	32.00	1.00	3.12
7	571	−4.01	0	−3.05	−2.54	0.50	4	2.49	30.00	1.00	3.02
39	566	−4.01	0	−3.12	−2.92	0.20	4	2.50	32.00	1.00	3.03
12	0	−4.06	0	−3.13	−2.85	0.27	4	2.49	36.00	1.00	2.71

Table SI22: Structural, energetic and electronic properties for Mo$_{13}$ cluster, as follows: configuration number (i), relative DFT total energy (ΔE_{tot}^{DFT}, in meV), binding energy (E_b, in eV), total magnetic moment (M_{tot}, in μ_B), HOMO energy (ε_{HOMO}, in eV), LUMO energy (ε_{LUMO}, in eV), HOMO-LUMO energy difference, (E_{gap}, in eV), total number of bonds (N_b), average bond length (d_{av}, in Å), average chemical order parameter (σ_{av}), average effective coordination number (ECN_{av}, NNN), and average radius (R_{av}, in Å).

i	ΔE_{tot}^{DFT}	E_b	M_{tot}	ε_{HOMO}	ε_{LUMO}	E_{gap}	ECN_{av}	d_{av}	N_b	σ_{av}	R_{av}
32	8047	−3.50	0	−3.09	−3.01	0.07	4	2.95	39.00	1.00	8.40
29	1952	−3.97	0	−3.31	−3.06	0.25	3	2.45	34.00	1.00	3.47
15	1921	−3.97	0	−3.25	−3.05	0.19	4	2.50	35.00	1.00	3.79
39	1802	−3.98	0	−3.34	−3.09	0.25	4	2.49	36.00	1.00	3.32
10	1645	−3.99	0	−3.21	−2.99	0.21	4	2.48	34.00	1.00	3.66
52	1590	−4.00	0	−3.18	−2.81	0.36	3	2.44	36.00	1.00	3.72
36	1542	−4.00	0	−3.15	−2.90	0.24	4	2.49	37.00	1.00	3.35
57	1530	−4.00	0	−3.19	−2.88	0.30	4	2.49	38.00	1.00	3.22
61	1523	−4.00	0	−3.21	−2.94	0.27	4	2.46	36.00	1.00	3.73
28	1510	−4.00	0	−3.20	−2.95	0.25	4	2.48	36.00	1.00	3.31
63	1484	−4.00	0	−3.18	−2.95	0.22	4	2.47	36.00	1.00	3.36
8	1457	−4.01	0	−3.15	−2.84	0.31	4	2.49	36.00	1.00	3.29
40	1416	−4.01	0	−3.17	−2.85	0.31	3	2.45	37.00	1.00	3.19
41	1416	−4.01	0	−3.26	−2.94	0.32	4	2.43	35.00	1.00	3.58
5	1388	−4.01	0	−3.07	−2.81	0.26	4	2.49	34.00	1.00	3.45
9	1372	−4.01	0	−3.21	−2.85	0.35	3	2.44	36.00	1.00	3.23
30	1366	−4.01	0	−3.24	−2.95	0.28	4	2.47	37.00	1.00	3.36
20	1365	−4.01	0	−3.08	−2.91	0.17	4	2.50	36.00	1.00	3.24
1	1352	−4.02	0	−2.92	−2.84	0.07	4	2.50	35.00	1.00	3.68
3	1340	−4.02	0	−3.21	−2.90	0.31	4	2.50	38.00	1.00	3.16
24	1305	−4.02	0	−3.22	−3.03	0.19	4	2.47	38.00	1.00	3.23
35	1300	−4.02	0	−3.08	−2.76	0.32	4	2.47	34.00	1.00	3.57
14	1299	−4.02	0	−3.35	−2.97	0.37	4	2.45	38.00	1.00	3.17
26	1293	−4.02	0	−3.25	−3.05	0.20	4	2.47	35.00	1.00	3.63
64	1273	−4.02	0	−3.24	−2.92	0.31	3	2.44	32.00	1.00	3.49
31	1208	−4.03	0	−3.27	−2.97	0.29	4	2.48	36.00	1.00	3.31
60	1198	−4.03	0	−3.26	−3.01	0.25	4	2.43	36.00	1.00	3.01
34	1195	−4.03	0	−3.00	−2.81	0.18	4	2.49	36.00	1.00	3.74
33	1108	−4.03	0	−2.95	−2.72	0.22	4	2.47	36.00	1.00	3.37
58	1090	−4.04	0	−3.24	−2.96	0.28	4	2.48	37.00	1.00	3.11
47	1054	−4.04	0	−3.10	−2.92	0.17	4	2.47	37.00	1.00	3.19
12	1053	−4.04	0	−3.12	−2.88	0.24	4	2.48	36.00	1.00	3.30
38	987	−4.04	0	−3.10	−2.82	0.27	4	2.48	35.00	1.00	3.30
4	982	−4.04	0	−3.06	−2.93	0.12	4	2.51	36.00	1.00	2.89
43	968	−4.04	0	−3.26	−3.00	0.26	4	2.46	35.00	1.00	3.25
37	963	−4.05	0	−3.09	−2.91	0.18	3	2.44	35.00	1.00	3.27
51	959	−4.05	0	−3.27	−2.93	0.34	4	2.49	37.00	1.00	3.09
22	959	−4.05	0	−3.27	−2.93	0.34	4	2.49	37.00	1.00	3.09
11	954	−4.05	0	−3.19	−2.91	0.28	4	2.47	35.00	1.00	3.23
62	899	−4.05	0	−2.94	−2.68	0.25	4	2.46	37.00	1.00	3.06
65	851	−4.05	0	−3.25	−2.87	0.37	4	2.46	35.00	1.00	3.10
45	820	−4.06	0	−3.38	−2.87	0.51	3	2.43	35.00	1.00	3.23
13	790	−4.06	0	−3.00	−2.77	0.22	4	2.50	38.00	1.00	2.86
19	773	−4.06	0	−3.04	−2.76	0.28	4	2.50	33.00	1.00	3.21
55	753	−4.06	0	−3.01	−2.82	0.18	4	2.48	36.00	1.00	3.37
42	684	−4.07	0	−3.15	−2.94	0.20	4	2.50	37.00	1.00	3.33
21	680	−4.07	0	−2.99	−2.79	0.19	4	2.49	35.00	1.00	3.28
25	678	−4.07	0	−2.99	−2.79	0.19	4	2.49	35.00	1.00	3.28
16	668	−4.07	0	−3.02	−2.81	0.20	4	2.47	35.00	1.00	3.16

27	666	−4.07	0	−3.02	−2.81	0.20	4	2.47	37.00	1.00	3.16
6	549	−4.08	0	−2.84	−2.72	0.12	4	2.49	35.00	1.00	3.29
44	518	−4.08	0	−3.11	−2.78	0.33	4	2.47	39.00	1.00	3.49
49	460	−4.08	0	−3.20	−2.92	0.28	4	2.51	34.00	1.00	3.16
50	440	−4.09	0	−3.21	−2.86	0.35	4	2.47	39.00	1.00	2.92
56	389	−4.09	0	−3.06	−2.75	0.30	4	2.47	34.00	1.00	3.14
53	387	−4.09	0	−3.08	−2.76	0.32	4	2.49	37.00	1.00	2.91
17	357	−4.09	0	−3.23	−2.79	0.43	4	2.49	36.00	1.00	3.04
48	307	−4.10	0	−3.09	−2.82	0.27	4	2.47	35.00	1.00	3.09
7	217	−4.10	0	−2.81	−2.60	0.21	4	2.49	33.00	1.00	3.20
54	179	−4.11	0	−3.00	−2.72	0.28	4	2.50	37.00	1.00	2.92
2	3	−4.12	0	−3.20	−2.85	0.34	4	2.48	39.00	1.00	2.75
59	2	−4.12	0	−3.20	−2.85	0.34	4	2.48	39.00	1.00	2.75
18	1	−4.12	0	−3.19	−2.85	0.34	4	2.48	39.00	1.00	2.75
23	0	−4.12	0	−3.20	−2.85	0.34	4	2.48	39.00	1.00	2.75

Table SI23: Structural, energetic and electronic properties for Mo_{14} cluster, as follows: configuration number (i), relative DFT total energy (ΔE_{tot}^{DFT}, in meV), binding energy (E_b, in eV), total magnetic moment (M_{tot}, in μ_B), HOMO energy (ε_{HOMO}, in eV), LUMO energy (ε_{LUMO}, in eV), HOMO-LUMO energy difference, (E_{gap}, in eV), total number of bonds (N_b), average bond length (d_{av}, in Å), average chemical order parameter (σ_{av}), average effective coordination number (ECN_{av}, NNN), and average radius (R_{av}, in Å).
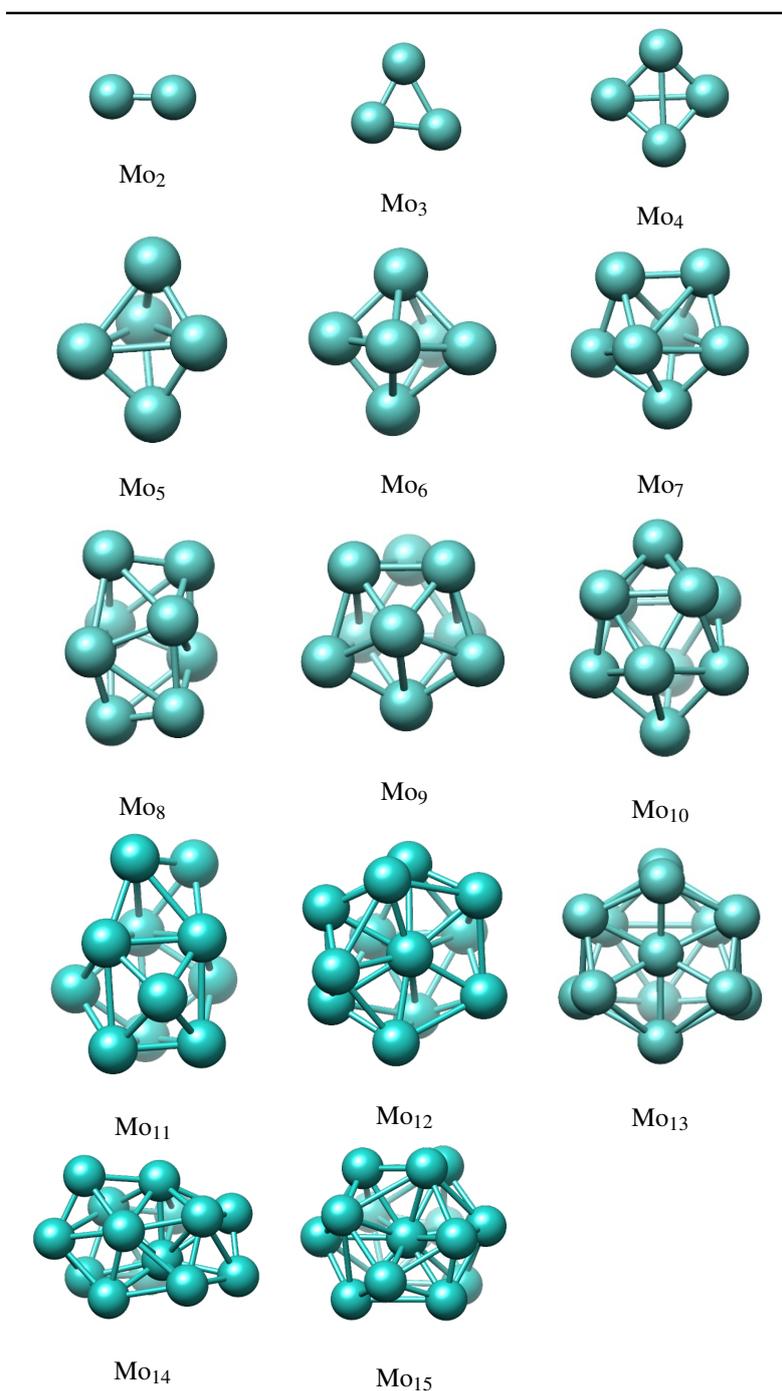
i	ΔE_{tot}^{DFT}	E_b	M_{tot}	ε_{HOMO}	ε_{LUMO}	E_{gap}	ECN_{av}	d_{av}	N_b	σ_{av}	R_{av}
9	2117	−4.00	0	−3.32	−3.00	0.31	4	2.49	37.00	1.00	3.44
28	1827	−4.02	0	−3.26	−3.02	0.24	4	2.49	38.00	1.00	3.48
19	1575	−4.04	0	−3.27	−3.10	0.16	4	2.51	41.00	1.00	3.73
23	1570	−4.04	0	−3.10	−2.89	0.20	4	2.43	38.00	1.00	3.69
20	1568	−4.04	0	−3.20	−2.97	0.23	4	2.48	38.00	1.00	3.78
24	1388	−4.06	0	−3.17	−2.89	0.27	4	2.48	40.00	1.00	3.36
21	1261	−4.06	0	−3.35	−2.97	0.37	4	2.46	37.00	1.00	3.70
03	1222	−4.07	0	−3.28	−3.04	0.24	4	2.49	39.00	1.00	3.57
15	1112	−4.08	0	−3.12	−3.00	0.12	4	2.50	39.00	1.00	3.11
6	1104	−4.08	0	−3.24	−2.99	0.25	4	2.45	41.00	1.00	3.58
1	1104	−4.08	0	−3.02	−2.79	0.23	4	2.50	38.00	1.00	3.64
29	1072	−4.08	0	−3.16	−2.88	0.27	4	2.46	39.00	1.00	3.64
26	952	−4.09	0	−3.41	−3.01	0.40	4	2.46	41.00	1.00	3.22
25	935	−4.09	0	−3.09	−2.88	0.21	4	2.49	39.00	1.00	3.71
4	932	−4.09	0	−3.22	−2.69	0.53	4	2.46	38.00	1.00	2.97
40	839	−4.10	0	−3.20	−2.90	0.30	4	2.49	40.00	1.00	3.60
37	839	−4.10	0	−3.13	−2.96	0.16	4	2.46	38.00	1.00	3.66
35	836	−4.10	0	−3.15	−3.00	0.14	4	2.51	37.00	1.00	3.41
18	817	−4.10	0	−3.31	−2.91	0.39	4	2.51	42.00	1.00	3.26
33	813	−4.10	0	−3.07	−2.74	0.32	4	2.47	40.00	1.00	3.87
8	807	−4.10	0	−3.13	−2.83	0.30	4	2.48	41.00	1.00	3.63
12	786	−4.10	0	−3.11	−2.96	0.15	4	2.49	39.00	1.00	3.17
34	758	−4.10	0	−3.17	−2.93	0.23	4	2.49	40.00	1.00	3.30
31	737	−4.10	0	−3.22	−2.89	0.32	4	2.51	42.00	1.00	3.64
11	701	−4.11	0	−3.23	−2.78	0.44	4	2.46	39.00	1.00	3.08
27	643	−4.11	0	−3.27	−2.96	0.30	4	2.44	41.00	1.00	3.25
22	627	−4.11	0	−3.04	−2.80	0.24	4	2.48	40.00	1.00	3.38
13	511	−4.12	0	−3.09	−2.91	0.17	4	2.49	40.00	1.00	3.19
10	343	−4.13	0	−3.17	−2.82	0.35	4	2.49	40.00	1.00	3.28
36	338	−4.13	0	−2.99	−2.70	0.28	4	2.51	38.00	1.00	3.37
7	302	−4.13	0	−2.90	−2.75	0.14	4	2.50	37.00	1.00	3.40
5	217	−4.14	0	−3.12	−2.90	0.22	4	2.50	43.00	1.00	3.31
17	157	−4.14	0	−3.14	−2.89	0.24	4	2.49	41.00	1.00	3.41
14	126	−4.15	0	−3.08	−2.84	0.24	4	2.47	41.00	1.00	3.41
39	126	−4.15	0	−3.07	−2.69	0.37	4	2.45	36.00	1.00	3.23
2	35	−4.15	0	−3.22	−3.02	0.19	4	2.52	42.00	1.00	2.98
16	22	−4.15	0	−3.02	−2.84	0.18	4	2.50	40.00	1.00	3.23
38	0	−4.16	0	−3.02	−2.79	0.23	4	2.51	40.00	1.00	3.12

Table SI24: Structural, energetic and electronic properties for Mo_{15} cluster, as follows: configuration number (i), relative DFT total energy (ΔE_{tot}^{DFT}, in meV), binding energy (E_b, in eV), total magnetic moment (M_{tot}, in μ_B), HOMO energy (ε_{HOMO}, in eV), LUMO energy (ε_{LUMO}, in eV), HOMO-LUMO energy difference, (E_{gap}, in eV), total number of bonds (N_b), average bond length (d_{av}, in Å), average chemical order parameter (σ_{av}), average effective coordination number (ECN_{av}, NNN), and average radius (R_{av}, in Å).

i	ΔE_{tot}^{DFT}	E_b	M_{tot}	ε_{HOMO}	ε_{LUMO}	E_{gap}	ECN_{av}	d_{av}	N_b	σ_{av}	R_{av}
35	3381	−4.04	0	−3.28	−3.10	0.18	4	2.49	42.00	1.00	3.91
16	2641	−4.09	0	−3.36	−3.05	0.31	4	2.51	42.00	1.00	3.75
31	2639	−4.09	0	−3.18	−2.96	0.22	4	2.51	42.00	1.00	4.41
18	2410	−4.10	0	−3.31	−3.01	0.30	4	2.50	42.00	1.00	4.13
24	2095	−4.12	0	−3.21	−3.02	0.19	4	2.52	41.00	1.00	3.46
9	2032	−4.13	0	−3.28	−2.91	0.36	4	2.49	42.00	1.00	3.52
10	1967	−4.13	0	−3.24	−2.96	0.27	4	2.52	46.00	1.00	3.39
21	1913	−4.14	0	−3.17	−2.87	0.29	4	2.50	42.00	1.00	3.97
29	1895	−4.14	0	−3.19	−2.88	0.31	4	2.45	42.00	1.00	3.51
26	1872	−4.14	0	−3.31	−2.92	0.38	4	2.48	43.00	1.00	3.75
38	1852	−4.14	0	−3.16	−2.79	0.36	4	2.49	43.00	1.00	3.55
15	1655	−4.15	0	−3.35	−3.09	0.25	4	2.51	46.00	1.00	3.22
01	1637	−4.15	0	−3.21	−2.88	0.32	4	2.49	42.00	1.00	3.52
34	1621	−4.16	0	−3.22	−2.97	0.25	4	2.46	42.00	1.00	3.63
33	1596	−4.16	0	−3.17	−2.86	0.30	4	2.50	42.00	1.00	3.64
6	1594	−4.16	0	−3.17	−2.87	0.30	4	2.50	42.00	1.00	3.64
23	1579	−4.16	0	−3.20	−3.01	0.19	4	2.50	44.00	1.00	3.57
20	1463	−4.17	0	−3.03	−2.79	0.23	4	2.51	41.00	1.00	3.67
28	1437	−4.17	0	−3.28	−2.96	0.32	4	2.49	44.00	1.00	3.50
22	1283	−4.18	0	−3.05	−2.84	0.21	4	2.50	43.00	1.00	3.46
12	1281	−4.18	0	−3.05	−2.84	0.21	4	2.50	43.00	1.00	3.46
7	1216	−4.18	0	−3.25	−2.96	0.29	4	2.51	42.00	1.00	3.37
37	1185	−4.19	0	−3.19	−2.95	0.24	4	2.51	43.00	1.00	3.65
36	1180	−4.19	0	−3.24	−2.85	0.39	4	2.45	40.00	1.00	3.74
40	1144	−4.19	0	−3.10	−2.84	0.26	4	2.50	45.00	1.00	3.38
32	1119	−4.19	0	−3.10	−2.92	0.17	4	2.51	46.00	1.00	3.52
8	1072	−4.19	0	−3.09	−2.88	0.20	4	2.47	39.00	1.00	3.36
11	1049	−4.19	0	−3.23	−2.93	0.29	4	2.49	46.00	1.00	3.52
2	1049	−4.19	0	−3.23	−2.93	0.29	4	2.49	46.00	1.00	3.52
19	1023	−4.20	0	−2.98	−2.81	0.16	4	2.51	40.00	1.00	3.39
25	941	−4.20	0	−3.20	−2.93	0.27	4	2.50	47.00	1.00	3.41
27	884	−4.21	0	−3.17	−2.97	0.19	4	2.51	44.00	1.00	3.27
17	752	−4.21	0	−2.91	−2.70	0.20	4	2.50	45.00	1.00	3.39
39	725	−4.22	0	−3.16	−2.97	0.18	4	2.49	49.00	1.00	3.15
14	659	−4.22	0	−3.18	−2.94	0.24	4	2.50	45.00	1.00	3.56
3	633	−4.22	0	−3.27	−2.93	0.34	4	2.44	44.00	1.00	3.53
5	502	−4.23	0	−3.14	−2.98	0.16	4	2.50	44.00	1.00	3.34
13	487	−4.23	0	−3.13	−2.96	0.16	5	2.54	49.00	1.00	3.05
4	0	−4.26	0	−3.14	−2.90	0.23	4	2.52	48.00	1.00	2.79

*Mo$_{15}$ configuration 30 was excluded from the set.

Table SI25: Lowest energy configurations for Mo$_n$ clusters with $n = 2 - 15$.

Mo$_2$

Mo$_3$

Mo$_4$

Mo$_5$

Mo$_6$

Mo$_7$

Mo$_8$

Mo$_9$

Mo$_{10}$

Mo$_{11}$

Mo$_{12}$

Mo$_{13}$

Mo$_{14}$

Mo$_{15}$
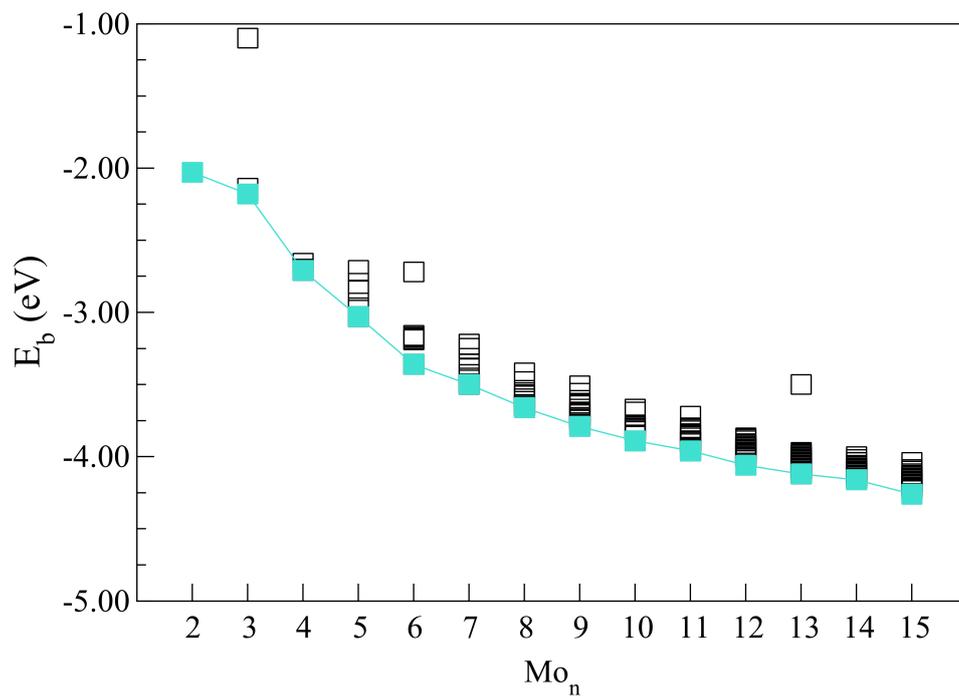
Figure SI11: Binding energy (E_b) for Mo$_n$ clusters with $n = 2 - 15$.
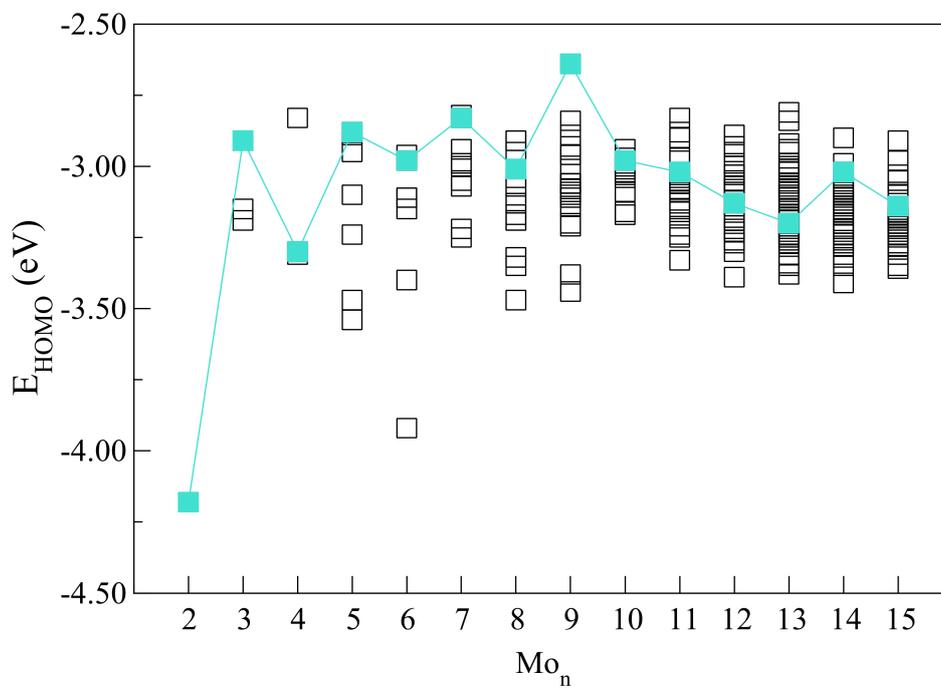
Figure SI12: HOMO energy (E_{HOMO}) for Mo$_n$ clusters with $n = 2 - 15$.
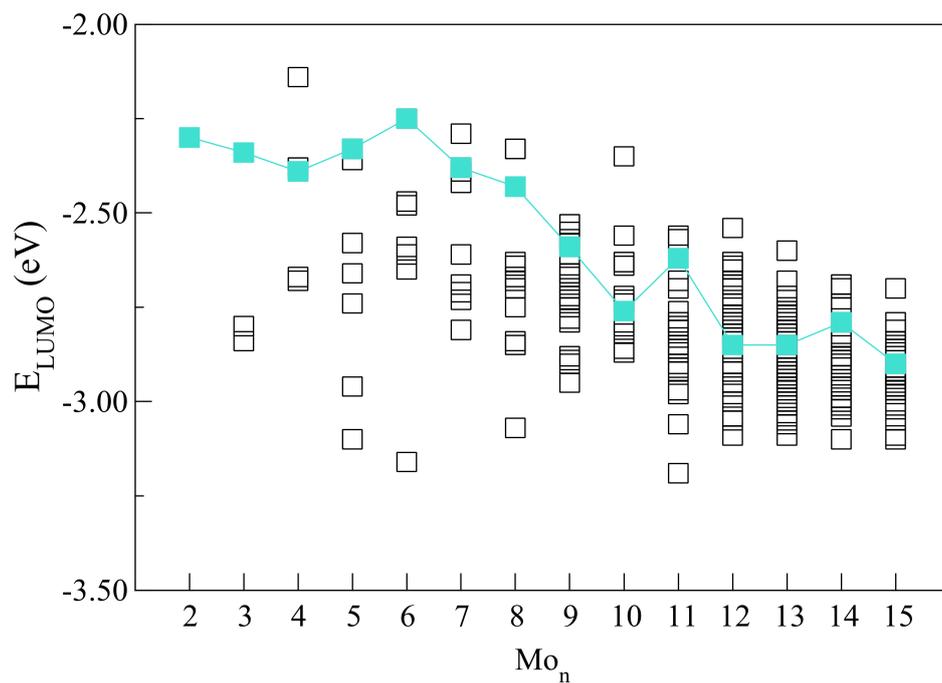
Figure SI13: LUMO energy (E_{HOMO}) for Mo$_n$ clusters with $n = 2 - 15$.
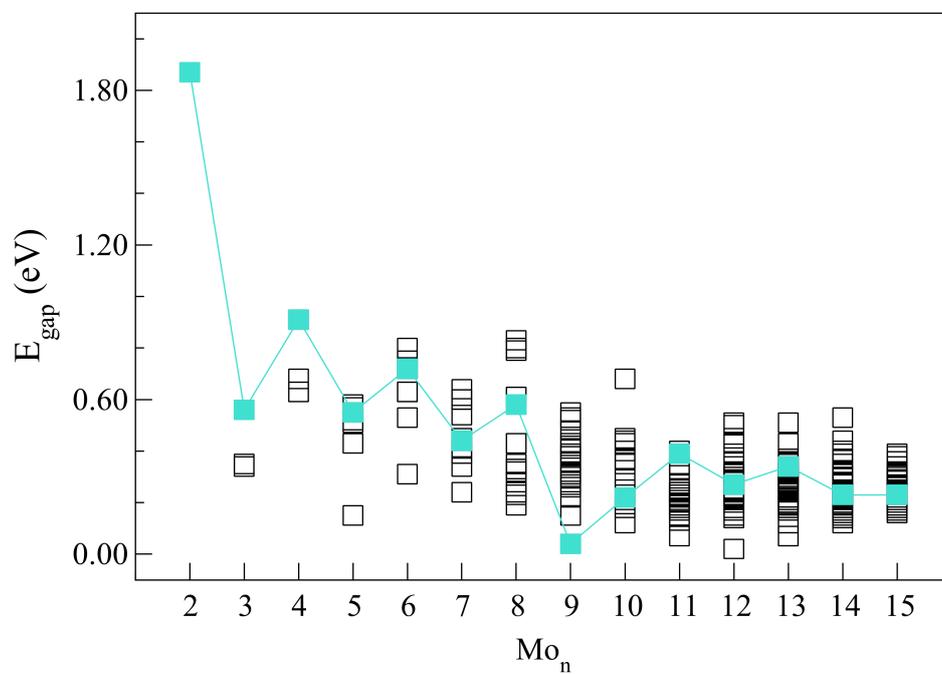
Figure SI14: HOMO-LUMO energy gap (E_{gap}) for Mo$_n$ clusters with $n = 2 - 15$.
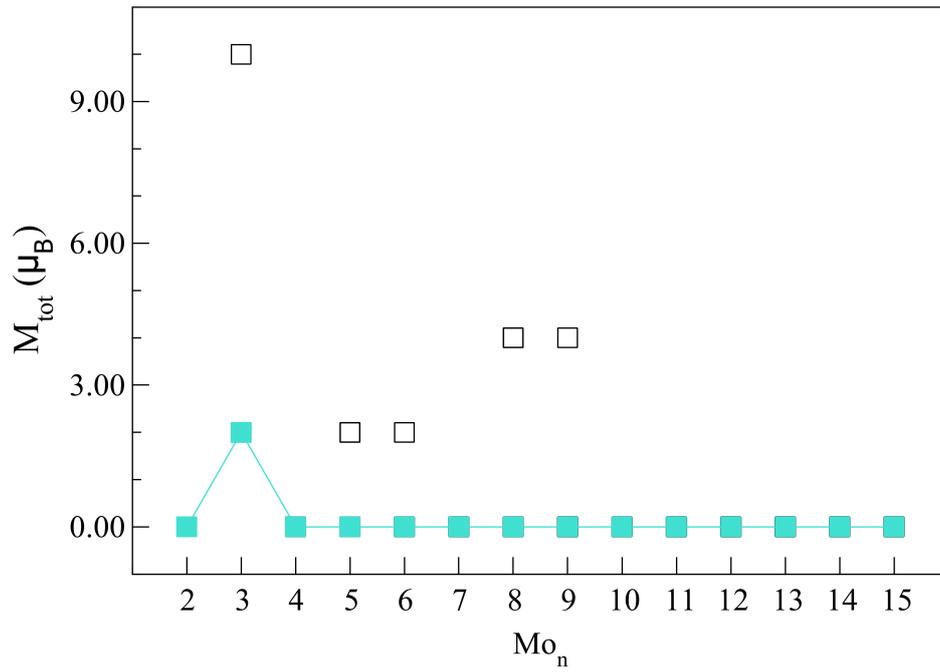
Figure SI15: Total magnetic moment (M_{tot}) for Mo$_n$ clusters with $n = 2 - 15$.
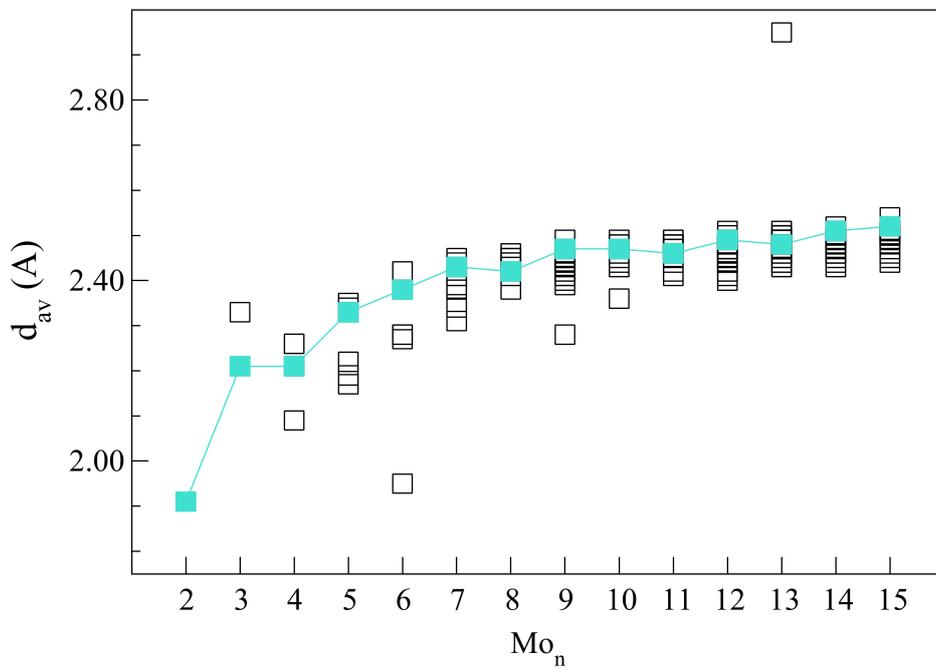
Figure SI16: Average bond length (d_{av}) for Mo$_n$ clusters with $n = 2 - 15$.

Figure SI17: Average effective coordination number (ECN_{av}) for Mo_n clusters with $n = 2 - 15$.

Figure SI18: Total number of bonds (N_b) for Mo_n clusters with $n = 2 - 15$.

Figure SI19: Average chemical order parameter (σ_{av}) for Mo$_n$ clusters with $n = 2 - 15$.

Figure SI20: Average radius (R_{av}) for Mo$_n$ clusters with $n = 2 - 15$.

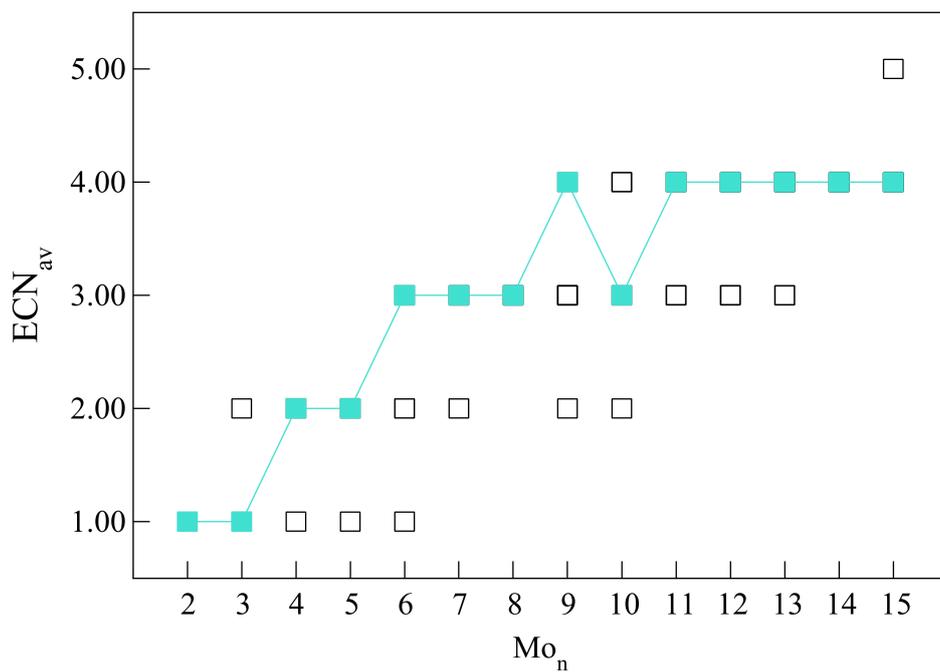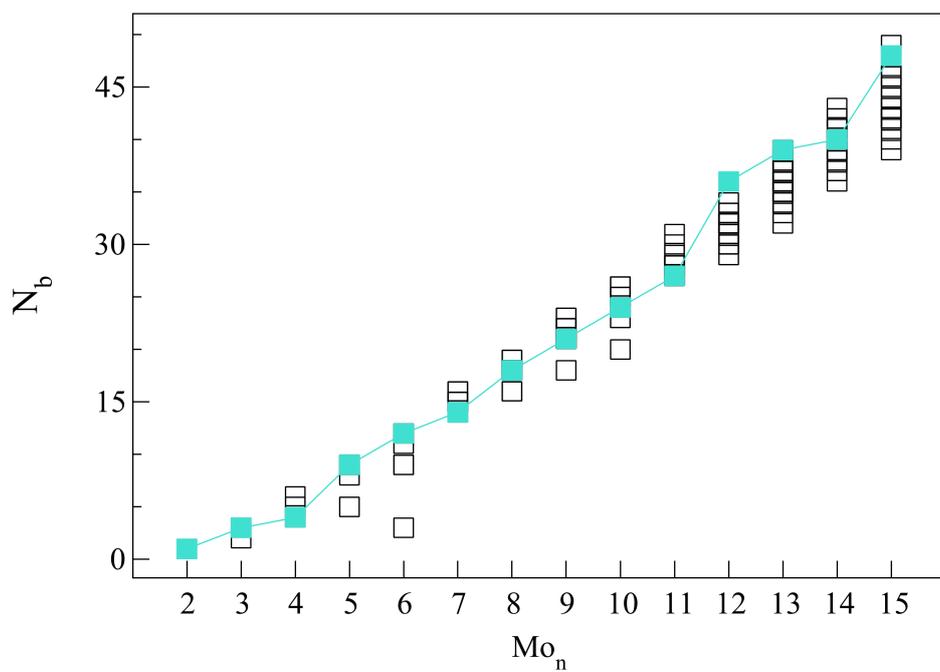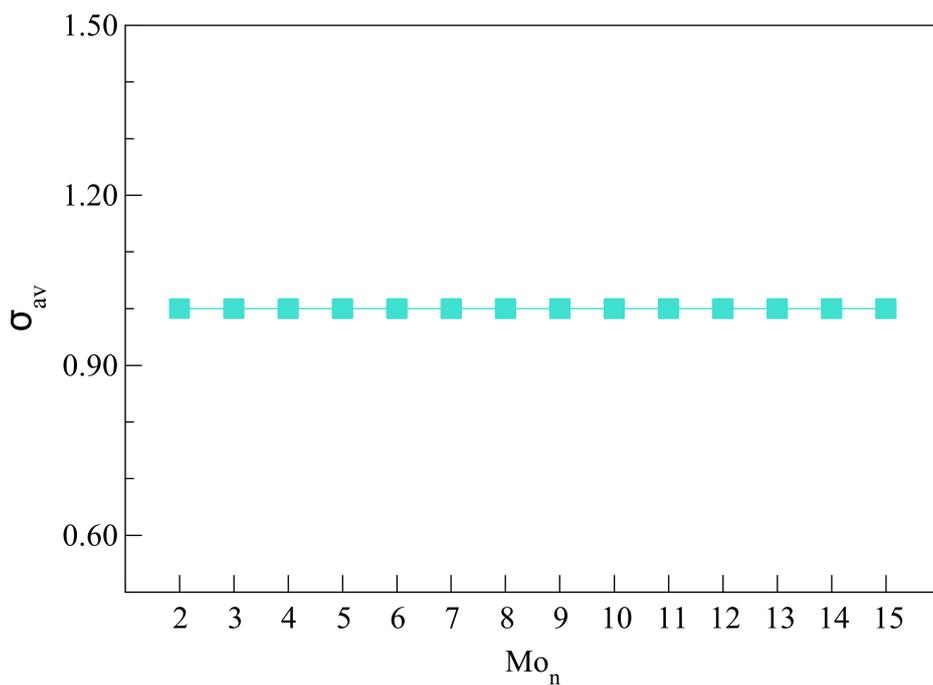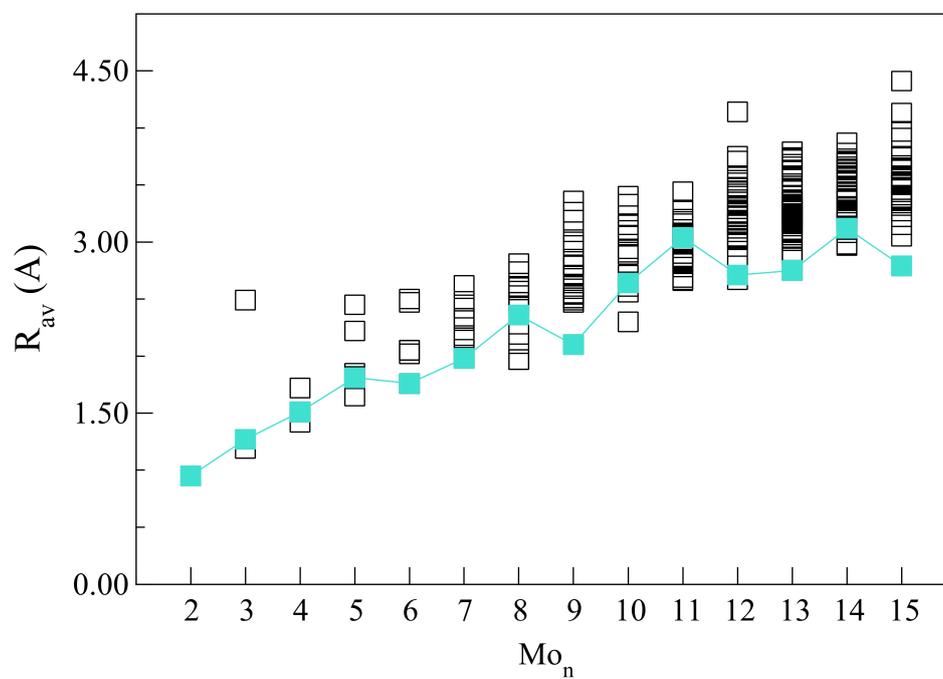# 4 Gas-phase Co$_n$Mo$_m$ Subnanoalloys

Table SI26: Structural, energetic and electronic properties for CoMo cluster, as follows: configuration number (i), relative DFT total energy (ΔE_{tot}^{DFT}, in meV), binding energy (E_b, in eV), excess energy (E_{exc}, in eV), stabilization energy (E_{stab}, in eV), total magnetic moment (M_{tot}, in μ_B), HOMO energy (ε_{HOMO}, in eV), LUMO energy (ε_{LUMO}, in eV), HOMO-LUMO energy difference, (E_{gap}, in eV), total number of bonds (N_b), average chemical order parameter (σ_{av}), average bond length (d_{av}, in Å), average effective coordination number (ECN_{av}, NNN), and average radius (R_{av}, in Å).

i	ΔE_{tot}^{DFT}	E_b	E_{exc}	E_{stab}	M_{tot}	ε_{HOMO}	ε_{LUMO}	E_{gap}	N_b	σ_{av}	d_{av}	ECN_{av}	R_{av}
2	0	−0.99	0.63	−0.99	3	−3.44	−3.05	0.38	1	−1.00	1.97	1.00	0.98
1	0	−0.99	0.63	−0.99	3	−3.44	−3.05	0.38	1	−1.00	1.97	1.00	0.98

Table SI27: Structural, energetic and electronic properties for Co$_2$Mo cluster, as follows: configuration number (i), relative DFT total energy (ΔE_{tot}^{DFT}, in meV), binding energy (E_b, in eV), excess energy (E_{exc}, in eV), stabilization energy (E_{stab}, in eV), total magnetic moment (M_{tot}, in μ_B), HOMO energy (ε_{HOMO}, in eV), LUMO energy (ε_{LUMO}, in eV), HOMO-LUMO energy difference, (E_{gap}, in eV), total number of bonds (N_b), average chemical order parameter (σ_{av}), average bond length (d_{av}, in Å), average effective coordination number (ECN_{av}, NNN), and average radius (R_{av}, in Å).

i	ΔE_{tot}^{DFT}	E_b	E_{exc}	E_{stab}	M_{tot}	ε_{HOMO}	ε_{LUMO}	E_{gap}	N_b	σ_{av}	d_{av}	ECN_{av}	R_{av}
2	121	−1.58	0.23	−0.74	4	−3.43	−3.03	0.39	3	−0.33	2.12	1.58	1.32
1	0	−1.62	0.19	−0.78	8	−3.64	−3.01	0.63	3	−0.33	2.22	1.85	1.28
3	0	−1.62	0.19	−0.78	8	−3.64	−3.01	0.63	3	−0.33	2.22	1.85	1.28

Table SI28: Structural, energetic and electronic properties for Co$_2$Mo$_2$ cluster, as follows: configuration number (i), relative DFT total energy (ΔE_{tot}^{DFT}, in meV), binding energy (E_b, in eV), excess energy (E_{exc}, in eV), stabilization energy (E_{stab}, in eV), total magnetic moment (M_{tot}, in μ_B), HOMO energy (ε_{HOMO}, in eV), LUMO energy (ε_{LUMO}, in eV), HOMO-LUMO energy difference, (E_{gap}, in eV), total number of bonds (N_b), average chemical order parameter (σ_{av}), average bond length (d_{av}, in Å), average effective coordination number (ECN_{av}, NNN), and average radius (R_{av}, in Å).

i	ΔE_{tot}^{DFT}	E_b	E_{exc}	E_{stab}	M_{tot}	ε_{HOMO}	ε_{LUMO}	E_{gap}	N_b	σ_{av}	d_{av}	ECN_{av}	R_{av}
2	724	−2.17	−0.12	−0.52	6	−3.04	−2.63	0.41	6	−0.33	2.28	2.71	1.40
5	723	−2.17	−0.12	−0.52	6	−3.04	−2.63	0.40	6	−0.33	2.28	2.71	1.40
6	1	−2.35	−0.05	−0.70	4	−3.29	−2.97	0.32	6	−0.33	2.20	2.14	1.49
3	0	−2.35	−0.05	−0.70	4	−3.29	−2.97	0.32	5	−0.20	2.20	2.13	1.49
4	0	−2.35	−0.05	−0.70	4	−3.29	−2.97	0.32	5	−0.20	2.20	2.13	1.49
1	0	−2.35	−0.05	−0.70	4	−3.29	−2.97	0.32	5	−0.20	2.20	2.14	1.49

Table SI29: Structural, energetic and electronic properties for Co_3Mo_2 cluster, as follows: configuration number (i), relative DFT total energy (ΔE_{tot}^{DFT}, in meV), binding energy (E_b, in eV), excess energy (E_{exc}, in eV), stabilization energy (E_{stab}, in eV), total magnetic moment (M_{tot}, in μ_B), HOMO energy (ε_{HOMO}, in eV), LUMO energy (ε_{LUMO}, in eV), HOMO-LUMO energy difference, (E_{gap}, in eV), total number of bonds (N_b), average chemical order parameter (σ_{av}), average bond length (d_{av}, in Å), average effective coordination number (ECN_{av}, NNN), and average radius (R_{av}, in Å).

i	ΔE_{tot}^{DFT}	E_b	E_{exc}	E_{stab}	M_{tot}	ε_{HOMO}	ε_{LUMO}	E_{gap}	N_b	σ_{av}	d_{av}	ECN_{av}	R_{av}
1	1315	−2.34	0.23	−0.52	7	−3.33	−3.20	0.12	9	−0.33	2.28	2.91	1.60
8	94	−2.59	−0.01	−0.76	5	−3.28	−2.83	0.45	9	−0.33	2.30	3.05	1.98
0	93	−2.59	−0.01	−0.76	5	−3.28	−2.83	0.45	9	−0.33	2.30	3.04	1.98
9	69	−2.59	−0.01	−0.77	7	−3.50	−3.25	0.24	9	−0.33	2.30	2.83	1.87
7	59	−2.59	−0.01	−0.77	7	−3.58	−3.22	0.36	9	−0.11	2.26	2.74	1.63
3	58	−2.59	−0.01	−0.77	7	−3.58	−3.22	0.35	9	−0.11	2.26	2.74	1.63
6	58	−2.59	−0.01	−0.77	7	−3.58	−3.22	0.36	9	−0.11	2.26	2.74	1.63
2	58	−2.59	−0.01	−0.77	7	−3.58	−3.22	0.36	9	−0.11	2.26	2.74	1.63
5	58	−2.59	−0.01	−0.77	7	−3.58	−3.22	0.36	9	−0.11	2.26	2.74	1.63
4	0	−2.61	−0.02	−0.78	7	−3.59	−3.36	0.22	9	−0.11	2.26	2.77	1.75

Table SI30: Structural, energetic and electronic properties for Co_3Mo_3 cluster, as follows: configuration number (i), relative DFT total energy (ΔE_{tot}^{DFT}, in meV), binding energy (E_b, in eV), excess energy (E_{exc}, in eV), stabilization energy (E_{stab}, in eV), total magnetic moment (M_{tot}, in μ_B), HOMO energy (ε_{HOMO}, in eV), LUMO energy (ε_{LUMO}, in eV), HOMO-LUMO energy difference, (E_{gap}, in eV), total number of bonds (N_b), average chemical order parameter (σ_{av}), average bond length (d_{av}, in Å), average effective coordination number (ECN_{av}, NNN), and average radius (R_{av}, in Å).

i	ΔE_{tot}^{DFT}	E_b	E_{exc}	E_{stab}	M_{tot}	ε_{HOMO}	ε_{LUMO}	E_{gap}	N_b	σ_{av}	d_{av}	ECN_{av}	R_{av}
19	643	−2.92	−0.22	−0.99	5	−3.15	−2.87	0.28	12	−0.33	2.34	3.97	1.68
13	643	−2.92	−0.22	−0.99	5	−3.15	−2.87	0.28	12	−0.33	2.34	3.97	1.68
5	643	−2.92	−0.22	−0.99	5	−3.15	−2.87	0.27	12	−0.33	2.34	3.97	1.68
9	643	−2.92	−0.22	−0.99	5	−3.15	−2.87	0.27	12	−0.33	2.34	3.97	1.68
3	643	−2.92	−0.22	−0.99	5	−3.15	−2.87	0.28	12	−0.33	2.34	3.97	1.68
7	642	−2.92	−0.22	−0.99	5	−3.15	−2.87	0.28	12	−0.33	2.34	3.97	1.68
12	642	−2.92	−0.22	−0.99	5	−3.15	−2.87	0.27	12	−0.33	2.34	3.97	1.68
14	642	−2.92	−0.22	−0.99	5	−3.15	−2.87	0.28	12	−0.33	2.34	3.97	1.68
18	642	−2.92	−0.22	−0.99	5	−3.15	−2.87	0.28	12	−0.33	2.34	3.97	1.68
16	642	−2.92	−0.22	−0.99	5	−3.15	−2.87	0.27	12	−0.33	2.34	3.97	1.68
8	642	−2.92	−0.22	−0.99	5	−3.15	−2.87	0.27	12	−0.33	2.34	3.97	1.68
2	642	−2.92	−0.22	−0.99	5	−3.15	−2.87	0.27	12	−0.33	2.34	3.97	1.68
10	0	−3.03	−0.33	−1.09	5	−3.42	−3.10	0.31	12	0.00	2.34	3.98	1.66
11	0	−3.03	−0.33	−1.09	5	−3.42	−3.10	0.31	12	0.00	2.34	3.98	1.66
1	0	−3.03	−0.33	−1.09	5	−3.42	−3.11	0.31	12	0.00	2.34	3.98	1.66
6	0	−3.03	−0.33	−1.09	5	−3.42	−3.10	0.31	12	0.00	2.34	3.98	1.66
17	0	−3.03	−0.33	−1.09	5	−3.42	−3.10	0.31	12	0.00	2.34	3.98	1.66
4	0	−3.03	−0.33	−1.09	5	−3.42	−3.10	0.31	12	0.00	2.34	3.98	1.66
20	0	−3.03	−0.33	−1.09	5	−3.42	−3.11	0.31	12	0.00	2.34	3.98	1.66
15	0	−3.03	−0.33	−1.09	5	−3.42	−3.10	0.31	12	0.00	2.34	3.98	1.66

Table SI31: Structural, energetic and electronic properties for Co$_4$Mo$_3$ cluster, as follows: configuration number (i), relative DFT total energy (ΔE_{tot}^{DFT}, in meV), binding energy (E_b, in eV), excess energy (E_{exc}, in eV), stabilization energy (E_{stab}, in eV), total magnetic moment (M_{tot}, in μ_B), HOMO energy (ε_{HOMO}, in eV), LUMO energy (ε_{LUMO}, in eV), HOMO-LUMO energy difference, (E_{gap}, in eV), total number of bonds (N_b), average chemical order parameter (σ_{av}), average bond length (d_{av}, in Å), average effective coordination number (ECN_{av}, NNN), and average radius (R_{av}, in Å).

i	ΔE_{tot}^{DFT}	E_b	E_{exc}	E_{stab}	M_{tot}	ε_{HOMO}	ε_{LUMO}	E_{gap}	N_b	σ_{av}	d_{av}	ECN_{av}	R_{av}
24	1616	−2.88	−0.09	−0.70	8	−3.64	−3.32	0.31	15	−0.20	2.33	4.18	2.25
30	1615	−2.88	−0.09	−0.70	8	−3.64	−3.32	0.31	15	−0.20	2.33	4.18	2.25
17	1615	−2.88	−0.09	−0.70	8	−3.64	−3.32	0.31	15	−0.20	2.33	4.18	2.25
20	1249	−2.93	−0.14	−0.75	6	−3.37	−3.06	0.30	15	−0.33	2.33	3.88	2.28
35	1249	−2.93	−0.14	−0.75	6	−3.37	−3.06	0.30	15	−0.33	2.33	3.88	2.28
7	1248	−2.93	−0.14	−0.75	6	−3.37	−3.06	0.30	15	−0.33	2.33	3.88	2.28
16	714	−3.01	−0.22	−0.82	8	−3.37	−3.09	0.27	15	−0.20	2.36	4.16	2.29
1	714	−3.01	−0.22	−0.82	8	−3.37	−3.09	0.27	15	−0.20	2.36	4.16	2.29
25	713	−3.01	−0.22	−0.82	8	−3.37	−3.09	0.27	15	−0.20	2.36	4.16	2.29
31	713	−3.01	−0.22	−0.82	8	−3.37	−3.09	0.27	15	−0.20	2.36	4.16	2.29
22	713	−3.01	−0.22	−0.82	8	−3.37	−3.09	0.27	15	−0.20	2.36	4.16	2.29
9	712	−3.01	−0.22	−0.82	8	−3.37	−3.09	0.27	15	−0.20	2.36	4.16	2.29
8	624	−3.02	−0.23	−0.84	6	−3.40	−3.14	0.25	15	−0.33	2.37	4.17	2.32
21	624	−3.02	−0.23	−0.84	6	−3.40	−3.14	0.26	15	−0.33	2.37	4.17	2.32
34	597	−3.02	−0.23	−0.84	8	−3.42	−3.14	0.28	15	−0.33	2.37	4.14	2.33
15	596	−3.02	−0.23	−0.84	8	−3.43	−3.14	0.28	15	−0.33	2.37	4.14	2.33
13	538	−3.03	−0.24	−0.85	8	−3.52	−3.27	0.24	15	0.06	2.35	3.97	2.27
32	537	−3.03	−0.24	−0.85	8	−3.52	−3.27	0.25	15	0.06	2.35	3.97	2.27
10	537	−3.03	−0.24	−0.85	8	−3.52	−3.26	0.25	15	0.06	2.35	3.97	2.27
3	497	−3.04	−0.25	−0.86	10	−3.32	−3.21	0.10	16	0.00	2.36	3.93	1.92
26	304	−3.06	−0.28	−0.88	8	−3.45	−3.12	0.33	16	0.00	2.36	4.06	1.89
23	304	−3.06	−0.28	−0.88	8	−3.46	−3.12	0.33	16	0.00	2.36	4.06	1.89
33	303	−3.06	−0.28	−0.88	8	−3.45	−3.12	0.33	16	0.00	2.36	4.06	1.89
29	303	−3.06	−0.28	−0.88	8	−3.46	−3.12	0.33	16	0.00	2.36	4.06	1.89
14	273	−3.07	−0.28	−0.89	8	−3.47	−3.16	0.30	15	0.06	2.34	3.83	2.07
05	272	−3.07	−0.28	−0.89	6	−3.27	−3.15	0.12	15	0.06	2.36	4.21	2.30
28	272	−3.07	−0.28	−0.89	6	−3.27	−3.15	0.11	15	0.06	2.36	4.21	2.30
4	135	−3.09	−0.30	−0.91	6	−3.35	−3.14	0.20	15	−0.06	2.36	4.19	2.22
12	134	−3.09	−0.30	−0.91	6	−3.35	−3.14	0.20	15	−0.06	2.36	4.19	2.21
27	97	−3.09	−0.30	−0.91	8	−3.56	−3.26	0.29	15	−0.06	2.37	4.08	2.19
18	84	−3.10	−0.31	−0.91	8	−3.48	−3.07	0.40	15	0.06	2.36	4.08	2.22
19	27	−3.10	−0.31	−0.92	8	−3.52	−3.15	0.37	15	0.20	2.36	4.21	2.25
11	0	−3.11	−0.32	−0.93	8	−3.68	−3.37	0.31	15	−0.20	2.39	4.25	2.35

Table SI32: Structural, energetic and electronic properties for Co$_4$Mo$_4$ cluster, as follows: configuration number (i), relative DFT total energy (ΔE_{tot}^{DFT}, in meV), binding energy (E_b, in eV), excess energy (E_{exc}, in eV), stabilization energy (E_{stab}, in eV), total magnetic moment (M_{tot}, in μ_B), HOMO energy (ε_{HOMO}, in eV), LUMO energy (ε_{LUMO}, in eV), HOMO-LUMO energy difference, (E_{gap}, in eV), total number of bonds (N_b), average chemical order parameter (σ_{av}), average bond length (d_{av}, in Å), average effective coordination number (ECN_{av}, NNN), and average radius (R_{av}, in Å).

i	ΔE_{tot}^{DFT}	E_b	E_{exc}	E_{stab}	M_{tot}	ε_{HOMO}	ε_{LUMO}	E_{gap}	N_b	σ_{av}	d_{av}	ECN_{av}	R_{av}
53	1059	−3.14	−0.29	−0.69	6	−3.18	−3.01	0.17	20	−0.20	2.37	4.36	2.20
56	1059	−3.14	−0.29	−0.69	6	−3.18	−3.00	0.17	20	−0.20	2.37	4.36	2.20

68	1058	−3.14	−0.29	−0.69	6	−3.18	−3.00	0.17	20	−0.20	2.37	4.36	2.20
30	1056	−3.14	−0.29	−0.69	6	−3.18	−3.01	0.17	20	−0.20	2.37	4.36	2.20
57	866	−3.16	−0.31	−0.72	6	−3.27	−2.99	0.28	20	−0.40	2.39	4.22	2.29
31	865	−3.16	−0.31	−0.72	6	−3.27	−2.99	0.28	20	−0.40	2.39	4.22	2.29
40	864	−3.16	−0.31	−0.72	6	−3.27	−2.99	0.28	20	−0.40	2.39	4.22	2.29
14	864	−3.16	−0.31	−0.72	6	−3.27	−2.99	0.28	20	−0.40	2.39	4.22	2.29
60	714	−3.18	−0.33	−0.74	8	−3.29	−3.15	0.14	18	−0.00	2.35	3.73	2.11
70	713	−3.18	−0.33	−0.74	8	−3.29	−3.15	0.13	18	−0.00	2.35	3.73	2.11
52	705	−3.18	−0.33	−0.74	8	−3.46	−3.16	0.30	18	−0.33	2.39	4.14	2.19
16	704	−3.18	−0.33	−0.74	8	−3.46	−3.16	0.30	18	−0.33	2.39	4.14	2.19
55	703	−3.18	−0.33	−0.74	8	−3.46	−3.16	0.30	18	−0.33	2.39	4.14	2.19
20	703	−3.18	−0.33	−0.74	8	−3.46	−3.16	0.30	18	−0.33	2.39	4.14	2.19
63	700	−3.18	−0.33	−0.74	8	−3.39	−3.12	0.27	20	−0.20	2.35	3.98	2.23
58	700	−3.18	−0.33	−0.74	8	−3.39	−3.12	0.27	20	−0.20	2.35	3.99	2.23
46	700	−3.18	−0.33	−0.74	8	−3.39	−3.12	0.27	20	−0.20	2.35	3.99	2.23
28	699	−3.18	−0.33	−0.74	8	−3.39	−3.12	0.27	20	−0.20	2.35	3.98	2.23
33	699	−3.18	−0.33	−0.74	8	−3.39	−3.12	0.27	20	−0.20	2.35	3.98	2.23
50	699	−3.18	−0.33	−0.74	8	−3.39	−3.12	0.27	20	−0.20	2.35	3.98	2.23
26	699	−3.18	−0.33	−0.74	10	−3.36	−3.18	0.18	19	−0.05	2.36	3.81	2.12
69	699	−3.18	−0.33	−0.74	8	−3.39	−3.12	0.27	20	−0.20	2.35	3.99	2.23
66	698	−3.18	−0.33	−0.74	8	−3.39	−3.12	0.27	20	−0.20	2.35	3.99	2.23
48	697	−3.18	−0.33	−0.74	10	−3.36	−3.18	0.18	19	−0.05	2.36	3.81	2.12
44	642	−3.19	−0.34	−0.74	6	−3.37	−3.06	0.31	19	−0.15	2.38	4.16	2.23
27	641	−3.19	−0.34	−0.74	6	−3.37	−3.06	0.31	20	−0.20	2.38	4.15	2.23
35	641	−3.19	−0.34	−0.74	6	−3.37	−3.07	0.30	19	−0.15	2.38	4.15	2.23
10	640	−3.19	−0.34	−0.74	6	−3.37	−3.06	0.31	20	−0.20	2.38	4.16	2.23
9	640	−3.19	−0.34	−0.74	6	−3.37	−3.05	0.31	20	−0.20	2.38	4.16	2.23
61	639	−3.19	−0.34	−0.74	6	−3.37	−3.06	0.31	18	−0.11	2.38	4.16	2.23
36	639	−3.19	−0.34	−0.74	6	−3.37	−3.06	0.31	20	−0.20	2.38	4.16	2.23
62	639	−3.19	−0.34	−0.74	6	−3.37	−3.06	0.31	19	−0.15	2.38	4.16	2.23
67	608	−3.19	−0.35	−0.75	10	−3.40	−3.11	0.29	20	−0.20	2.36	4.07	2.21
22	559	−3.20	−0.35	−0.75	6	−3.27	−3.01	0.26	19	−0.26	2.39	4.41	2.15
49	558	−3.20	−0.35	−0.75	6	−3.27	−3.01	0.26	19	−0.26	2.39	4.41	2.15
17	337	−3.23	−0.38	−0.78	6	−3.32	−2.99	0.32	20	0.20	2.39	4.41	2.22
54	337	−3.23	−0.38	−0.78	6	−3.31	−2.99	0.32	20	0.20	2.39	4.41	2.22
41	206	−3.24	−0.40	−0.80	6	−3.36	−3.12	0.24	19	−0.15	2.40	4.37	2.29
23	199	−3.24	−0.40	−0.80	8	−3.40	−3.14	0.25	20	0.00	2.39	4.32	2.17
45	163	−3.25	−0.40	−0.80	6	−3.36	−3.14	0.22	19	0.05	2.40	4.43	2.18
1	163	−3.25	−0.40	−0.80	6	−3.36	−3.14	0.21	20	0.00	2.40	4.43	2.18
11	162	−3.25	−0.40	−0.80	6	−3.36	−3.14	0.22	20	0.00	2.40	4.43	2.18
38	161	−3.25	−0.40	−0.80	6	−3.42	−3.12	0.29	19	−0.15	2.42	4.45	2.26
65	161	−3.25	−0.40	−0.80	8	−3.18	−2.98	0.19	18	0.11	2.38	4.20	2.13
13	161	−3.25	−0.40	−0.80	6	−3.42	−3.12	0.29	19	−0.15	2.42	4.45	2.26
8	161	−3.25	−0.40	−0.80	6	−3.42	−3.12	0.29	19	−0.15	2.42	4.45	2.26
2	161	−3.25	−0.40	−0.80	6	−3.42	−3.12	0.29	19	−0.15	2.42	4.45	2.26
5	161	−3.25	−0.40	−0.80	6	−3.42	−3.12	0.29	19	−0.15	2.42	4.45	2.26
21	161	−3.25	−0.40	−0.80	6	−3.42	−3.12	0.29	19	−0.15	2.42	4.45	2.26
43	161	−3.25	−0.40	−0.80	6	−3.42	−3.12	0.29	19	−0.15	2.42	4.45	2.26
25	159	−3.25	−0.40	−0.80	6	−3.42	−3.12	0.29	19	−0.15	2.42	4.45	2.26
39	136	−3.25	−0.40	−0.81	8	−3.23	−3.00	0.22	19	0.05	2.38	4.20	2.16
06	135	−3.25	−0.40	−0.81	8	−3.23	−3.00	0.22	19	0.05	2.38	4.20	2.16
32	133	−3.25	−0.40	−0.81	8	−3.23	−3.00	0.22	18	0.11	2.38	4.20	2.16
15	118	−3.25	−0.41	−0.81	6	−3.40	−3.05	0.35	20	−0.20	2.38	4.09	2.31
18	118	−3.25	−0.41	−0.81	6	−3.40	−3.05	0.35	20	−0.20	2.38	4.09	2.31
12	75	−3.26	−0.41	−0.82	6	−3.26	−3.00	0.26	20	0.00	2.37	4.21	2.24
42	73	−3.26	−0.41	−0.82	6	−3.26	−3.00	0.26	20	0.00	2.37	4.21	2.24
64	73	−3.26	−0.41	−0.82	6	−3.26	−3.00	0.26	19	0.05	2.37	4.21	2.24

i	ΔE_{tot}^{DFT}	E_b	E_{exc}	E_{stab}	M_{tot}	ε_{HOMO}	ε_{LUMO}	E_{gap}	N_b	σ_{av}	d_{av}	ECN_{av}	R_{av}
29	72	−3.26	−0.41	−0.82	6	−3.26	−3.00	0.25	20	0.00	2.37	4.21	2.24
37	72	−3.26	−0.41	−0.82	6	−3.26	−3.00	0.25	19	0.05	2.37	4.21	2.24
59	72	−3.26	−0.41	−0.82	6	−3.26	−3.00	0.25	19	0.05	2.37	4.21	2.24
34	72	−3.26	−0.41	−0.82	6	−3.26	−3.00	0.26	19	0.05	2.37	4.21	2.24
7	71	−3.26	−0.41	−0.82	6	−3.26	−3.00	0.26	20	0.00	2.37	4.21	2.24
4	0	−3.27	−0.42	−0.82	6	−3.42	−3.12	0.29	20	−0.20	2.40	4.47	2.18

Table SI33: Structural, energetic and electronic properties for Co_5Mo_4 cluster, as follows: configuration number (i), relative DFT total energy (ΔE_{tot}^{DFT}, in meV), binding energy (E_b, in eV), excess energy (E_{exc}, in eV), stabilization energy (E_{stab}, in eV), total magnetic moment (M_{tot}, in μ_B), HOMO energy (ε_{HOMO}, in eV), LUMO energy (ε_{LUMO}, in eV), HOMO-LUMO energy difference, (E_{gap}, in eV), total number of bonds (N_b), average chemical order parameter (σ_{av}), average bond length (d_{av}, in Å), average effective coordination number (ECN_{av}, NNN), and average radius (R_{av}, in Å).

i	ΔE_{tot}^{DFT}	E_b	E_{exc}	E_{stab}	M_{tot}	ε_{HOMO}	ε_{LUMO}	E_{gap}	N_b	σ_{av}	d_{av}	ECN_{av}	R_{av}
17	1335	−3.19	−0.28	−0.61	5	−3.23	−3.04	0.18	21	−0.23	2.35	4.36	2.20
91	1334	−3.19	−0.28	−0.61	5	−3.23	−3.04	0.19	21	−0.23	2.35	4.36	2.20
16	920	−3.24	−0.33	−0.66	5	−3.29	−3.11	0.17	21	−0.14	2.36	4.30	2.29
88	919	−3.24	−0.33	−0.66	5	−3.29	−3.11	0.17	21	−0.14	2.36	4.30	2.29
56	919	−3.24	−0.33	−0.66	5	−3.29	−3.11	0.17	21	−0.14	2.36	4.30	2.29
7	855	−3.24	−0.33	−0.66	5	−3.22	−3.17	0.05	21	−0.33	2.36	4.42	2.29
52	855	−3.24	−0.33	−0.66	5	−3.22	−3.17	0.05	21	−0.33	2.36	4.43	2.29
66	752	−3.25	−0.34	−0.67	7	−3.38	−3.21	0.17	21	−0.14	2.35	4.14	2.27
39	751	−3.25	−0.34	−0.67	7	−3.38	−3.21	0.17	21	−0.14	2.35	4.14	2.27
87	751	−3.25	−0.34	−0.67	7	−3.38	−3.21	0.17	21	−0.14	2.35	4.14	2.27
42	750	−3.25	−0.34	−0.67	7	−3.38	−3.21	0.17	21	−0.14	2.35	4.14	2.27
25	658	−3.26	−0.36	−0.68	7	−3.48	−3.11	0.37	21	−0.33	2.36	4.33	2.28
31	658	−3.26	−0.36	−0.68	7	−3.48	−3.11	0.37	21	−0.33	2.36	4.33	2.28
94	647	−3.27	−0.36	−0.69	9	−3.39	−3.16	0.23	21	−0.04	2.35	3.98	2.29
73	647	−3.27	−0.36	−0.69	9	−3.39	−3.16	0.23	21	−0.04	2.35	3.97	2.29
64	647	−3.27	−0.36	−0.69	9	−3.39	−3.16	0.23	21	−0.04	2.35	3.98	2.29
41	647	−3.27	−0.36	−0.69	5	−3.46	−3.04	0.41	21	−0.14	2.36	4.52	2.26
96	646	−3.27	−0.36	−0.69	5	−3.46	−3.04	0.41	21	−0.14	2.36	4.52	2.26
32	646	−3.27	−0.36	−0.69	9	−3.39	−3.16	0.23	21	−0.04	2.35	3.97	2.29
53	646	−3.27	−0.36	−0.69	9	−3.39	−3.16	0.23	21	−0.04	2.35	3.98	2.29
46	646	−3.27	−0.36	−0.69	9	−3.39	−3.16	0.23	21	−0.04	2.35	3.97	2.29
19	646	−3.27	−0.36	−0.69	5	−3.46	−3.05	0.41	21	−0.14	2.36	4.52	2.26
85	646	−3.27	−0.36	−0.69	9	−3.39	−3.16	0.23	21	−0.04	2.35	3.98	2.29
43	646	−3.27	−0.36	−0.69	9	−3.39	−3.15	0.23	21	−0.04	2.35	3.97	2.29
37	646	−3.27	−0.36	−0.69	9	−3.39	−3.16	0.23	21	−0.04	2.35	3.98	2.29
40	646	−3.27	−0.36	−0.69	5	−3.46	−3.05	0.41	21	−0.14	2.36	4.52	2.26
57	645	−3.27	−0.36	−0.69	5	−3.46	−3.05	0.41	21	−0.14	2.36	4.52	2.26
89	645	−3.27	−0.36	−0.69	9	−3.39	−3.16	0.23	21	−0.04	2.35	3.97	2.29
86	645	−3.27	−0.36	−0.69	5	−3.47	−3.05	0.41	21	−0.14	2.36	4.52	2.26
59	629	−3.27	−0.36	−0.69	7	−3.46	−3.20	0.26	21	−0.14	2.35	4.21	2.28
76	629	−3.27	−0.36	−0.69	7	−3.46	−3.20	0.26	21	−0.14	2.35	4.21	2.28
18	629	−3.27	−0.36	−0.69	7	−3.46	−3.20	0.26	21	−0.14	2.35	4.21	2.28
14	628	−3.27	−0.36	−0.69	9	−3.40	−3.20	0.20	21	−0.14	2.37	4.28	2.24
47	559	−3.28	−0.37	−0.70	7	−3.36	−3.05	0.31	21	−0.23	2.39	4.57	2.27
74	558	−3.28	−0.37	−0.70	7	−3.36	−3.05	0.31	21	−0.23	2.39	4.57	2.27
10	558	−3.28	−0.37	−0.70	7	−3.36	−3.05	0.31	21	−0.23	2.39	4.57	2.27
26	476	−3.28	−0.38	−0.70	5	−3.38	−3.12	0.25	21	−0.23	2.39	4.55	2.28
27	475	−3.29	−0.38	−0.70	5	−3.38	−3.12	0.25	21	−0.23	2.39	4.55	2.28

60	438	−3.29	−0.38	−0.71	5	−3.39	−3.17	0.21	21	−0.23	2.37	4.46	2.26
78	438	−3.29	−0.38	−0.71	5	−3.39	−3.17	0.21	21	−0.23	2.37	4.46	2.26
0	438	−3.29	−0.38	−0.71	5	−3.39	−3.17	0.21	21	−0.23	2.37	4.46	2.26
38	438	−3.29	−0.38	−0.71	5	−3.39	−3.17	0.21	21	−0.23	2.37	4.46	2.26
51	425	−3.29	−0.38	−0.71	7	−3.39	−3.12	0.26	21	−0.04	2.37	4.31	2.28
71	424	−3.29	−0.38	−0.71	7	−3.39	−3.12	0.26	21	−0.04	2.37	4.31	2.28
12	424	−3.29	−0.38	−0.71	7	−3.39	−3.12	0.26	21	−0.04	2.37	4.31	2.28
34	424	−3.29	−0.38	−0.71	7	−3.39	−3.12	0.26	21	−0.04	2.37	4.31	2.28
03	423	−3.29	−0.38	−0.71	7	−3.39	−3.12	0.26	21	−0.04	2.37	4.31	2.28
54	423	−3.29	−0.38	−0.71	7	−3.39	−3.12	0.26	21	−0.04	2.37	4.31	2.28
61	423	−3.29	−0.38	−0.71	7	−3.39	−3.12	0.26	21	−0.04	2.37	4.31	2.28
35	422	−3.29	−0.38	−0.71	7	−3.39	−3.12	0.26	21	−0.04	2.37	4.31	2.28
65	402	−3.29	−0.38	−0.71	7	−3.46	−3.25	0.20	21	−0.23	2.37	4.31	2.31
80	402	−3.29	−0.38	−0.71	7	−3.46	−3.25	0.20	21	−0.23	2.37	4.31	2.31
9	402	−3.29	−0.38	−0.71	7	−3.46	−3.25	0.20	21	−0.23	2.37	4.31	2.31
24	402	−3.29	−0.38	−0.71	7	−3.46	−3.25	0.20	21	−0.23	2.37	4.31	2.31
62	401	−3.29	−0.38	−0.71	7	−3.46	−3.25	0.20	21	−0.23	2.37	4.31	2.31
4	373	−3.30	−0.39	−0.72	5	−3.39	−3.08	0.31	22	−0.18	2.38	4.47	2.30
36	373	−3.30	−0.39	−0.72	5	−3.39	−3.08	0.31	22	−0.18	2.38	4.47	2.30
2	372	−3.30	−0.39	−0.72	5	−3.39	−3.08	0.31	22	−0.18	2.38	4.47	2.30
55	372	−3.30	−0.39	−0.72	5	−3.39	−3.08	0.31	21	−0.23	2.38	4.47	2.30
99	372	−3.30	−0.39	−0.72	5	−3.39	−3.08	0.31	21	−0.23	2.38	4.47	2.30
84	372	−3.30	−0.39	−0.72	5	−3.39	−3.08	0.31	21	−0.23	2.38	4.47	2.30
20	367	−3.30	−0.39	−0.72	7	−3.36	−3.16	0.20	21	−0.14	2.40	4.61	2.30
72	364	−3.30	−0.39	−0.72	7	−3.31	−3.26	0.05	21	−0.14	2.38	4.55	2.25
15	363	−3.30	−0.39	−0.72	7	−3.31	−3.26	0.05	21	−0.14	2.38	4.55	2.26
22	320	−3.30	−0.39	−0.72	5	−3.43	−3.24	0.18	21	−0.33	2.39	4.50	2.34
21	265	−3.31	−0.40	−0.73	9	−3.45	−3.18	0.27	21	−0.14	2.40	4.55	2.28
68	247	−3.31	−0.40	−0.73	7	−3.31	−3.02	0.28	21	−0.14	2.39	4.58	2.28
92	246	−3.31	−0.40	−0.73	7	−3.31	−3.02	0.28	22	−0.18	2.39	4.57	2.28
44	246	−3.31	−0.40	−0.73	7	−3.31	−3.02	0.28	22	−0.18	2.39	4.58	2.28
48	245	−3.31	−0.40	−0.73	7	−3.31	−3.02	0.28	22	−0.18	2.39	4.58	2.28
69	245	−3.31	−0.40	−0.73	7	−3.31	−3.02	0.28	22	−0.18	2.39	4.58	2.28
33	245	−3.31	−0.40	−0.73	7	−3.31	−3.02	0.28	21	−0.14	2.39	4.58	2.28
01	245	−3.31	−0.40	−0.73	7	−3.31	−3.02	0.28	21	−0.14	2.39	4.58	2.28
83	245	−3.31	−0.40	−0.73	7	−3.31	−3.02	0.28	21	−0.14	2.39	4.57	2.28
95	242	−3.31	−0.40	−0.73	5	−3.51	−3.17	0.33	21	−0.33	2.39	4.44	2.34
75	242	−3.31	−0.40	−0.73	5	−3.51	−3.17	0.33	21	−0.33	2.39	4.44	2.34
5	242	−3.31	−0.40	−0.73	5	−3.51	−3.17	0.33	21	−0.33	2.39	4.44	2.34
58	241	−3.31	−0.40	−0.73	5	−3.50	−3.17	0.33	21	−0.33	2.39	4.44	2.34
93	238	−3.31	−0.40	−0.73	5	−3.34	−3.15	0.18	23	−0.13	2.41	4.52	2.38
67	89	−3.33	−0.42	−0.75	7	−3.33	−3.08	0.24	21	−0.14	2.39	4.59	2.28
13	89	−3.33	−0.42	−0.75	7	−3.33	−3.08	0.24	21	−0.14	2.39	4.59	2.28
77	88	−3.33	−0.42	−0.75	7	−3.33	−3.08	0.24	21	−0.14	2.39	4.59	2.28
11	88	−3.33	−0.42	−0.75	7	−3.33	−3.08	0.24	21	−0.14	2.39	4.59	2.28
50	79	−3.33	−0.42	−0.75	7	−3.34	−3.06	0.27	21	−0.14	2.38	4.38	2.29
98	78	−3.33	−0.42	−0.75	7	−3.34	−3.06	0.27	21	−0.14	2.38	4.38	2.29
70	76	−3.33	−0.42	−0.75	7	−3.34	−3.06	0.27	21	−0.14	2.38	4.38	2.29
08	76	−3.33	−0.42	−0.75	7	−3.34	−3.06	0.27	21	−0.14	2.38	4.38	2.29
28	0	−3.34	−0.43	−0.76	9	−3.22	−2.90	0.31	21	−0.23	2.35	4.15	2.28
23	0	−3.34	−0.43	−0.76	9	−3.22	−2.90	0.31	21	−0.23	2.35	4.15	2.28
30	0	−3.34	−0.43	−0.76	9	−3.22	−2.90	0.31	21	−0.23	2.35	4.15	2.28

Table SI34: Structural, energetic and electronic properties for Co_5Mo_5 cluster, as follows: configuration number (i), relative DFT total energy (ΔE_{tot}^{DFT}, in meV), binding energy (E_b, in eV), excess energy (E_{exc}, in eV), stabilization energy (E_{stab}, in eV), total magnetic moment (M_{tot}, in μ_B), HOMO energy (ε_{HOMO}, in eV), LUMO energy (ε_{LUMO}, in eV), HOMO-LUMO energy difference, (E_{gap}, in eV), total number of bonds (N_b), average chemical order parameter (σ_{av}), average bond length (d_{av}, in Å), average effective coordination number (ECN_{av}, NNN), and average radius (R_{av}, in Å).

i	ΔE_{tot}^{DFT}	E_b	E_{exc}	E_{stab}	M_{tot}	ε_{HOMO}	ε_{LUMO}	E_{gap}	N_b	σ_{av}	d_{av}	ECN_{av}	R_{av}
44	3006	−3.17	−0.16	−0.42	8	−3.41	−3.40	0.00	25	−0.20	2.31	4.94	2.63
42	2846	−3.18	−0.17	−0.43	9	−3.47	−3.43	0.04	25	0.12	2.31	4.94	2.63
45	2835	−3.19	−0.17	−0.43	7	−3.44	−3.43	0.01	25	0.12	2.31	4.94	2.63
96	2125	−3.26	−0.25	−0.50	7	−3.39	−3.34	0.04	25	−0.12	2.31	4.94	2.63
67	2125	−3.26	−0.25	−0.50	6	−3.36	−3.34	0.01	25	−0.12	2.31	4.94	2.63
27	1122	−3.36	−0.35	−0.60	11	−3.57	−3.50	0.07	27	−0.11	2.42	4.79	2.81
31	1021	−3.37	−0.36	−0.61	9	−3.33	−3.13	0.19	26	0.00	2.39	4.58	2.79
11	1015	−3.37	−0.36	−0.61	5	−3.14	−2.98	0.15	26	−0.23	2.38	4.84	2.73
61	1010	−3.37	−0.36	−0.61	7	−3.33	−3.11	0.22	26	−0.15	2.38	4.69	2.72
53	1009	−3.37	−0.36	−0.61	7	−3.33	−3.11	0.22	26	−0.15	2.38	4.69	2.72
50	964	−3.37	−0.36	−0.62	9	−3.41	−3.30	0.11	25	−0.36	2.40	4.81	2.80
04	963	−3.37	−0.36	−0.62	9	−3.41	−3.30	0.11	25	−0.36	2.40	4.81	2.79
12	940	−3.38	−0.36	−0.62	7	−3.10	−2.92	0.18	26	0.00	2.37	4.74	2.69
80	910	−3.38	−0.37	−0.62	11	−3.20	−3.09	0.11	25	−0.20	2.38	4.60	2.73
37	887	−3.38	−0.37	−0.63	5	−3.23	−3.10	0.12	25	0.04	2.38	4.80	2.79
70	886	−3.38	−0.37	−0.63	5	−3.23	−3.10	0.13	25	0.04	2.38	4.80	2.79
97	884	−3.38	−0.37	−0.63	5	−3.23	−3.10	0.13	25	0.04	2.38	4.80	2.79
06	882	−3.38	−0.37	−0.63	5	−3.49	−3.19	0.30	25	−0.20	2.37	4.66	2.81
26	875	−3.38	−0.37	−0.63	9	−3.15	−2.95	0.20	25	0.12	2.39	4.81	2.72
60	875	−3.38	−0.37	−0.63	9	−3.15	−2.95	0.20	25	0.12	2.39	4.81	2.72
46	862	−3.38	−0.37	−0.63	9	−3.38	−3.19	0.18	25	−0.12	2.39	4.59	2.81
29	860	−3.38	−0.37	−0.63	9	−3.22	−3.05	0.17	26	−0.15	2.37	4.53	2.77
65	859	−3.38	−0.37	−0.63	9	−3.38	−3.19	0.19	26	−0.07	2.39	4.60	2.80
52	842	−3.39	−0.37	−0.63	9	−3.18	−3.08	0.10	25	−0.20	2.37	4.56	2.74
83	842	−3.39	−0.37	−0.63	9	−3.18	−3.08	0.10	25	−0.20	2.37	4.56	2.74
35	841	−3.39	−0.37	−0.63	9	−3.18	−3.08	0.10	25	−0.20	2.37	4.56	2.74
84	841	−3.39	−0.37	−0.63	9	−3.18	−3.08	0.10	25	−0.20	2.37	4.56	2.74
05	811	−3.39	−0.38	−0.63	9	−3.43	−3.26	0.16	25	−0.28	2.39	4.65	2.75
81	811	−3.39	−0.38	−0.63	9	−3.43	−3.26	0.16	25	−0.28	2.39	4.66	2.75
23	791	−3.39	−0.38	−0.64	7	−3.39	−3.19	0.19	25	−0.28	2.41	4.67	2.82
51	788	−3.39	−0.38	−0.64	7	−3.39	−3.19	0.19	26	−0.23	2.41	4.67	2.82
30	769	−3.39	−0.38	−0.64	7	−3.28	−3.10	0.17	26	−0.30	2.38	4.54	2.84
69	745	−3.39	−0.38	−0.64	7	−3.41	−3.23	0.17	25	−0.20	2.41	4.67	2.78
57	745	−3.39	−0.38	−0.64	7	−3.41	−3.23	0.17	25	−0.20	2.41	4.67	2.78
95	744	−3.40	−0.38	−0.64	7	−3.41	−3.23	0.17	25	−0.20	2.41	4.67	2.78
32	721	−3.40	−0.39	−0.64	7	−3.33	−3.18	0.15	25	−0.28	2.39	4.73	2.78
82	721	−3.40	−0.39	−0.64	7	−3.33	−3.18	0.15	25	−0.28	2.39	4.73	2.78
59	721	−3.40	−0.39	−0.64	9	−3.48	−3.14	0.34	27	−0.18	2.41	4.46	2.81
20	720	−3.40	−0.39	−0.64	9	−3.48	−3.14	0.34	27	−0.18	2.41	4.46	2.81
01	656	−3.40	−0.39	−0.65	5	−3.27	−3.13	0.13	25	−0.12	2.38	4.67	2.83
08	623	−3.41	−0.40	−0.65	5	−3.21	−3.14	0.06	25	−0.20	2.39	4.68	2.78
75	621	−3.41	−0.40	−0.65	9	−3.39	−3.21	0.17	25	0.04	2.39	4.56	2.80
13	621	−3.41	−0.40	−0.65	9	−3.39	−3.21	0.17	26	0.07	2.39	4.56	2.80
92	620	−3.41	−0.40	−0.65	9	−3.39	−3.21	0.17	25	0.04	2.39	4.57	2.80
74	569	−3.41	−0.40	−0.66	9	−3.45	−3.24	0.20	25	−0.04	2.38	4.40	2.78
22	568	−3.41	−0.40	−0.66	9	−3.45	−3.24	0.20	25	−0.04	2.38	4.40	2.78
36	529	−3.42	−0.41	−0.66	9	−3.36	−3.15	0.21	25	0.12	2.38	4.56	2.78
77	526	−3.42	−0.41	−0.66	9	−3.36	−3.15	0.21	25	0.12	2.38	4.56	2.78

38	525	−3.42	−0.41	−0.66	7	−3.25	−3.03	0.21	25	−0.04	2.37	4.76	2.74
58	524	−3.42	−0.41	−0.66	7	−3.25	−3.03	0.21	25	−0.04	2.37	4.76	2.74
55	524	−3.42	−0.41	−0.66	7	−3.25	−3.03	0.21	25	−0.04	2.37	4.76	2.74
28	520	−3.42	−0.41	−0.66	7	−3.60	−3.42	0.17	25	−0.20	2.40	4.72	2.80
88	518	−3.42	−0.41	−0.66	7	−3.43	−3.23	0.19	25	−0.20	2.41	4.69	2.76
41	517	−3.42	−0.41	−0.66	7	−3.43	−3.23	0.19	25	−0.20	2.41	4.69	2.76
86	517	−3.42	−0.41	−0.66	7	−3.43	−3.23	0.19	25	−0.20	2.41	4.69	2.76
94	517	−3.42	−0.41	−0.66	7	−3.43	−3.24	0.18	25	−0.20	2.41	4.69	2.76
43	515	−3.42	−0.41	−0.66	7	−3.43	−3.23	0.19	26	−0.15	2.41	4.69	2.76
89	515	−3.42	−0.41	−0.66	7	−3.43	−3.23	0.19	25	−0.20	2.41	4.69	2.76
16	499	−3.42	−0.41	−0.67	5	−3.34	−3.07	0.26	25	−0.12	2.38	4.73	2.78
62	496	−3.42	−0.41	−0.67	5	−3.34	−3.07	0.26	25	−0.12	2.38	4.73	2.78
34	434	−3.43	−0.41	−0.67	9	−3.40	−3.17	0.22	25	−0.20	2.39	4.65	2.74
71	432	−3.43	−0.42	−0.67	9	−3.40	−3.17	0.22	25	−0.20	2.39	4.65	2.74
90	429	−3.43	−0.42	−0.67	9	−3.36	−3.12	0.24	25	−0.04	2.40	4.76	2.77
63	428	−3.43	−0.42	−0.67	9	−3.38	−3.18	0.19	25	0.12	2.40	4.75	2.78
64	428	−3.43	−0.42	−0.67	9	−3.36	−3.12	0.23	25	−0.04	2.40	4.76	2.77
99	426	−3.43	−0.42	−0.67	9	−3.38	−3.18	0.19	25	0.12	2.40	4.75	2.78
00	426	−3.43	−0.42	−0.67	9	−3.36	−3.12	0.24	25	−0.04	2.40	4.76	2.77
68	425	−3.43	−0.42	−0.67	9	−3.38	−3.18	0.19	25	0.12	2.40	4.75	2.78
47	423	−3.43	−0.42	−0.67	7	−3.58	−3.36	0.22	26	−0.15	2.39	4.50	2.92
56	423	−3.43	−0.42	−0.67	7	−3.58	−3.36	0.22	25	−0.20	2.39	4.49	2.92
10	412	−3.43	−0.42	−0.67	9	−3.46	−3.15	0.30	25	−0.36	2.39	4.65	2.73
25	408	−3.43	−0.42	−0.68	7	−3.30	−3.09	0.20	25	−0.04	2.38	4.58	2.77
03	407	−3.43	−0.42	−0.68	7	−3.30	−3.10	0.20	25	−0.04	2.38	4.58	2.78
21	406	−3.43	−0.42	−0.68	7	−3.30	−3.10	0.20	25	−0.04	2.38	4.58	2.78
66	399	−3.43	−0.42	−0.68	7	−3.15	−2.95	0.20	25	−0.12	2.37	4.68	2.72
24	397	−3.43	−0.42	−0.68	7	−3.16	−2.95	0.20	25	−0.12	2.37	4.68	2.73
76	386	−3.43	−0.42	−0.68	7	−3.25	−3.11	0.14	25	−0.20	2.39	4.61	2.76
72	385	−3.43	−0.42	−0.68	7	−3.25	−3.11	0.14	25	−0.20	2.39	4.61	2.76
14	385	−3.43	−0.42	−0.68	7	−3.25	−3.11	0.14	25	−0.20	2.39	4.61	2.76
02	384	−3.43	−0.42	−0.68	7	−3.25	−3.11	0.14	25	−0.20	2.39	4.61	2.77
78	371	−3.43	−0.42	−0.68	7	−3.17	−2.91	0.25	25	0.04	2.36	4.52	2.72
15	369	−3.43	−0.42	−0.68	7	−3.17	−2.91	0.25	25	0.04	2.36	4.52	2.72
54	130	−3.46	−0.45	−0.70	9	−3.48	−3.31	0.17	27	−0.03	2.42	4.65	2.83
73	130	−3.46	−0.45	−0.70	9	−3.60	−3.26	0.33	26	−0.15	2.41	4.62	2.79
07	130	−3.46	−0.45	−0.70	9	−3.59	−3.26	0.33	26	−0.15	2.41	4.63	2.79
91	129	−3.46	−0.45	−0.70	9	−3.59	−3.26	0.33	26	−0.15	2.41	4.63	2.79
09	129	−3.46	−0.45	−0.70	9	−3.48	−3.31	0.17	26	0.00	2.42	4.65	2.83
87	129	−3.46	−0.45	−0.70	9	−3.60	−3.26	0.33	26	−0.15	2.41	4.63	2.79
49	63	−3.46	−0.45	−0.71	9	−3.41	−3.23	0.17	26	0.07	2.40	4.48	2.82
79	63	−3.46	−0.45	−0.71	9	−3.41	−3.23	0.17	26	0.07	2.40	4.48	2.82
19	48	−3.46	−0.45	−0.71	9	−3.20	−2.96	0.24	26	0.23	2.38	4.32	2.75
48	47	−3.46	−0.45	−0.71	9	−3.20	−2.96	0.24	26	0.23	2.38	4.32	2.75
93	1	−3.47	−0.46	−0.72	9	−3.56	−3.35	0.20	25	0.04	2.42	4.62	2.75
17	1	−3.47	−0.46	−0.72	9	−3.55	−3.35	0.20	25	0.04	2.42	4.62	2.75
85	1	−3.47	−0.46	−0.72	9	−3.55	−3.35	0.20	25	0.04	2.42	4.62	2.75
98	0	−3.47	−0.46	−0.72	9	−3.56	−3.35	0.20	25	0.04	2.42	4.62	2.75

Table SI35: Structural, energetic and electronic properties for Co_6Mo_5 cluster, as follows: configuration number (i), relative DFT total energy (ΔE_{tot}^{DFT}, in meV), binding energy (E_b, in eV), excess energy (E_{exc}, in eV), stabilization energy (E_{stab}, in eV), total magnetic moment (M_{tot}, in μ_B), HOMO energy (ε_{HOMO}, in eV), LUMO energy (ε_{LUMO}, in eV), HOMO-LUMO energy difference, (E_{gap}, in eV), total number of bonds (N_b), average chemical order parameter (σ_{av}), average bond length (d_{av}, in Å), average effective coordination number (ECN_{av}, NNN), and average radius (R_{av}, in Å).

i	ΔE_{tot}^{DFT}	E_b	E_{exc}	E_{stab}	M_{tot}	ε_{HOMO}	ε_{LUMO}	E_{gap}	N_b	σ_{av}	d_{av}	ECN_{av}	R_{av}
55	2489	−3.29	−0.24	−0.37	8	−3.46	−3.25	0.21	29	−0.24	2.40	4.91	3.09
22	2050	−3.33	−0.28	−0.41	8	−3.41	−3.21	0.19	29	−0.03	2.40	4.98	3.14
12	1972	−3.33	−0.29	−0.41	8	−3.36	−3.13	0.23	30	−0.20	2.39	4.94	3.22
68	1951	−3.33	−0.29	−0.41	6	−3.23	−3.04	0.19	29	−0.03	2.37	5.02	3.16
51	1946	−3.34	−0.29	−0.42	10	−3.45	−3.29	0.16	30	0.13	2.40	4.90	3.20
89	1882	−3.34	−0.30	−0.42	10	−3.47	−3.34	0.12	29	−0.17	2.41	4.90	3.10
88	1787	−3.35	−0.31	−0.43	10	−3.43	−3.25	0.17	29	−0.17	2.38	4.82	3.22
34	1772	−3.35	−0.31	−0.43	6	−3.31	−3.14	0.16	29	0.03	2.39	4.97	3.16
36	1751	−3.35	−0.31	−0.43	8	−3.26	−2.99	0.26	30	−0.06	2.38	4.69	3.24
7	1731	−3.35	−0.31	−0.43	10	−3.41	−3.19	0.21	29	0.17	2.40	4.87	3.23
97	1701	−3.36	−0.32	−0.44	8	−3.43	−3.20	0.22	30	−0.26	2.38	4.84	3.23
64	1667	−3.36	−0.32	−0.44	8	−3.32	−3.17	0.15	29	0.03	2.39	4.75	3.14
31	1599	−3.37	−0.33	−0.45	10	−3.46	−3.23	0.23	29	−0.03	2.42	4.92	3.17
46	1593	−3.37	−0.33	−0.45	8	−3.22	−2.99	0.22	29	0.17	2.38	4.96	3.01
70	1590	−3.37	−0.33	−0.45	10	−3.53	−3.26	0.26	29	0.03	2.38	4.41	3.14
15	1573	−3.37	−0.33	−0.45	8	−3.34	−3.10	0.23	30	−0.13	2.37	4.53	3.29
77	1559	−3.37	−0.33	−0.45	8	−3.27	−3.14	0.13	29	−0.17	2.38	4.90	3.21
42	1547	−3.37	−0.33	−0.45	6	−3.16	−3.00	0.16	29	−0.03	2.35	4.57	3.36
71	1508	−3.38	−0.33	−0.46	8	−3.39	−3.15	0.23	29	0.03	2.38	4.80	3.16
54	1470	−3.38	−0.34	−0.46	10	−3.32	−3.18	0.13	29	0.10	2.37	4.42	3.22
41	1469	−3.38	−0.34	−0.46	10	−3.39	−3.20	0.19	29	−0.10	2.39	4.79	3.16
80	1463	−3.38	−0.34	−0.46	10	−3.48	−3.31	0.17	29	−0.17	2.40	4.61	3.19
26	1456	−3.38	−0.34	−0.46	10	−3.44	−3.26	0.18	29	−0.17	2.39	4.72	3.18
16	1404	−3.38	−0.34	−0.46	10	−3.44	−3.22	0.21	29	−0.31	2.38	4.74	3.32
95	1383	−3.39	−0.35	−0.47	8	−3.23	−2.99	0.23	30	0.06	2.35	4.60	3.34
63	1381	−3.39	−0.35	−0.47	8	−3.41	−3.15	0.26	29	−0.17	2.38	4.85	3.17
79	1380	−3.39	−0.35	−0.47	10	−3.37	−3.13	0.23	29	−0.10	2.38	4.70	3.11
29	1348	−3.39	−0.35	−0.47	12	−3.28	−3.18	0.09	29	0.17	2.39	4.79	3.20
21	1317	−3.39	−0.35	−0.47	8	−3.35	−3.23	0.12	29	−0.03	2.39	4.70	3.39
86	1313	−3.39	−0.35	−0.47	8	−3.31	−3.12	0.18	30	−0.20	2.38	4.74	3.24
76	1305	−3.39	−0.35	−0.47	10	−3.36	−3.06	0.30	29	0.17	2.38	4.93	3.20
6	1299	−3.39	−0.35	−0.47	10	−3.38	−3.19	0.19	30	−0.06	2.36	4.51	3.22
25	1284	−3.40	−0.35	−0.48	10	−3.36	−3.17	0.18	29	0.03	2.36	4.50	3.20
83	1275	−3.40	−0.36	−0.48	8	−3.58	−3.35	0.22	30	−0.20	2.40	4.84	3.22
23	1252	−3.40	−0.36	−0.48	10	−3.42	−3.17	0.25	29	−0.10	2.37	4.58	3.25
18	1245	−3.40	−0.36	−0.48	10	−3.29	−3.07	0.21	29	0.03	2.37	4.64	3.10
60	1242	−3.40	−0.36	−0.48	6	−3.29	−3.04	0.25	30	−0.20	2.38	4.70	3.24
9	1239	−3.40	−0.36	−0.48	10	−3.55	−3.30	0.25	29	−0.17	2.40	4.56	3.15
14	1227	−3.40	−0.36	−0.48	6	−3.33	−3.09	0.24	30	−0.06	2.38	4.67	2.95
84	1215	−3.40	−0.36	−0.48	8	−3.15	−2.91	0.24	29	−0.10	2.36	4.52	2.95
82	1208	−3.40	−0.36	−0.48	8	−3.25	−3.08	0.16	29	−0.24	2.37	4.66	3.23
78	1185	−3.40	−0.36	−0.48	8	−3.49	−3.24	0.24	29	−0.24	2.39	4.77	3.15
39	1172	−3.41	−0.36	−0.49	10	−3.43	−3.28	0.15	29	−0.03	2.39	4.55	3.27
20	1154	−3.41	−0.37	−0.49	6	−3.41	−3.17	0.24	30	−0.20	2.38	4.80	3.05
58	1128	−3.41	−0.37	−0.49	10	−3.55	−3.30	0.25	30	0.06	2.39	4.64	3.16
57	1117	−3.41	−0.37	−0.49	8	−3.50	−3.21	0.29	30	−0.20	2.38	4.62	3.31
50	1098	−3.41	−0.37	−0.49	10	−3.46	−3.21	0.24	29	0.03	2.40	4.81	3.13
30	1093	−3.41	−0.37	−0.49	8	−3.13	−2.96	0.16	29	0.10	2.36	4.76	3.04

i	ΔE_{tot}^{DFT}	E_b	E_{exc}	E_{stab}	M_{tot}	ε_{HOMO}	ε_{LUMO}	E_{gap}	N_b	σ_{av}	d_{av}	ECN_{av}	R_{av}
53	1092	−3.41	−0.37	−0.49	10	−3.37	−3.19	0.18	29	0.10	2.37	4.50	3.35
8	1051	−3.42	−0.38	−0.50	10	−3.49	−3.30	0.19	29	−0.31	2.42	4.87	3.10
10	1042	−3.42	−0.38	−0.50	8	−3.32	−3.16	0.16	29	−0.17	2.38	4.78	3.23
33	1022	−3.42	−0.38	−0.50	8	−3.44	−3.18	0.25	29	−0.03	2.37	4.55	3.28
74	1003	−3.42	−0.38	−0.50	6	−3.41	−3.14	0.27	29	−0.24	2.38	4.81	3.32
98	995	−3.42	−0.38	−0.50	10	−3.48	−3.34	0.13	29	−0.03	2.39	4.68	3.12
1	992	−3.42	−0.38	−0.50	10	−3.45	−3.22	0.22	30	−0.13	2.38	4.57	3.32
75	954	−3.43	−0.38	−0.51	12	−3.59	−3.37	0.22	29	−0.10	2.42	4.73	3.04
13	938	−3.43	−0.39	−0.51	10	−3.49	−3.28	0.20	29	−0.24	2.43	4.94	3.19
93	938	−3.43	−0.39	−0.51	4	−3.42	−3.22	0.20	30	−0.26	2.40	4.93	3.26
17	934	−3.43	−0.39	−0.51	8	−3.23	−3.13	0.09	30	−0.20	2.37	4.59	2.81
99	931	−3.43	−0.39	−0.51	10	−3.51	−3.32	0.19	29	−0.24	2.42	4.75	2.99
94	909	−3.43	−0.39	−0.51	8	−3.21	−3.06	0.14	29	0.10	2.39	5.00	3.13
66	905	−3.43	−0.39	−0.51	10	−3.44	−3.29	0.15	29	−0.10	2.41	4.72	3.21
40	903	−3.43	−0.39	−0.51	8	−3.50	−3.19	0.30	30	−0.06	2.37	4.55	3.23
62	896	−3.43	−0.39	−0.51	8	−3.35	−3.13	0.22	29	0.03	2.35	4.61	3.26
24	883	−3.43	−0.39	−0.51	8	−3.51	−3.24	0.26	29	−0.17	2.38	4.65	3.23
69	857	−3.43	−0.39	−0.51	6	−3.35	−3.14	0.20	28	0.00	2.39	4.81	2.88
3	809	−3.44	−0.40	−0.52	8	−3.45	−3.20	0.25	30	−0.20	2.41	4.84	3.24
44	806	−3.44	−0.40	−0.52	10	−3.43	−3.19	0.24	29	−0.03	2.40	4.85	3.16
45	803	−3.44	−0.40	−0.52	10	−3.47	−3.26	0.21	29	0.03	2.41	4.80	3.25
61	786	−3.44	−0.40	−0.52	10	−3.32	−3.12	0.20	29	0.37	2.39	4.72	3.24
28	764	−3.44	−0.40	−0.52	10	−3.52	−3.23	0.28	30	−0.06	2.42	4.66	3.10
19	746	−3.44	−0.40	−0.52	8	−3.31	−3.15	0.16	30	0.20	2.41	4.77	3.15
92	741	−3.44	−0.40	−0.52	10	−3.44	−3.24	0.19	29	0.24	2.39	4.67	3.25
87	739	−3.44	−0.40	−0.53	10	−3.47	−3.21	0.26	30	0.00	2.41	4.66	3.15
11	734	−3.45	−0.40	−0.53	10	−3.44	−3.21	0.22	30	−0.13	2.42	4.71	2.75
5	716	−3.45	−0.41	−0.53	8	−3.52	−3.28	0.23	29	−0.10	2.42	4.89	3.25
32	693	−3.45	−0.41	−0.53	12	−3.53	−3.32	0.20	28	0.07	2.39	4.50	2.86
43	650	−3.45	−0.41	−0.53	10	−3.49	−3.30	0.18	29	0.03	2.39	4.48	3.28
49	649	−3.45	−0.41	−0.53	10	−3.35	−3.06	0.29	29	0.17	2.39	4.67	3.15
81	641	−3.45	−0.41	−0.53	10	−3.48	−3.22	0.25	30	0.20	2.40	4.67	3.20
38	598	−3.46	−0.42	−0.54	10	−3.51	−3.29	0.21	29	−0.10	2.40	4.61	3.32
47	558	−3.46	−0.42	−0.54	8	−3.29	−3.11	0.18	28	−0.07	2.39	4.73	2.80
56	530	−3.46	−0.42	−0.54	8	−3.40	−3.13	0.27	30	0.06	2.41	4.79	3.36
2	487	−3.47	−0.43	−0.55	8	−3.33	−3.03	0.30	29	−0.03	2.38	4.75	2.80
90	431	−3.47	−0.43	−0.55	10	−3.52	−3.27	0.24	30	−0.13	2.40	4.81	2.88
96	287	−3.49	−0.44	−0.57	8	−3.44	−3.33	0.10	29	0.03	2.42	4.82	3.34
4	284	−3.49	−0.45	−0.57	10	−3.48	−3.32	0.15	27	0.11	2.38	4.39	2.96
37	0	−3.51	−0.47	−0.59	10	−3.53	−3.26	0.26	29	−0.03	2.43	4.85	3.22

Table SI36: Structural, energetic and electronic properties for Co_6Mo_6 cluster, as follows: configuration number (i), relative DFT total energy (ΔE_{tot}^{DFT}, in meV), binding energy (E_b, in eV), excess energy (E_{exc}, in eV), stabilization energy (E_{stab}, in eV), total magnetic moment (M_{tot}, in μ_B), HOMO energy (ε_{HOMO}, in eV), LUMO energy (ε_{LUMO}, in eV), HOMO-LUMO energy difference, (E_{gap}, in eV), total number of bonds (N_b), average chemical order parameter (σ_{av}), average bond length (d_{av}, in Å), average effective coordination number (ECN_{av}, NNN), and average radius (R_{av}, in Å).

i	ΔE_{tot}^{DFT}	E_b	E_{exc}	E_{stab}	M_{tot}	ε_{HOMO}	ε_{LUMO}	E_{gap}	N_b	σ_{av}	d_{av}	ECN_{av}	R_{av}
12	1775	−3.48	−0.34	−0.38	12	−3.40	−3.31	0.08	33	−0.21	2.42	5.06	2.91
72	1704	−3.48	−0.35	−0.39	8	−3.33	−3.11	0.22	33	0.03	2.38	4.72	2.88
50	1686	−3.49	−0.35	−0.39	6	−3.26	−3.03	0.22	32	0.06	2.38	4.93	2.77
99	1682	−3.49	−0.35	−0.39	6	−3.35	−3.20	0.15	33	−0.09	2.39	5.07	2.80

51	1682	−3.49	−0.35	−0.39	6	−3.35	−3.20	0.15	33	−0.09	2.39	5.07	2.80
0	1579	−3.49	−0.36	−0.40	8	−3.33	−3.21	0.12	33	−0.03	2.39	4.84	2.79
31	1541	−3.50	−0.36	−0.40	8	−3.29	−3.10	0.19	33	−0.03	2.38	4.79	2.80
23	1521	−3.50	−0.36	−0.40	10	−3.33	−3.13	0.20	34	−0.17	2.41	5.01	2.94
97	1510	−3.50	−0.36	−0.40	6	−3.39	−3.17	0.21	34	−0.05	2.39	4.92	2.96
8	1506	−3.50	−0.36	−0.40	8	−3.50	−3.20	0.30	32	−0.12	2.39	4.89	2.79
63	1456	−3.50	−0.37	−0.41	8	−3.34	−3.11	0.23	34	−0.05	2.40	4.83	2.98
95	1452	−3.51	−0.37	−0.41	4	−3.26	−3.08	0.17	33	0.09	2.39	5.05	2.82
34	1401	−3.51	−0.37	−0.41	8	−3.26	−3.07	0.19	33	−0.09	2.38	4.94	2.82
14	1400	−3.51	−0.37	−0.41	8	−3.53	−3.28	0.25	34	−0.17	2.39	4.83	2.87
61	1395	−3.51	−0.37	−0.41	10	−3.36	−3.18	0.17	34	−0.17	2.41	4.97	2.92
58	1319	−3.52	−0.38	−0.42	8	−3.45	−3.12	0.32	34	−0.05	2.39	4.76	3.00
71	1303	−3.52	−0.38	−0.42	8	−3.36	−3.15	0.21	34	−0.11	2.38	4.84	2.88
67	1293	−3.52	−0.38	−0.42	10	−3.33	−3.16	0.16	34	−0.11	2.39	4.76	3.00
16	1290	−3.52	−0.38	−0.42	8	−3.35	−3.17	0.17	34	−0.23	2.39	4.79	2.75
87	1287	−3.52	−0.38	−0.42	8	−3.41	−3.19	0.21	31	−0.22	2.38	4.77	2.80
88	1232	−3.52	−0.39	−0.43	8	−3.52	−3.32	0.20	33	−0.21	2.39	4.54	2.83
48	1226	−3.52	−0.39	−0.43	10	−3.44	−3.30	0.13	34	−0.17	2.41	4.95	2.90
24	1217	−3.52	−0.39	−0.43	8	−3.35	−3.19	0.16	34	−0.05	2.41	5.08	2.94
55	1188	−3.53	−0.39	−0.43	10	−3.35	−3.14	0.20	33	0.03	2.37	4.59	2.87
84	1184	−3.53	−0.39	−0.43	10	−3.42	−3.23	0.18	33	−0.09	2.42	4.93	2.91
11	1168	−3.53	−0.39	−0.43	8	−3.37	−3.04	0.33	32	−0.25	2.38	4.88	2.96
4	1142	−3.53	−0.39	−0.44	8	−3.49	−3.30	0.18	32	−0.06	2.41	4.92	2.95
40	1132	−3.53	−0.39	−0.44	8	−3.16	−3.04	0.11	33	−0.15	2.39	4.99	2.90
56	1103	−3.53	−0.40	−0.44	8	−3.40	−3.23	0.16	33	−0.21	2.41	4.87	2.91
20	1081	−3.54	−0.40	−0.44	8	−3.27	−3.15	0.11	34	−0.05	2.39	4.75	2.78
01	1080	−3.54	−0.40	−0.44	8	−3.37	−3.23	0.13	34	−0.29	2.40	4.87	2.82
13	1049	−3.54	−0.40	−0.44	8	−3.30	−3.15	0.14	33	−0.09	2.40	4.92	2.96
78	1047	−3.54	−0.40	−0.44	10	−3.30	−3.10	0.19	32	0.00	2.40	5.01	2.84
60	1021	−3.54	−0.40	−0.45	10	−3.39	−3.24	0.14	33	−0.15	2.43	4.99	2.76
81	1010	−3.54	−0.40	−0.45	8	−3.34	−3.14	0.20	33	−0.21	2.40	4.94	2.89
43	966	−3.55	−0.41	−0.45	8	−3.48	−3.32	0.15	33	−0.15	2.41	4.96	2.81
75	961	−3.55	−0.41	−0.45	10	−3.33	−3.19	0.13	34	0.05	2.41	4.89	2.94
37	942	−3.55	−0.41	−0.45	8	−3.40	−3.14	0.25	34	−0.29	2.41	4.95	2.85
92	930	−3.55	−0.41	−0.45	8	−3.34	−3.08	0.26	34	−0.05	2.39	4.85	2.88
85	929	−3.55	−0.41	−0.45	8	−3.37	−3.22	0.14	33	−0.09	2.42	4.91	2.96
73	929	−3.55	−0.41	−0.45	10	−3.45	−3.29	0.16	33	−0.03	2.42	4.85	2.83
64	925	−3.55	−0.41	−0.45	8	−3.41	−3.15	0.25	34	−0.23	2.40	4.87	2.82
45	903	−3.55	−0.41	−0.45	8	−3.46	−3.27	0.18	34	−0.11	2.41	4.74	2.78
22	900	−3.55	−0.41	−0.46	10	−3.46	−3.25	0.20	32	−0.12	2.43	4.88	2.90
74	861	−3.55	−0.42	−0.46	8	−3.37	−3.15	0.22	32	0.12	2.41	4.99	2.89
26	843	−3.56	−0.42	−0.46	8	−3.24	−3.04	0.20	33	−0.09	2.39	4.93	2.88
86	817	−3.56	−0.42	−0.46	10	−3.38	−3.20	0.18	33	0.03	2.39	4.83	2.89
42	798	−3.56	−0.42	−0.46	10	−3.41	−3.16	0.25	32	0.12	2.43	4.97	2.81
98	776	−3.56	−0.42	−0.47	10	−3.45	−3.19	0.26	32	0.00	2.41	4.99	2.87
79	776	−3.56	−0.42	−0.47	10	−3.45	−3.18	0.26	33	0.03	2.41	4.99	2.87
32	773	−3.56	−0.42	−0.47	10	−3.40	−3.18	0.21	35	−0.14	2.41	4.64	2.92
30	771	−3.56	−0.42	−0.47	8	−3.41	−3.20	0.20	34	−0.05	2.43	4.95	2.86
69	769	−3.56	−0.42	−0.47	8	−3.20	−3.02	0.18	34	0.29	2.39	4.85	2.82
53	765	−3.56	−0.42	−0.47	10	−3.32	−3.01	0.30	31	0.16	2.38	4.59	2.78
82	762	−3.56	−0.42	−0.47	8	−3.35	−3.09	0.25	31	−0.22	2.40	4.89	2.85
38	747	−3.56	−0.43	−0.47	10	−3.32	−3.25	0.06	32	−0.31	2.42	4.74	2.86
29	744	−3.56	−0.43	−0.47	10	−3.27	−3.07	0.19	34	0.17	2.41	4.98	2.91
3	708	−3.57	−0.43	−0.47	6	−3.27	−3.05	0.22	33	−0.03	2.41	4.98	2.87
25	705	−3.57	−0.43	−0.47	6	−3.27	−3.05	0.22	33	−0.03	2.41	4.98	2.87
93	684	−3.57	−0.43	−0.47	10	−3.40	−3.14	0.25	33	−0.03	2.42	4.85	2.97
10	667	−3.57	−0.43	−0.47	8	−3.26	−3.05	0.20	33	−0.09	2.40	5.06	2.88

33	663	−3.57	−0.43	−0.47	8	−3.32	−3.17	0.15	32	−0.06	2.41	5.01	2.90
9	642	−3.57	−0.43	−0.48	8	−3.50	−3.29	0.21	34	−0.23	2.39	4.76	2.96
89	586	−3.58	−0.44	−0.48	8	−3.33	−3.12	0.21	33	0.03	2.40	4.89	2.84
90	586	−3.58	−0.44	−0.48	8	−3.33	−3.12	0.21	33	0.03	2.40	4.89	2.84
47	584	−3.58	−0.44	−0.48	8	−3.41	−3.25	0.16	33	−0.21	2.41	4.79	2.89
52	583	−3.58	−0.44	−0.48	8	−3.55	−3.24	0.31	34	−0.23	2.43	4.84	2.96
36	576	−3.58	−0.44	−0.48	10	−3.26	−3.04	0.21	32	0.06	2.41	4.86	2.84
15	575	−3.58	−0.44	−0.48	8	−3.28	−3.17	0.11	32	0.00	2.39	4.78	2.83
5	551	−3.58	−0.44	−0.48	10	−3.34	−3.19	0.14	33	0.27	2.42	4.87	2.86
7	548	−3.58	−0.44	−0.48	8	−3.47	−3.25	0.22	32	−0.06	2.43	4.92	2.96
70	527	−3.58	−0.44	−0.49	10	−3.43	−3.25	0.18	33	0.09	2.44	4.90	2.98
6	519	−3.58	−0.44	−0.49	8	−3.43	−3.15	0.28	33	−0.09	2.39	4.92	2.88
65	508	−3.58	−0.45	−0.49	10	−3.59	−3.31	0.28	32	−0.12	2.40	4.66	2.85
94	501	−3.58	−0.45	−0.49	8	−3.39	−3.28	0.10	35	−0.20	2.43	4.79	3.00
59	425	−3.59	−0.45	−0.49	10	−3.52	−3.29	0.22	34	0.00	2.43	4.78	2.94
46	418	−3.59	−0.45	−0.50	10	−3.41	−3.21	0.19	34	0.29	2.40	4.84	2.91
80	417	−3.59	−0.45	−0.50	10	−3.44	−3.23	0.20	35	0.02	2.45	4.97	2.99
21	415	−3.59	−0.45	−0.50	8	−3.50	−3.30	0.20	34	0.00	2.42	4.71	2.94
28	408	−3.59	−0.45	−0.50	10	−3.51	−3.32	0.19	33	0.09	2.42	4.73	2.97
76	392	−3.59	−0.46	−0.50	10	−3.42	−3.21	0.20	33	−0.15	2.41	4.82	2.89
2	376	−3.59	−0.46	−0.50	10	−3.58	−3.37	0.21	32	−0.12	2.43	4.85	2.91
66	362	−3.60	−0.46	−0.50	10	−3.54	−3.28	0.26	33	0.03	2.41	4.81	2.90
17	360	−3.60	−0.46	−0.50	8	−3.41	−3.23	0.18	32	0.00	2.39	4.67	2.93
57	351	−3.60	−0.46	−0.50	8	−3.53	−3.29	0.24	33	−0.09	2.43	4.94	2.89
27	316	−3.60	−0.46	−0.50	10	−3.41	−3.19	0.22	33	−0.15	2.42	4.89	2.94
49	298	−3.60	−0.46	−0.51	8	−3.36	−3.10	0.25	33	0.03	2.41	4.74	2.93
91	288	−3.60	−0.46	−0.51	8	−3.43	−3.18	0.24	32	−0.12	2.43	5.00	2.85
18	282	−3.60	−0.46	−0.51	10	−3.52	−3.33	0.18	33	−0.09	2.44	4.96	3.02
35	105	−3.62	−0.48	−0.52	10	−3.54	−3.37	0.17	32	0.12	2.42	4.84	3.07
44	78	−3.62	−0.48	−0.52	10	−3.48	−3.21	0.26	33	0.03	2.44	4.79	2.97
83	16	−3.62	−0.49	−0.53	8	−3.52	−3.33	0.18	34	0.05	2.42	4.83	3.04
62	0	−3.63	−0.49	−0.53	8	−3.35	−3.10	0.25	32	0.18	2.42	5.04	2.83

Table SI37: Structural, energetic and electronic properties for Co_7Mo_6 cluster, as follows: configuration number (i), relative DFT total energy (ΔE_{tot}^{DFT}, in meV), binding energy (E_b, in eV), excess energy (E_{exc}, in eV), stabilization energy (E_{stab}, in eV), total magnetic moment (M_{tot}, in μ_B), HOMO energy (ε_{HOMO}, in eV), LUMO energy (ε_{LUMO}, in eV), HOMO-LUMO energy difference, (E_{gap}, in eV), total number of bonds (N_b), average chemical order parameter (σ_{av}), average bond length (d_{av}, in Å), average effective coordination number (ECN_{av}, NNN), and average radius (R_{av}, in Å).

i	ΔE_{tot}^{DFT}	E_b	E_{exc}	E_{stab}	M_{tot}	ε_{HOMO}	ε_{LUMO}	E_{gap}	N_b	σ_{av}	d_{av}	ECN_{av}	R_{av}
99	1786	−3.55	−0.34	−0.45	11	−3.20	−3.05	0.14	36	0.05	2.38	5.13	2.88
36	1771	−3.55	−0.34	−0.45	9	−3.16	−3.05	0.11	36	0.05	2.39	5.18	2.85
16	1677	−3.56	−0.35	−0.45	9	−3.48	−3.27	0.20	36	0.05	2.40	5.30	2.91
7	1653	−3.56	−0.35	−0.46	13	−3.33	−3.22	0.11	36	−0.16	2.41	5.18	2.91
40	1641	−3.56	−0.35	−0.46	11	−3.21	−2.99	0.22	36	0.05	2.39	5.19	2.87
33	1639	−3.56	−0.35	−0.46	9	−3.37	−3.24	0.13	36	0.16	2.38	5.08	2.98
35	1594	−3.56	−0.35	−0.46	11	−3.45	−3.26	0.18	37	−0.02	2.42	5.39	2.93
28	1586	−3.57	−0.35	−0.46	9	−3.16	−3.05	0.11	36	−0.05	2.38	5.30	2.87
20	1583	−3.57	−0.36	−0.46	9	−3.42	−3.27	0.14	36	−0.11	2.40	5.36	2.92
44	1582	−3.57	−0.36	−0.46	9	−3.46	−3.29	0.17	36	−0.05	2.40	5.20	2.96
93	1537	−3.57	−0.36	−0.46	9	−3.31	−3.16	0.14	37	−0.24	2.41	5.27	2.91
43	1532	−3.57	−0.36	−0.47	9	−3.35	−3.17	0.17	36	−0.05	2.38	5.03	2.98

8	1528	−3.57	−0.36	−0.47	11	−3.40	−3.30	0.10	36	0.11	2.38	5.09	2.97
31	1506	−3.57	−0.36	−0.47	9	−3.39	−3.17	0.22	36	0.05	2.40	5.35	2.90
58	1488	−3.57	−0.36	−0.47	9	−3.39	−3.18	0.20	36	−0.05	2.39	5.23	2.89
1	1452	−3.58	−0.37	−0.47	9	−3.48	−3.29	0.18	36	−0.11	2.41	5.28	2.93
56	1446	−3.58	−0.37	−0.47	7	−3.37	−3.18	0.19	36	−0.05	2.38	5.26	2.98
86	1412	−3.58	−0.37	−0.47	9	−3.37	−3.20	0.17	36	−0.05	2.39	5.27	2.90
68	1404	−3.58	−0.37	−0.48	9	−3.24	−3.15	0.09	36	−0.05	2.39	5.16	2.89
50	1400	−3.58	−0.37	−0.48	11	−3.45	−3.21	0.24	37	−0.29	2.42	5.23	2.97
81	1389	−3.58	−0.37	−0.48	9	−3.35	−3.16	0.18	36	−0.11	2.40	5.33	2.89
41	1376	−3.58	−0.37	−0.48	11	−3.50	−3.32	0.18	36	−0.16	2.42	5.19	2.90
88	1363	−3.58	−0.37	−0.48	9	−3.31	−3.07	0.23	36	−0.22	2.40	5.23	2.88
95	1326	−3.59	−0.37	−0.48	9	−3.44	−3.34	0.09	38	−0.10	2.41	5.10	2.97
73	1324	−3.59	−0.38	−0.48	9	−3.38	−3.20	0.17	36	−0.16	2.41	5.23	2.91
94	1317	−3.59	−0.38	−0.48	9	−3.50	−3.26	0.24	36	−0.22	2.40	5.21	2.94
90	1314	−3.59	−0.38	−0.48	9	−3.40	−3.16	0.23	36	−0.11	2.39	5.26	2.95
21	1308	−3.59	−0.38	−0.48	9	−3.34	−3.14	0.20	36	−0.16	2.41	5.34	2.89
34	1297	−3.59	−0.38	−0.48	9	−3.33	−3.18	0.14	37	−0.02	2.40	5.08	2.91
54	1267	−3.59	−0.38	−0.49	11	−3.45	−3.27	0.17	38	−0.21	2.42	5.17	2.96
57	1261	−3.59	−0.38	−0.49	9	−3.47	−3.30	0.17	37	0.02	2.41	5.08	2.91
18	1256	−3.59	−0.38	−0.49	9	−3.50	−3.34	0.15	37	−0.13	2.41	5.03	2.94
98	1255	−3.59	−0.38	−0.49	9	−3.58	−3.34	0.23	36	−0.11	2.41	5.22	2.89
80	1242	−3.59	−0.38	−0.49	11	−3.40	−3.14	0.26	36	−0.11	2.38	5.02	2.96
59	1239	−3.59	−0.38	−0.49	11	−3.48	−3.29	0.19	36	0.11	2.40	5.11	2.91
26	1182	−3.60	−0.39	−0.49	11	−3.57	−3.30	0.26	37	−0.02	2.41	4.99	3.02
70	1168	−3.60	−0.39	−0.49	9	−3.34	−3.06	0.27	36	−0.16	2.40	5.28	2.88
10	1164	−3.60	−0.39	−0.49	9	−3.54	−3.33	0.21	37	−0.18	2.42	5.31	2.92
66	1162	−3.60	−0.39	−0.49	11	−3.45	−3.21	0.23	37	0.08	2.40	5.01	2.87
32	1157	−3.60	−0.39	−0.49	9	−3.48	−3.29	0.18	38	−0.21	2.42	5.13	2.93
84	1152	−3.60	−0.39	−0.49	7	−3.57	−3.30	0.27	38	−0.10	2.40	5.21	2.96
52	1149	−3.60	−0.39	−0.49	9	−3.62	−3.37	0.24	36	−0.11	2.42	5.23	2.88
13	1148	−3.60	−0.39	−0.49	9	−3.59	−3.40	0.19	37	−0.18	2.43	5.29	2.95
51	1140	−3.60	−0.39	−0.50	7	−3.31	−3.13	0.18	37	−0.08	2.40	5.27	2.87
75	1133	−3.60	−0.39	−0.50	9	−3.48	−3.17	0.30	37	−0.18	2.40	5.25	2.87
12	1098	−3.60	−0.39	−0.50	7	−3.36	−3.22	0.13	37	−0.18	2.40	5.34	2.90
72	1094	−3.60	−0.39	−0.50	7	−3.42	−3.15	0.27	37	−0.24	2.39	5.14	2.87
64	1090	−3.60	−0.39	−0.50	9	−3.38	−3.24	0.13	38	−0.05	2.40	5.03	2.92
3	1090	−3.60	−0.39	−0.50	9	−3.52	−3.31	0.20	37	−0.13	2.41	5.25	2.94
30	1089	−3.60	−0.39	−0.50	9	−3.41	−3.33	0.07	37	−0.13	2.42	5.13	2.91
78	1086	−3.60	−0.39	−0.50	7	−3.38	−3.28	0.10	37	−0.18	2.41	5.20	2.90
79	1077	−3.60	−0.39	−0.50	11	−3.44	−3.27	0.17	38	−0.05	2.40	5.15	2.87
37	1071	−3.61	−0.39	−0.50	7	−3.43	−3.27	0.15	37	−0.18	2.41	5.28	2.88
42	1052	−3.61	−0.40	−0.50	7	−3.36	−3.10	0.25	36	−0.22	2.39	5.18	2.93
91	1033	−3.61	−0.40	−0.50	9	−3.36	−3.20	0.15	36	0.00	2.40	5.28	2.89
23	1016	−3.61	−0.40	−0.50	11	−3.37	−3.14	0.22	36	0.16	2.40	5.15	2.93
25	1013	−3.61	−0.40	−0.51	9	−3.37	−3.20	0.17	37	−0.24	2.41	5.16	2.91
77	1006	−3.61	−0.40	−0.51	9	−3.43	−3.28	0.14	37	−0.02	2.42	5.13	2.96
60	1004	−3.61	−0.40	−0.51	9	−3.53	−3.30	0.23	36	−0.33	2.41	5.27	2.89
65	996	−3.61	−0.40	−0.51	11	−3.44	−3.29	0.15	36	−0.16	2.42	5.19	2.91
46	985	−3.61	−0.40	−0.51	11	−3.37	−3.19	0.17	37	−0.13	2.41	5.07	2.97
45	979	−3.61	−0.40	−0.51	11	−3.49	−3.34	0.15	37	−0.13	2.43	5.21	2.89
4	962	−3.61	−0.40	−0.51	11	−3.47	−3.23	0.24	36	0.22	2.40	5.09	3.04
15	959	−3.61	−0.40	−0.51	9	−3.42	−3.33	0.09	36	−0.05	2.41	5.20	2.94
89	933	−3.62	−0.41	−0.51	11	−3.54	−3.25	0.28	36	0.05	2.41	5.14	2.95
96	905	−3.62	−0.41	−0.51	11	−3.61	−3.36	0.25	36	−0.11	2.44	5.15	2.89
5	901	−3.62	−0.41	−0.51	9	−3.55	−3.42	0.13	36	0.11	2.42	5.25	2.95
6	890	−3.62	−0.41	−0.51	9	−3.36	−3.20	0.15	36	0.11	2.41	5.32	2.94
55	888	−3.62	−0.41	−0.51	9	−3.52	−3.41	0.10	36	0.11	2.42	5.25	2.97

47	873	−3.62	−0.41	−0.52	9	−3.51	−3.22	0.28	37	−0.18	2.40	5.05	2.99
83	853	−3.62	−0.41	−0.52	9	−3.27	−3.12	0.15	36	0.11	2.40	5.23	2.92
2	844	−3.62	−0.41	−0.52	11	−3.46	−3.22	0.23	38	0.05	2.41	5.06	2.95
38	814	−3.62	−0.41	−0.52	9	−3.45	−3.24	0.21	37	−0.24	2.41	5.25	2.88
29	787	−3.63	−0.42	−0.52	11	−3.39	−3.15	0.23	36	0.27	2.41	5.16	2.95
48	784	−3.63	−0.42	−0.52	11	−3.43	−3.20	0.22	39	0.12	2.41	4.86	2.93
62	776	−3.63	−0.42	−0.52	11	−3.56	−3.35	0.21	36	−0.05	2.42	5.22	2.98
24	768	−3.63	−0.42	−0.52	11	−3.52	−3.35	0.17	36	−0.22	2.43	5.30	2.91
71	768	−3.63	−0.42	−0.52	9	−3.31	−3.09	0.21	36	0.00	2.40	5.30	2.88
61	768	−3.63	−0.42	−0.52	9	−3.40	−3.21	0.18	37	−0.08	2.40	5.13	2.97
22	760	−3.63	−0.42	−0.52	9	−3.48	−3.27	0.20	37	−0.18	2.40	4.97	3.07
76	744	−3.63	−0.42	−0.53	9	−3.49	−3.27	0.21	37	−0.02	2.41	5.17	2.90
82	663	−3.64	−0.43	−0.53	11	−3.48	−3.24	0.24	36	−0.05	2.42	5.27	2.87
63	651	−3.64	−0.43	−0.53	9	−3.44	−3.28	0.16	37	−0.13	2.42	5.08	2.91
0	646	−3.64	−0.43	−0.53	9	−3.49	−3.36	0.12	36	−0.05	2.42	5.26	2.95
53	611	−3.64	−0.43	−0.54	11	−3.40	−3.24	0.15	36	0.16	2.41	4.95	2.95
97	588	−3.64	−0.43	−0.54	9	−3.24	−3.11	0.13	36	0.11	2.39	5.10	2.88
39	587	−3.64	−0.43	−0.54	11	−3.65	−3.33	0.32	36	−0.11	2.44	5.19	2.93
11	579	−3.64	−0.43	−0.54	9	−3.38	−3.12	0.26	37	−0.02	2.40	5.18	2.92
14	557	−3.64	−0.43	−0.54	9	−3.41	−3.30	0.10	37	−0.08	2.40	5.05	2.88
74	506	−3.65	−0.44	−0.54	11	−3.48	−3.18	0.29	36	−0.05	2.41	5.08	2.91
67	493	−3.65	−0.44	−0.55	13	−3.61	−3.36	0.24	36	0.27	2.41	4.91	3.06
85	482	−3.65	−0.44	−0.55	11	−3.56	−3.33	0.22	37	−0.13	2.42	5.06	2.93
87	467	−3.65	−0.44	−0.55	11	−3.52	−3.36	0.16	36	0.16	2.42	4.91	3.01
49	445	−3.65	−0.44	−0.55	9	−3.46	−3.22	0.24	36	−0.11	2.41	5.14	2.89
92	405	−3.66	−0.45	−0.55	9	−3.62	−3.37	0.24	36	−0.05	2.42	5.15	2.88
27	404	−3.66	−0.45	−0.55	11	−3.53	−3.38	0.14	36	−0.11	2.44	5.16	2.92
19	392	−3.66	−0.45	−0.55	11	−3.55	−3.33	0.22	37	−0.02	2.42	5.16	2.88
9	360	−3.66	−0.45	−0.56	9	−3.54	−3.30	0.24	37	−0.13	2.42	5.13	2.93
17	0	−3.69	−0.48	−0.58	9	−3.54	−3.45	0.08	36	0.05	2.44	5.13	2.99

Table SI38: Structural, energetic and electronic properties for Co$_7$Mo$_7$ cluster, as follows: configuration number (i), relative DFT total energy (ΔE_{tot}^{DFT}, in meV), binding energy (E_b, in eV), excess energy (E_{exc}, in eV), stabilization energy (E_{stab}, in eV), total magnetic moment (M_{tot}, in μ_B), HOMO energy (ε_{HOMO}, in eV), LUMO energy (ε_{LUMO}, in eV), HOMO-LUMO energy difference, (E_{gap}, in eV), total number of bonds (N_b), average chemical order parameter (σ_{av}), average bond length (d_{av}, in Å), average effective coordination number (ECN_{av}, NNN), and average radius (R_{av}, in Å).

i	ΔE_{tot}^{DFT}	E_b	E_{exc}	E_{stab}	M_{tot}	ε_{HOMO}	ε_{LUMO}	E_{gap}	N_b	σ_{av}	d_{av}	ECN_{av}	R_{av}
47	1971	−3.60	−0.39	−0.41	9	−3.35	−3.26	0.09	40	0.00	2.39	5.16	3.25
27	1941	−3.60	−0.39	−0.41	9	−3.40	−3.20	0.19	40	−0.10	2.41	5.30	3.27
88	1938	−3.60	−0.39	−0.41	11	−3.35	−3.26	0.09	40	−0.05	2.40	5.09	3.20
28	1896	−3.61	−0.39	−0.42	11	−3.52	−3.31	0.21	39	−0.28	2.44	5.29	3.31
44	1864	−3.61	−0.40	−0.42	7	−3.45	−3.24	0.21	41	−0.21	2.40	5.13	3.18
59	1803	−3.61	−0.40	−0.42	7	−3.36	−3.26	0.10	40	0.05	2.39	5.20	3.26
57	1655	−3.62	−0.41	−0.43	9	−3.55	−3.34	0.20	39	−0.17	2.40	5.13	3.32
53	1587	−3.63	−0.41	−0.44	11	−3.31	−3.25	0.05	41	−0.21	2.42	5.15	3.25
74	1532	−3.63	−0.42	−0.44	9	−3.33	−3.07	0.25	40	−0.20	2.41	5.22	3.25
56	1515	−3.63	−0.42	−0.44	13	−3.51	−3.23	0.28	39	−0.02	2.42	5.18	3.28
30	1503	−3.63	−0.42	−0.44	7	−3.35	−3.14	0.21	42	−0.14	2.40	5.01	3.21
81	1502	−3.63	−0.42	−0.44	11	−3.49	−3.32	0.17	41	−0.12	2.42	5.22	3.31
96	1487	−3.64	−0.42	−0.44	9	−3.34	−3.13	0.20	41	−0.21	2.41	5.31	3.25
8	1451	−3.64	−0.42	−0.45	9	−3.52	−3.30	0.22	40	−0.25	2.42	5.14	3.23

99	1372	−3.64	−0.43	−0.45	9	−3.31	−3.18	0.13	39	0.17	2.40	5.10	3.33
95	1310	−3.65	−0.43	−0.46	5	−3.29	−3.07	0.22	39	−0.33	2.38	5.16	3.30
69	1306	−3.65	−0.44	−0.46	11	−3.27	−3.11	0.16	41	−0.02	2.41	5.21	3.23
04	1304	−3.65	−0.44	−0.46	11	−3.32	−3.07	0.25	40	−0.15	2.42	5.20	3.19
06	1294	−3.65	−0.44	−0.46	11	−3.40	−3.23	0.16	40	0.00	2.41	5.01	3.32
91	1279	−3.65	−0.44	−0.46	9	−3.60	−3.40	0.19	39	−0.07	2.42	5.12	3.27
24	1271	−3.65	−0.44	−0.46	9	−3.44	−3.29	0.15	42	−0.09	2.42	5.21	3.30
55	1248	−3.65	−0.44	−0.46	7	−3.28	−3.05	0.23	41	−0.12	2.40	5.21	3.25
11	1233	−3.65	−0.44	−0.46	5	−3.34	−3.16	0.17	40	−0.10	2.39	5.28	3.32
80	1226	−3.65	−0.44	−0.46	7	−3.39	−3.19	0.19	39	−0.17	2.40	5.20	3.32
3	1216	−3.66	−0.44	−0.46	9	−3.49	−3.21	0.28	41	−0.07	2.40	4.91	3.10
84	1204	−3.66	−0.44	−0.46	7	−3.32	−3.15	0.17	39	−0.28	2.41	5.28	3.34
37	1196	−3.66	−0.44	−0.47	9	−3.34	−3.15	0.19	41	−0.12	2.42	5.40	3.24
61	1174	−3.66	−0.44	−0.47	9	−3.45	−3.34	0.11	41	−0.17	2.42	5.20	3.35
16	1160	−3.66	−0.45	−0.47	11	−3.39	−3.13	0.25	40	0.00	2.42	5.28	3.27
40	1113	−3.66	−0.45	−0.47	9	−3.34	−3.19	0.14	40	0.05	2.42	5.25	3.36
77	1085	−3.66	−0.45	−0.47	9	−3.33	−3.15	0.18	40	−0.10	2.39	4.99	3.44
76	1046	−3.67	−0.45	−0.48	7	−3.42	−3.25	0.16	39	−0.07	2.40	5.25	3.40
63	1036	−3.67	−0.45	−0.48	9	−3.36	−3.12	0.24	40	−0.15	2.41	5.26	3.34
58	1036	−3.67	−0.45	−0.48	7	−3.27	−3.11	0.15	42	−0.04	2.41	5.21	2.96
51	1034	−3.67	−0.45	−0.48	7	−3.31	−3.14	0.17	40	−0.20	2.40	5.23	3.26
97	1028	−3.67	−0.45	−0.48	11	−3.55	−3.25	0.29	39	−0.02	2.42	5.17	3.33
38	1006	−3.67	−0.46	−0.48	11	−3.45	−3.29	0.16	41	0.07	2.42	4.99	3.31
22	993	−3.67	−0.46	−0.48	11	−3.45	−3.26	0.18	40	−0.15	2.41	5.03	3.29
62	978	−3.67	−0.46	−0.48	9	−3.27	−3.08	0.18	39	−0.02	2.38	5.06	3.40
19	976	−3.67	−0.46	−0.48	9	−3.36	−3.12	0.23	40	0.10	2.40	4.96	3.24
5	972	−3.67	−0.46	−0.48	7	−3.50	−3.32	0.17	39	−0.12	2.41	5.13	3.33
46	967	−3.67	−0.46	−0.48	11	−3.40	−3.24	0.16	41	0.02	2.43	5.00	3.18
85	963	−3.67	−0.46	−0.48	9	−3.54	−3.44	0.09	39	−0.07	2.43	5.21	3.40
21	953	−3.67	−0.46	−0.48	9	−3.39	−3.28	0.11	41	−0.21	2.42	5.27	3.25
9	944	−3.67	−0.46	−0.48	11	−3.56	−3.30	0.25	40	−0.20	2.44	5.23	3.23
42	928	−3.68	−0.46	−0.48	11	−3.49	−3.22	0.26	40	−0.05	2.43	5.14	3.35
98	918	−3.68	−0.46	−0.48	9	−3.40	−3.21	0.19	39	−0.02	2.41	5.24	3.27
10	915	−3.68	−0.46	−0.49	7	−3.36	−3.19	0.17	39	−0.28	2.41	5.18	3.28
29	885	−3.68	−0.47	−0.49	9	−3.43	−3.23	0.20	40	−0.10	2.41	5.20	3.35
45	882	−3.68	−0.47	−0.49	9	−3.40	−3.19	0.20	40	−0.10	2.42	5.14	3.32
26	874	−3.68	−0.47	−0.49	7	−3.25	−3.11	0.14	40	−0.10	2.41	5.12	3.23
52	872	−3.68	−0.47	−0.49	9	−3.36	−3.17	0.19	40	−0.15	2.42	5.22	3.31
65	865	−3.68	−0.47	−0.49	9	−3.43	−3.29	0.13	40	−0.15	2.42	5.17	3.30
90	860	−3.68	−0.47	−0.49	9	−3.46	−3.27	0.19	40	−0.10	2.41	5.10	3.30
54	854	−3.68	−0.47	−0.49	9	−3.36	−3.19	0.16	40	−0.10	2.42	5.03	3.31
72	805	−3.68	−0.47	−0.49	13	−3.44	−3.26	0.17	40	−0.05	2.40	4.81	3.23
79	803	−3.68	−0.47	−0.49	7	−3.42	−3.31	0.10	39	0.02	2.42	5.24	3.41
49	785	−3.69	−0.47	−0.49	9	−3.55	−3.34	0.20	40	−0.10	2.43	5.11	3.49
43	777	−3.69	−0.47	−0.50	7	−3.39	−3.21	0.18	40	−0.20	2.42	5.08	3.26
48	773	−3.69	−0.47	−0.50	9	−3.59	−3.38	0.20	39	−0.12	2.43	5.19	3.29
39	770	−3.69	−0.47	−0.50	7	−3.37	−3.18	0.18	40	−0.30	2.40	5.13	3.32
01	769	−3.69	−0.47	−0.50	11	−3.38	−3.27	0.11	40	−0.05	2.42	5.09	3.41
73	740	−3.69	−0.48	−0.50	9	−3.56	−3.36	0.19	40	−0.05	2.43	5.21	3.36
02	723	−3.69	−0.48	−0.50	7	−3.46	−3.25	0.20	43	−0.25	2.44	5.25	2.75
31	701	−3.69	−0.48	−0.50	11	−3.58	−3.33	0.25	40	−0.25	2.43	5.05	3.46
50	692	−3.69	−0.48	−0.50	9	−3.42	−3.22	0.20	41	−0.17	2.42	5.14	3.36
34	677	−3.69	−0.48	−0.50	7	−3.64	−3.36	0.27	39	−0.17	2.42	5.15	3.38
60	664	−3.69	−0.48	−0.50	9	−3.35	−3.15	0.19	39	−0.12	2.40	4.94	3.38
92	618	−3.70	−0.48	−0.51	11	−3.52	−3.41	0.10	40	−0.10	2.44	5.08	3.42
14	603	−3.70	−0.49	−0.51	11	−3.46	−3.36	0.10	40	−0.20	2.42	5.11	3.14
41	591	−3.70	−0.49	−0.51	9	−3.53	−3.36	0.16	39	−0.02	2.42	5.11	3.35

68	563	−3.70	−0.49	−0.51	9	−3.43	−3.28	0.15	40	0.05	2.44	5.22	3.17
66	554	−3.70	−0.49	−0.51	7	−3.48	−3.26	0.21	40	−0.05	2.41	5.19	3.33
64	547	−3.70	−0.49	−0.51	9	−3.44	−3.20	0.24	39	−0.17	2.43	5.24	3.49
23	519	−3.71	−0.49	−0.51	11	−3.39	−3.21	0.18	39	0.33	2.40	5.04	3.30
67	508	−3.71	−0.49	−0.51	11	−3.54	−3.44	0.10	39	0.07	2.43	5.00	3.48
70	490	−3.71	−0.49	−0.52	9	−3.42	−3.20	0.21	40	−0.05	2.42	5.10	3.31
86	480	−3.71	−0.49	−0.52	11	−3.47	−3.28	0.18	41	−0.02	2.44	5.12	2.84
12	457	−3.71	−0.50	−0.52	13	−3.61	−3.50	0.10	39	−0.12	2.44	5.06	3.28
32	448	−3.71	−0.50	−0.52	7	−3.41	−3.26	0.15	40	−0.10	2.41	5.20	3.25
82	446	−3.71	−0.50	−0.52	9	−3.44	−3.24	0.20	41	−0.02	2.43	5.10	3.29
20	350	−3.72	−0.50	−0.53	11	−3.49	−3.31	0.17	40	0.10	2.42	4.61	3.29
18	328	−3.72	−0.50	−0.53	9	−3.41	−3.24	0.17	40	−0.05	2.42	5.21	3.17
15	247	−3.72	−0.51	−0.53	9	−3.48	−3.24	0.24	39	−0.02	2.43	5.09	3.44
93	240	−3.73	−0.51	−0.53	9	−3.56	−3.41	0.14	41	−0.02	2.44	5.05	3.41
87	223	−3.73	−0.51	−0.53	9	−3.62	−3.42	0.19	39	−0.02	2.43	5.05	3.41
78	144	−3.73	−0.52	−0.54	9	−3.53	−3.30	0.22	39	0.02	2.42	5.14	3.40
75	123	−3.73	−0.52	−0.54	5	−3.36	−3.12	0.23	40	−0.15	2.38	4.91	3.05
71	0	−3.74	−0.53	−0.55	9	−3.49	−3.14	0.34	39	−0.07	2.42	5.20	3.44

Table SI39: Structural, energetic and electronic properties for Co_8Mo_7 cluster, as follows: configuration number (i), relative DFT total energy (ΔE_{tot}^{DFT}, in meV), binding energy (E_b, in eV), excess energy (E_{exc}, in eV), stabilization energy (E_{stab}, in eV), total magnetic moment (M_{tot}, in μ_B), HOMO energy (ε_{HOMO}, in eV), LUMO energy (ε_{LUMO}, in eV), HOMO-LUMO energy difference, (E_{gap}, in eV), total number of bonds (N_b), average chemical order parameter (σ_{av}), average bond length (d_{av}, in Å), average effective coordination number (ECN_{av}, NNN), and average radius (R_{av}, in Å).

i	ΔE_{tot}^{DFT}	E_b	E_{exc}	E_{stab}	M_{tot}	ε_{HOMO}	ε_{LUMO}	E_{gap}	N_b	σ_{av}	d_{av}	ECN_{av}	R_{av}
57	1788	−3.63	−0.40	−0.40	10	−3.44	−3.28	0.16	44	−0.09	2.40	5.27	3.41
40	1728	−3.63	−0.40	−0.41	10	−3.55	−3.38	0.16	43	−0.20	2.42	5.55	3.36
28	1668	−3.64	−0.40	−0.41	10	−3.48	−3.31	0.16	43	−0.06	2.40	5.34	3.40
20	1547	−3.65	−0.41	−0.42	10	−3.41	−3.32	0.08	44	−0.13	2.39	5.23	3.50
14	1471	−3.65	−0.42	−0.42	8	−3.51	−3.32	0.18	44	0.00	2.40	5.31	3.48
12	1394	−3.66	−0.42	−0.43	8	−3.50	−3.30	0.19	43	−0.25	2.40	5.34	3.32
21	1378	−3.66	−0.42	−0.43	8	−3.44	−3.32	0.11	44	−0.18	2.39	5.27	3.38
37	1320	−3.66	−0.43	−0.43	8	−3.53	−3.40	0.12	44	−0.27	2.40	5.14	3.41
35	1301	−3.66	−0.43	−0.43	12	−3.46	−3.30	0.16	45	−0.06	2.43	5.30	3.41
08	1287	−3.66	−0.43	−0.44	10	−3.50	−3.32	0.17	44	−0.13	2.41	5.31	3.46
97	1277	−3.66	−0.43	−0.44	10	−3.41	−3.32	0.09	46	−0.21	2.41	5.27	3.48
32	1251	−3.67	−0.43	−0.44	8	−3.48	−3.28	0.20	43	−0.11	2.41	5.40	3.41
1	1237	−3.67	−0.43	−0.44	8	−3.45	−3.25	0.19	43	−0.20	2.40	5.32	3.42
53	1229	−3.67	−0.43	−0.44	8	−3.42	−3.21	0.20	44	−0.09	2.39	5.40	3.34
25	1200	−3.67	−0.44	−0.44	10	−3.60	−3.34	0.25	44	−0.18	2.41	5.41	3.45
48	1198	−3.67	−0.44	−0.44	12	−3.64	−3.42	0.22	44	−0.22	2.44	5.32	3.56
70	1196	−3.67	−0.44	−0.44	12	−3.46	−3.25	0.20	44	0.04	2.41	5.32	3.36
4	1190	−3.67	−0.44	−0.44	10	−3.49	−3.25	0.24	44	−0.04	2.41	5.39	3.38
93	1189	−3.67	−0.44	−0.44	14	−3.57	−3.30	0.27	45	−0.06	2.42	5.40	3.39
50	1189	−3.67	−0.44	−0.44	10	−3.45	−3.25	0.20	44	−0.09	2.40	5.38	3.46
24	1188	−3.67	−0.44	−0.44	10	−3.41	−3.30	0.10	43	0.02	2.42	5.51	3.35
58	1149	−3.67	−0.44	−0.44	12	−3.50	−3.32	0.17	44	0.13	2.42	5.27	3.42
42	1130	−3.67	−0.44	−0.45	12	−3.53	−3.31	0.22	46	−0.04	2.41	5.26	3.47
47	1123	−3.67	−0.44	−0.45	10	−3.46	−3.26	0.20	44	−0.09	2.42	5.38	3.44
52	1089	−3.68	−0.44	−0.45	12	−3.53	−3.34	0.19	44	−0.09	2.42	5.35	3.37
82	1081	−3.68	−0.44	−0.45	12	−3.58	−3.36	0.22	43	−0.06	2.44	5.42	3.34

17	1061	−3.68	−0.45	−0.45	12	−3.45	−3.29	0.15	45	0.11	2.40	5.27	3.45
30	1056	−3.68	−0.45	−0.45	10	−3.62	−3.41	0.21	43	−0.06	2.41	5.13	3.39
90	1045	−3.68	−0.45	−0.45	10	−3.46	−3.31	0.15	44	−0.04	2.41	5.39	3.48
72	1042	−3.68	−0.45	−0.45	10	−3.44	−3.29	0.14	44	−0.13	2.42	5.21	3.41
15	1037	−3.68	−0.45	−0.45	10	−3.52	−3.35	0.17	45	0.02	2.43	5.37	3.46
13	1035	−3.68	−0.45	−0.45	10	−3.60	−3.35	0.24	44	−0.13	2.43	5.46	3.39
27	1026	−3.68	−0.45	−0.45	12	−3.37	−3.20	0.16	44	−0.09	2.40	5.29	3.46
67	1006	−3.68	−0.45	−0.45	8	−3.46	−3.27	0.18	44	0.00	2.41	5.34	3.31
54	995	−3.68	−0.45	−0.45	8	−3.46	−3.27	0.18	44	−0.04	2.42	5.43	3.44
38	989	−3.68	−0.45	−0.45	6	−3.38	−3.21	0.17	44	−0.13	2.40	5.45	3.40
0	981	−3.68	−0.45	−0.46	8	−3.40	−3.16	0.24	45	−0.20	2.40	5.27	3.45
36	980	−3.68	−0.45	−0.46	10	−3.50	−3.35	0.14	44	−0.04	2.41	5.29	3.37
56	958	−3.69	−0.45	−0.46	10	−3.50	−3.34	0.15	45	−0.11	2.43	5.25	3.34
75	951	−3.69	−0.45	−0.46	12	−3.45	−3.33	0.11	44	−0.04	2.41	5.26	3.45
49	934	−3.69	−0.45	−0.46	10	−3.57	−3.42	0.14	44	−0.09	2.43	5.33	3.30
19	933	−3.69	−0.45	−0.46	10	−3.41	−3.22	0.19	44	0.04	2.40	5.37	3.42
92	907	−3.69	−0.46	−0.46	12	−3.52	−3.36	0.16	43	−0.06	2.41	5.25	3.47
87	890	−3.69	−0.46	−0.46	10	−3.54	−3.35	0.18	45	−0.02	2.42	5.08	3.28
31	888	−3.69	−0.46	−0.46	10	−3.42	−3.30	0.11	44	−0.09	2.40	5.13	3.43
23	880	−3.69	−0.46	−0.46	10	−3.47	−3.27	0.20	43	−0.02	2.40	5.32	3.40
78	870	−3.69	−0.46	−0.46	12	−3.44	−3.26	0.17	44	0.13	2.40	5.31	3.43
71	848	−3.69	−0.46	−0.46	10	−3.37	−3.19	0.18	44	0.04	2.40	5.28	3.37
66	815	−3.69	−0.46	−0.47	10	−3.49	−3.30	0.19	45	−0.11	2.41	5.19	3.45
60	807	−3.70	−0.46	−0.47	8	−3.42	−3.25	0.17	44	−0.22	2.41	5.40	3.39
29	793	−3.70	−0.46	−0.47	12	−3.45	−3.29	0.15	44	0.09	2.42	5.38	3.43
79	747	−3.70	−0.47	−0.47	10	−3.55	−3.34	0.21	44	−0.13	2.41	5.26	3.42
84	722	−3.70	−0.47	−0.47	8	−3.32	−3.17	0.14	44	−0.22	2.40	5.23	3.39
99	713	−3.70	−0.47	−0.47	10	−3.45	−3.25	0.19	45	0.33	2.40	5.17	3.44
89	708	−3.70	−0.47	−0.47	10	−3.40	−3.30	0.10	43	0.11	2.42	5.44	3.41
85	708	−3.70	−0.47	−0.47	12	−3.57	−3.30	0.26	43	−0.02	2.43	5.48	3.43
51	701	−3.70	−0.47	−0.47	12	−3.57	−3.40	0.16	44	−0.09	2.41	5.15	3.33
16	672	−3.70	−0.47	−0.48	10	−3.60	−3.41	0.19	44	−0.13	2.43	5.23	3.40
68	650	−3.71	−0.47	−0.48	10	−3.55	−3.42	0.13	45	−0.15	2.43	5.23	3.43
44	635	−3.71	−0.47	−0.48	10	−3.45	−3.29	0.16	46	0.00	2.42	5.39	3.42
41	620	−3.71	−0.47	−0.48	12	−3.59	−3.40	0.19	45	−0.06	2.44	5.26	3.45
59	597	−3.71	−0.48	−0.48	12	−3.53	−3.30	0.23	44	0.00	2.40	5.05	3.41
83	592	−3.71	−0.48	−0.48	10	−3.47	−3.23	0.24	45	−0.06	2.41	5.22	3.36
33	530	−3.71	−0.48	−0.49	14	−3.47	−3.39	0.08	45	−0.06	2.42	5.23	3.36
91	521	−3.71	−0.48	−0.49	12	−3.49	−3.36	0.13	44	−0.09	2.43	5.34	3.43
74	505	−3.72	−0.48	−0.49	10	−3.43	−3.26	0.16	45	−0.11	2.44	5.31	3.40
34	497	−3.72	−0.48	−0.49	10	−3.57	−3.37	0.19	44	−0.04	2.43	5.29	3.42
6	467	−3.72	−0.48	−0.49	12	−3.50	−3.36	0.14	45	−0.06	2.43	5.15	3.46
63	459	−3.72	−0.49	−0.49	12	−3.44	−3.27	0.16	45	0.02	2.44	5.38	3.44
73	454	−3.72	−0.49	−0.49	10	−3.39	−3.18	0.21	46	−0.04	2.41	5.02	3.32
09	444	−3.72	−0.49	−0.49	10	−3.49	−3.32	0.17	44	−0.04	2.41	5.26	3.54
77	439	−3.72	−0.49	−0.49	12	−3.55	−3.35	0.20	45	−0.06	2.43	5.32	3.42
64	428	−3.72	−0.49	−0.49	10	−3.48	−3.28	0.19	46	−0.04	2.41	5.08	3.43
10	415	−3.72	−0.49	−0.49	12	−3.56	−3.37	0.18	45	0.11	2.40	5.21	3.58
86	397	−3.72	−0.49	−0.49	10	−3.52	−3.36	0.16	44	−0.18	2.42	5.10	3.38
2	381	−3.72	−0.49	−0.50	8	−3.43	−3.23	0.20	45	−0.11	2.41	5.05	3.27
3	364	−3.72	−0.49	−0.50	10	−3.51	−3.27	0.23	43	−0.06	2.42	5.36	3.31
7	247	−3.73	−0.50	−0.50	8	−3.46	−3.25	0.20	43	−0.16	2.41	5.21	3.31
81	238	−3.73	−0.50	−0.51	8	−3.39	−3.24	0.15	45	−0.11	2.43	5.12	3.38
88	225	−3.73	−0.50	−0.51	12	−3.60	−3.38	0.21	46	−0.04	2.41	4.75	3.31
43	224	−3.73	−0.50	−0.51	10	−3.49	−3.30	0.18	44	−0.13	2.43	5.42	3.45
76	215	−3.73	−0.50	−0.51	10	−3.50	−3.26	0.24	44	−0.27	2.42	5.20	3.31
65	200	−3.74	−0.50	−0.51	10	−3.52	−3.27	0.24	44	0.04	2.43	5.31	3.45

| 80 | 173 | −3.74 | −0.50 | −0.51 | 10 | −3.49 | −3.31 | 0.18 | 44 | −0.04 | 2.43 | 5.30 | 3.36 |
| 18 | 0 | −3.75 | −0.52 | −0.52 | 12 | −3.52 | −3.38 | 0.14 | 44 | −0.04 | 2.44 | 5.27 | 3.43 |

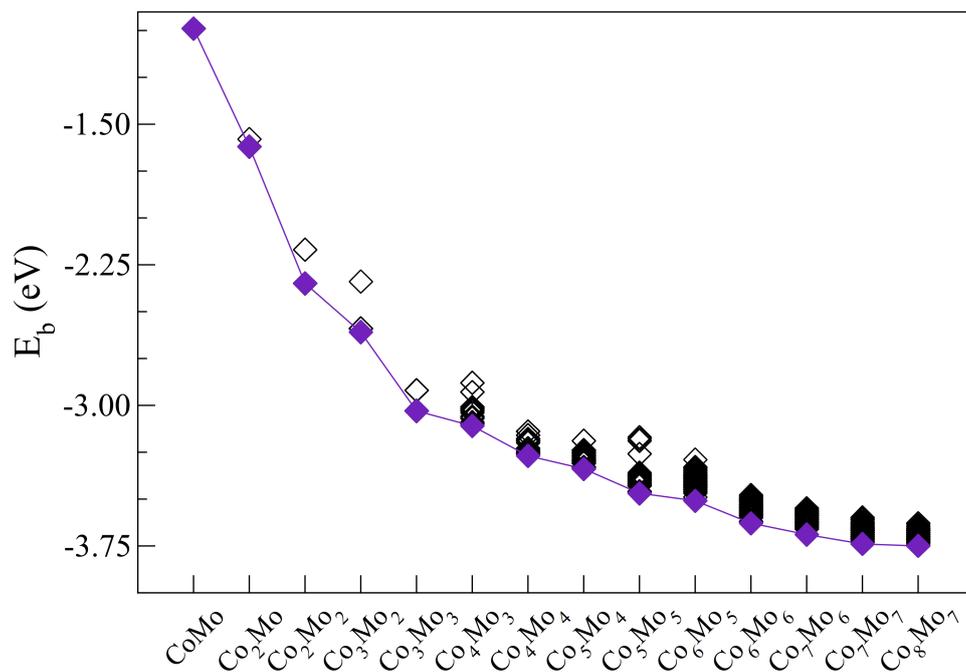Table SI40: Lowest energy configurations for the near-equiatomic Co_nMo_m subnanoalloys with $n+m = 2-15$.
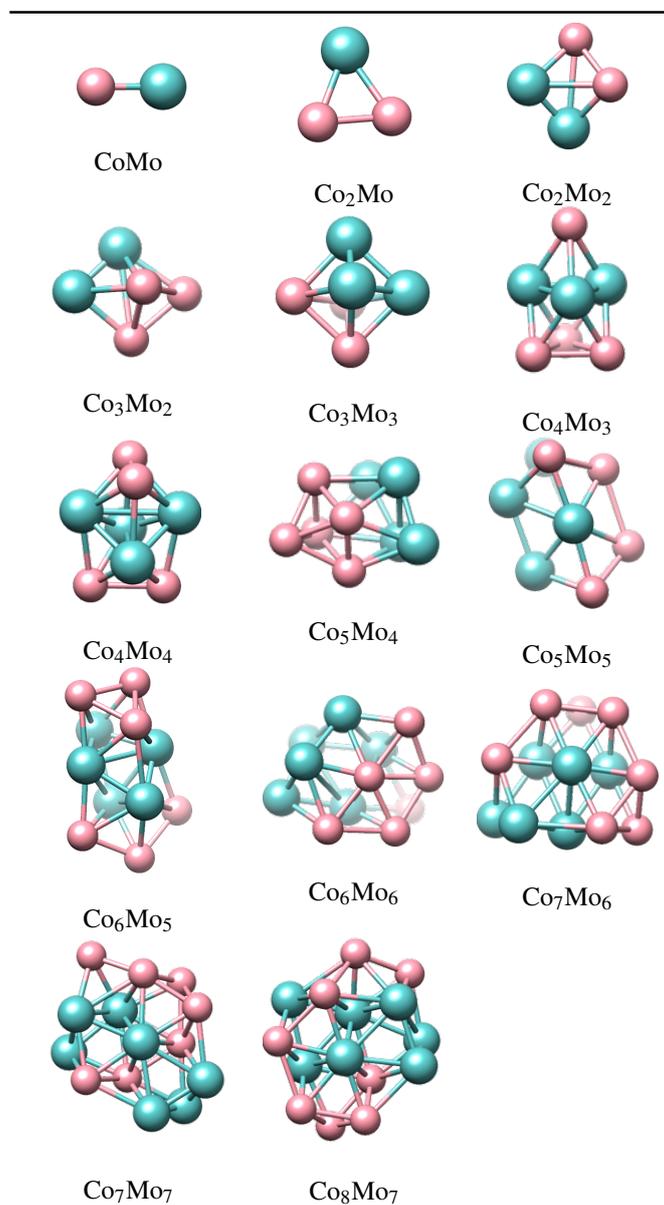
Figure SI21: Binding energy (E_b) for the near-equiatomic Co_nMo_m subnanoalloys with $n + m = 2 - 15$.
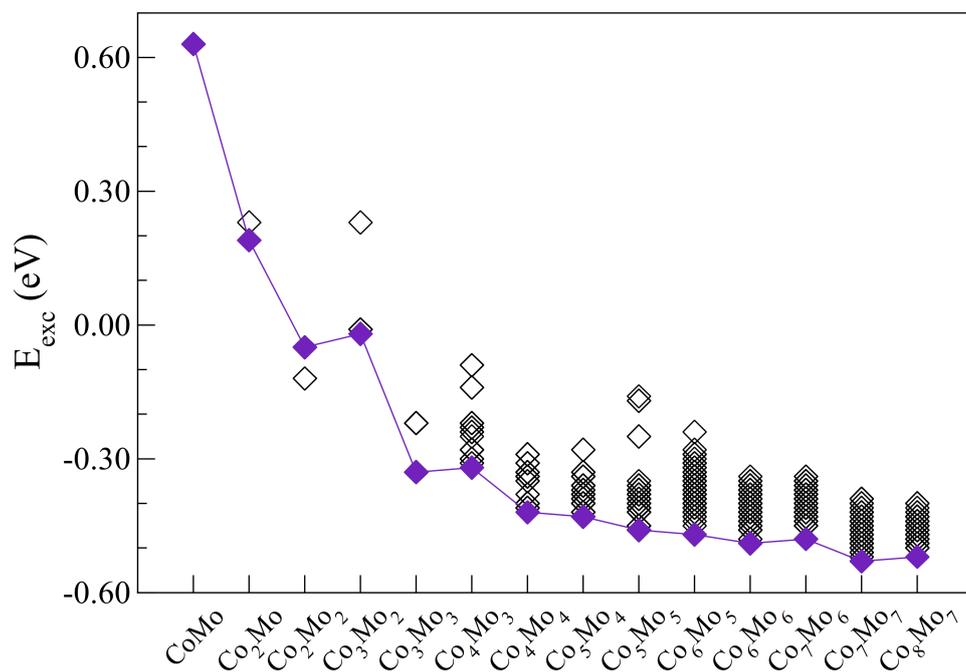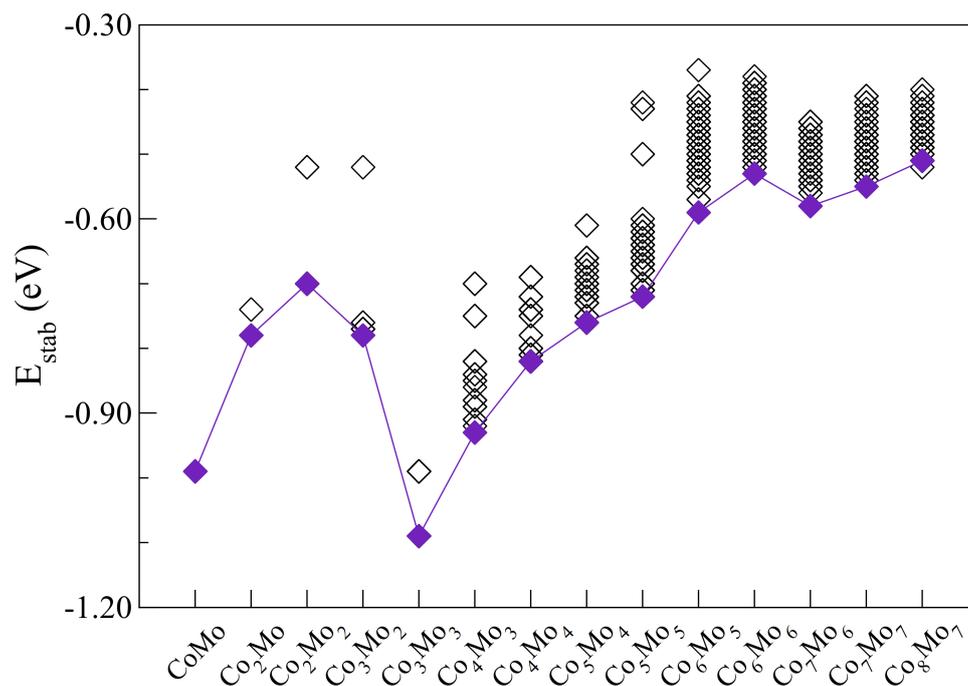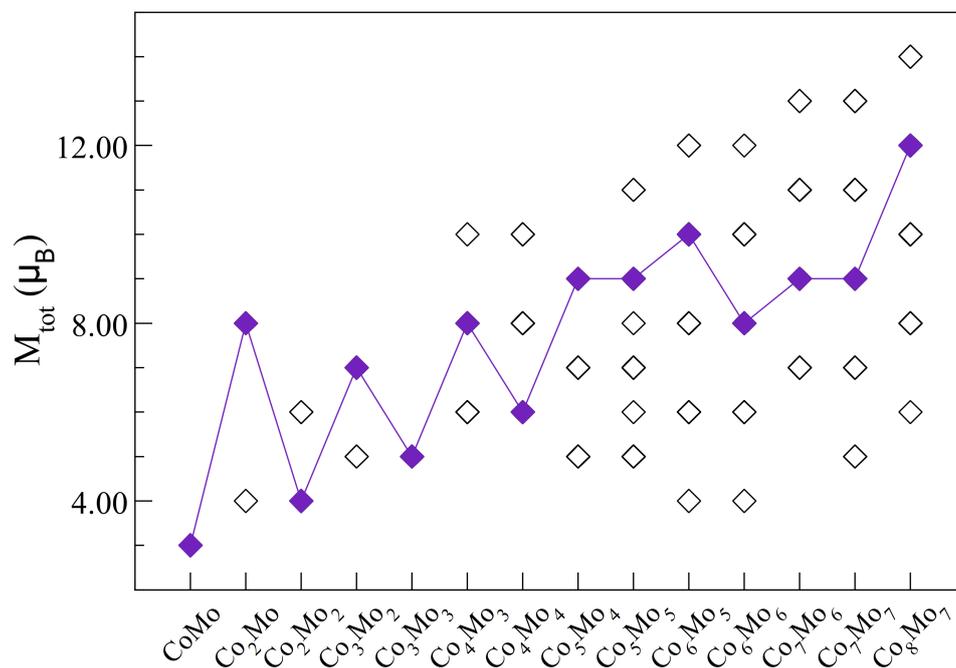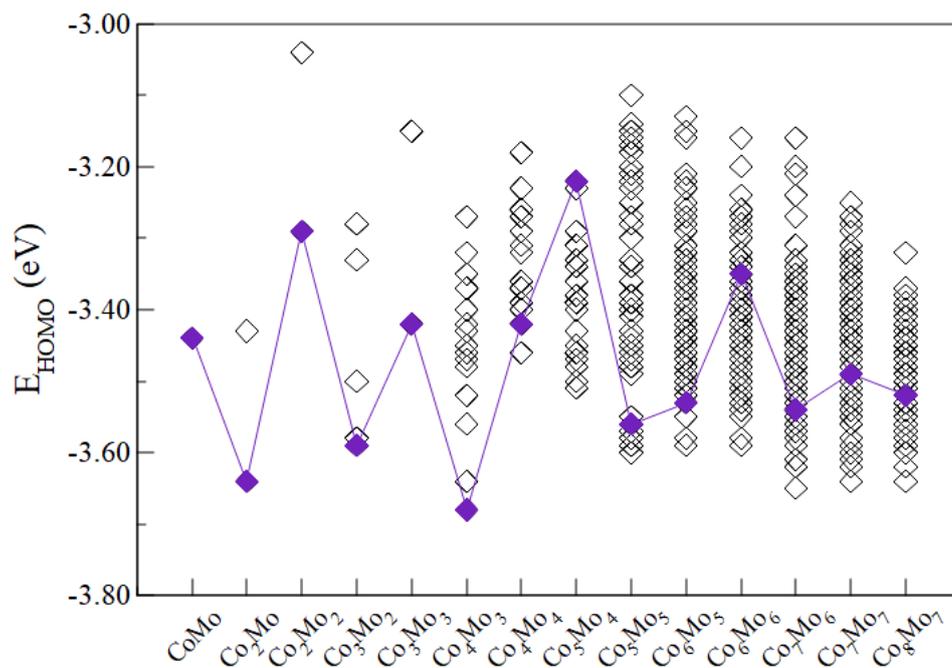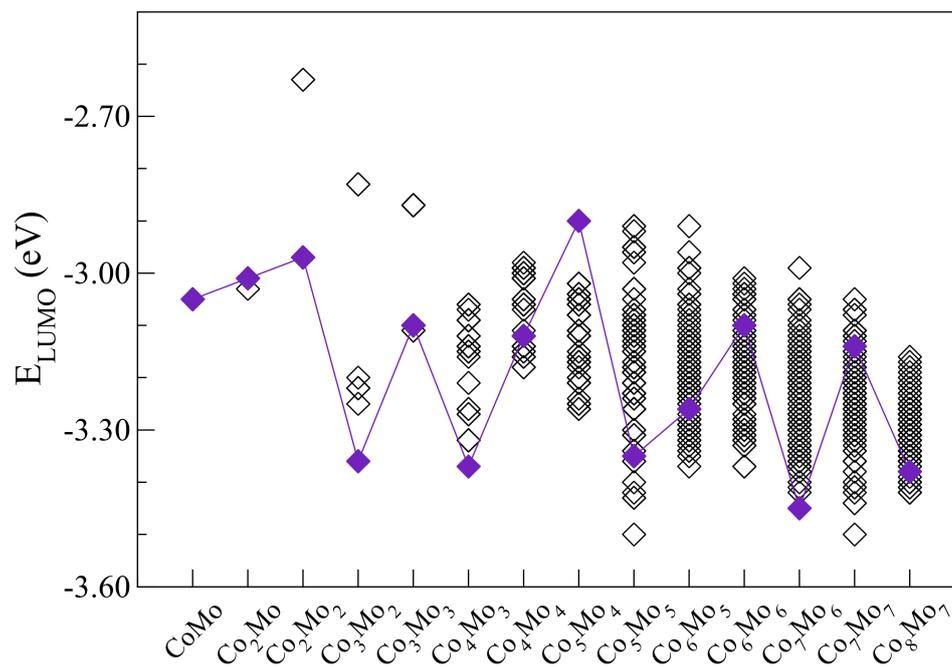

Figure SI22: Excess energy (E_{exc}) for the near-equiatomic Co_nMo_m subnanoalloys with $n + m = 2 - 15$.

Figure SI23: Stabilization energy (E_{stab}) for the near-equiatomic Co_nMo_m subnanoalloys with $n+m = 2-15$.

Figure SI24: Total magnetic moment (M_{tot}) for the near-equiatomic Co_nMo_m subnanoalloys with $n+m = 2-15$.

Figure SI25: HOMO energy (E_{HOMO}) for the near-equiatomic Co_nMo_m subnanoalloys with $n+m = 2-15$.

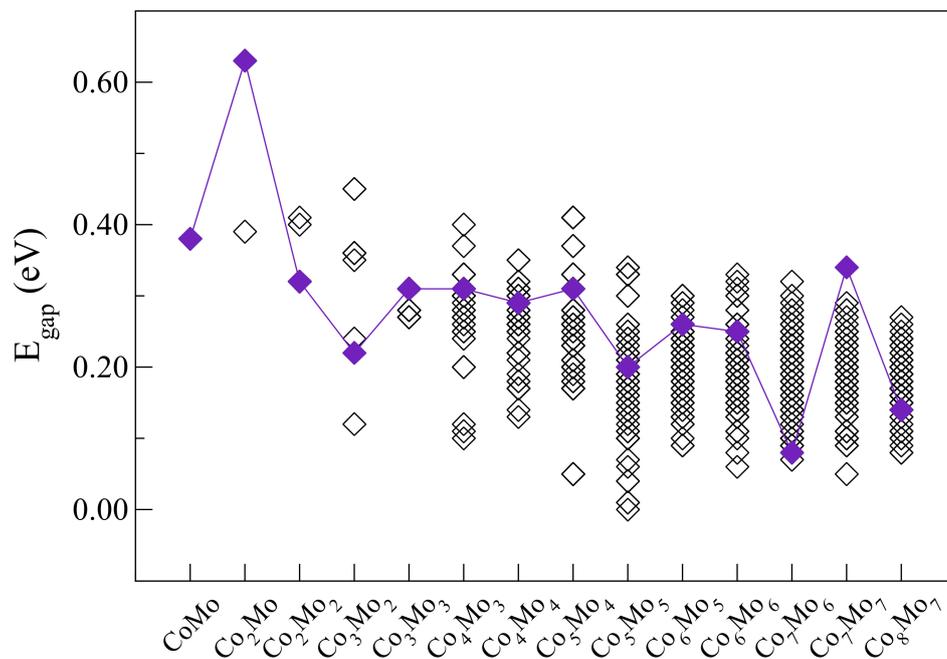Figure SI26: LUMO energy (E_{LUMO}) for the near-equiatomic Co_nMo_m subnanoalloys with $n+m = 2-15$.

Figure SI27: HOMO-LUMO energy gap (E_{gap}) for the near-equiatomic Co_nMo_m subnanoalloys with $n+m = 2-15$.
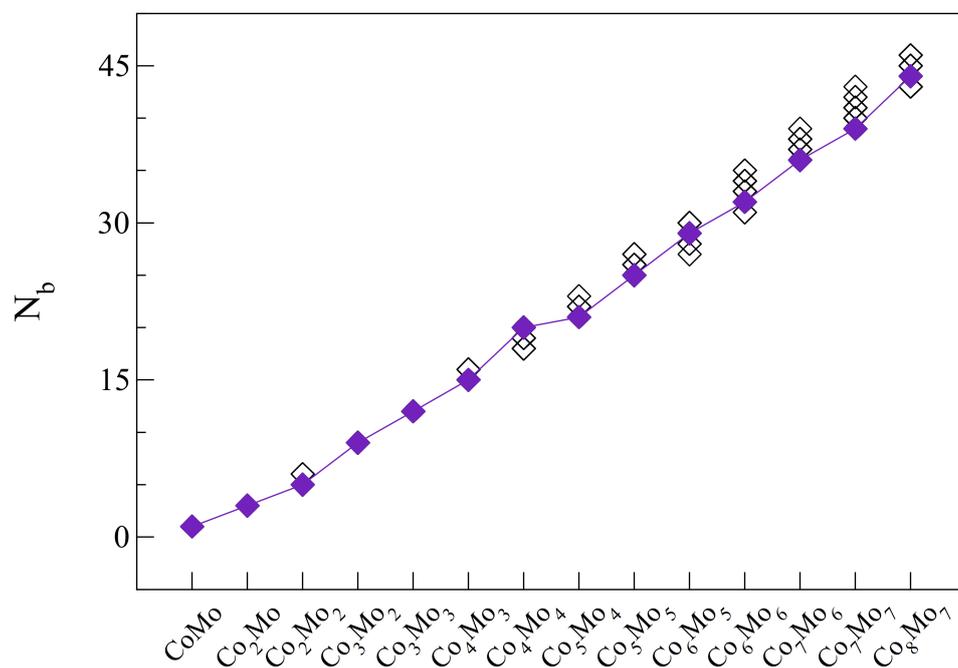

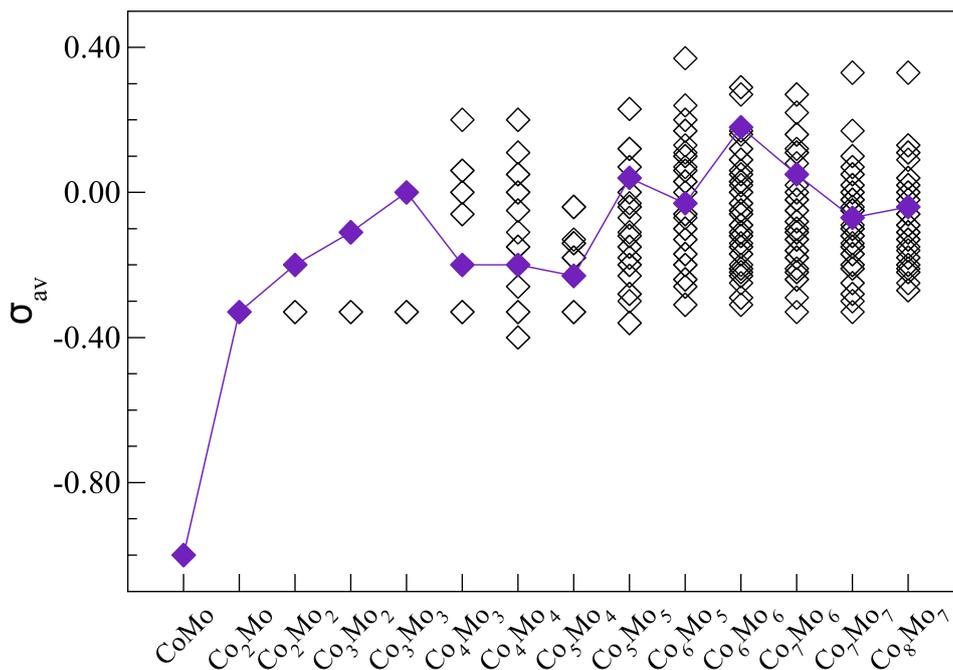Figure SI28: Total number of bonds (N_b) for the near-equiatomic Co_nMo_m subnanoalloys with $n+m = 2-15$.

Figure SI29: Average chemical order parameter (σ_{av}) for the near-equiatomic Co_nMo_m subnanoalloys with $n + m = 2 - 15$.
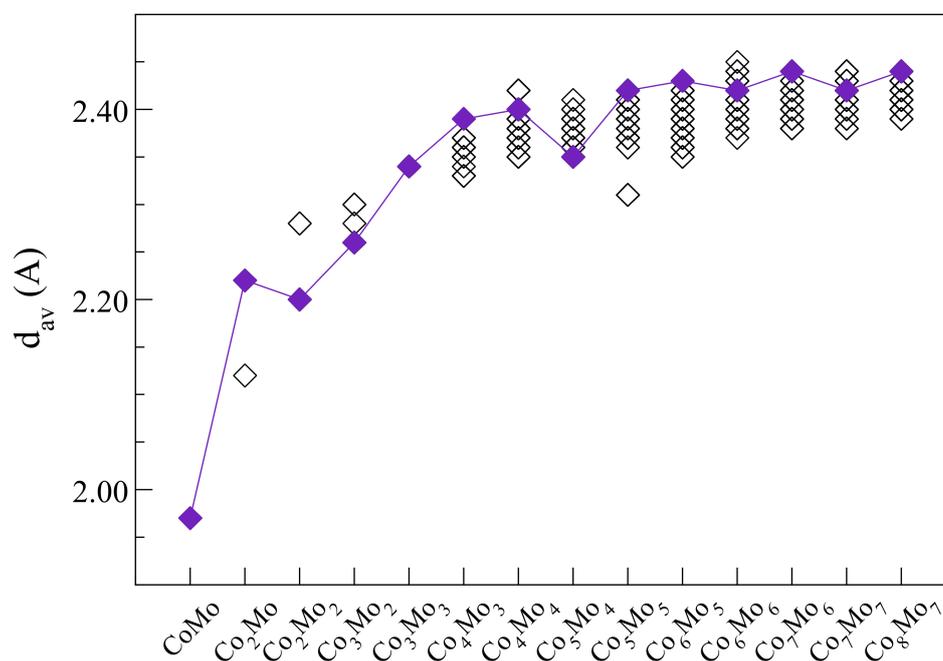

Figure SI30: Average bond length (d_{av}) for the near-equiatomic Co_nMo_m subnanoalloys with $n + m = 2 - 15$.
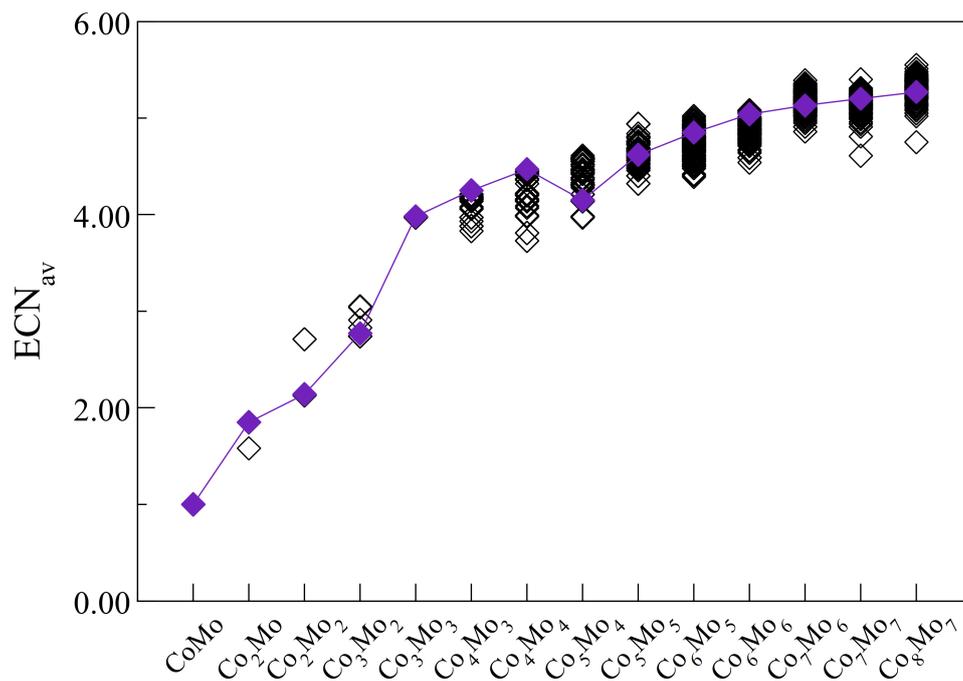
Figure SI31: Average effective coordination number (ECN_{av}) for the near-equiatomic Co_nMo_m subnanoalloys with $n + m = 2 - 15$.
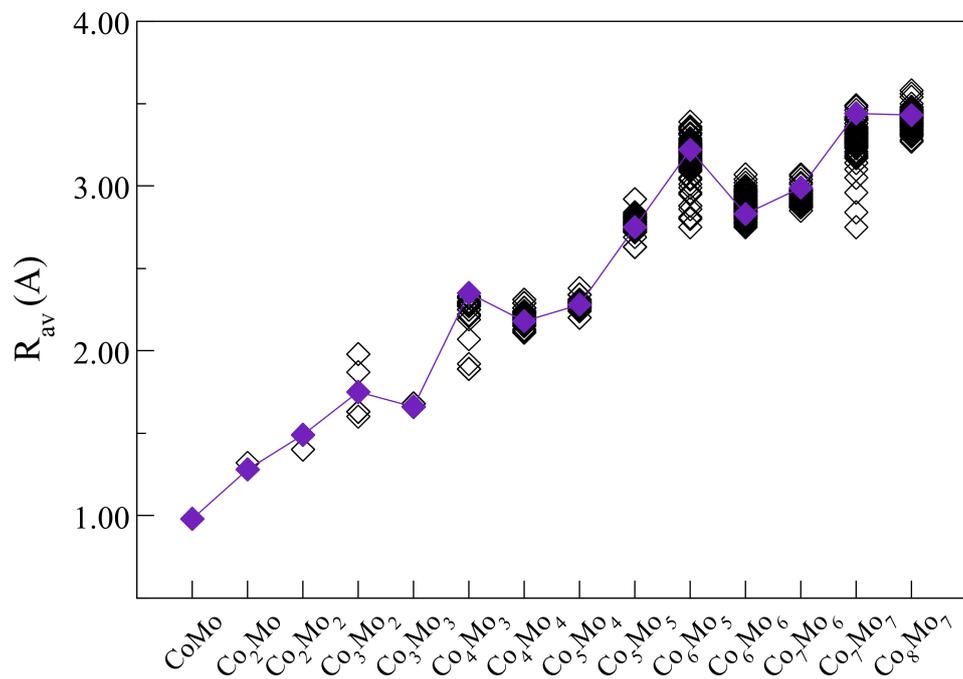

Figure SI32: Average radius (R_{av}) for the near-equiatomic Co_nMo_m subnanoalloys with $n + m = 2 - 15$.

5 Gas-phase Mo$_n$Co$_m$ Subnanoalloys

Table SI41: Structural, energetic and electronic properties for MoCo cluster, as follows: configuration number (i), relative DFT total energy (ΔE_{tot}^{DFT}, in meV), binding energy (E_b, in eV), excess energy (E_{exc}, in eV), stabilization energy (E_{stab}, in eV), total magnetic moment (M_{tot}, in μ_B), HOMO energy (ε_{HOMO}, in eV), LUMO energy (ε_{LUMO}, in eV), HOMO-LUMO energy difference, (E_{gap}, in eV), total number of bonds (N_b), average chemical order parameter (σ_{av}), average bond length (d_{av}, in Å), average effective coordination number (ECN_{av}, NNN), and average radius (R_{av}, in Å).

i	ΔE_{tot}^{DFT}	E_b	E_{exc}	E_{stab}	M_{tot}	ε_{HOMO}	ε_{LUMO}	E_{gap}	N_b	σ_{av}	d_{av}	ECN_{av}	R_{av}
2	0	−0.99	0.64	−0.99	3	−3.44	−3.05	0.38	1	−1.00	1.97	1.00	0.98
1	0	−0.99	0.64	−0.99	3	−3.44	−3.05	0.38	1	−1.00	1.97	1.00	0.98

Table SI42: Structural, energetic and electronic properties for Mo$_2$Co cluster, as follows: configuration number (i), relative DFT total energy (ΔE_{tot}^{DFT}, in meV), binding energy (E_b, in eV), excess energy (E_{exc}, in eV), stabilization energy (E_{stab}, in eV), total magnetic moment (M_{tot}, in μ_B), HOMO energy (ε_{HOMO}, in eV), LUMO energy (ε_{LUMO}, in eV), HOMO-LUMO energy difference, (E_{gap}, in eV), total number of bonds (N_b), average chemical order parameter (σ_{av}), average bond length (d_{av}, in Å), average effective coordination number (ECN_{av}, NNN), and average radius (R_{av}, in Å).

i	ΔE_{tot}^{DFT}	E_b	E_{exc}	E_{stab}	M_{tot}	ε_{HOMO}	ε_{LUMO}	E_{gap}	N_b	σ_{av}	d_{av}	ECN_{av}	R_{av}
3	2	−2.11	−0.09	−0.75	1	−2.90	−2.45	0.45	3	−0.33	2.16	1.66	1.32
1	1	−2.11	−0.09	−0.75	1	−2.89	−2.45	0.44	3	−0.33	2.16	1.66	1.31
2	0	−2.11	−0.09	−0.75	1	−2.90	−2.45	0.45	3	−0.33	2.16	1.65	1.32

Table SI43: Structural, energetic and electronic properties for Mo$_2$Co$_2$ cluster, as follows: configuration number (i), relative DFT total energy (ΔE_{tot}^{DFT}, in meV), binding energy (E_b, in eV), excess energy (E_{exc}, in eV), stabilization energy (E_{stab}, in eV), total magnetic moment (M_{tot}, in μ_B), HOMO energy (ε_{HOMO}, in eV), LUMO energy (ε_{LUMO}, in eV), HOMO-LUMO energy difference, (E_{gap}, in eV), total number of bonds (N_b), average chemical order parameter (σ_{av}), average bond length (d_{av}, in Å), average effective coordination number (ECN_{av}, NNN), and average radius (R_{av}, in Å).

i	ΔE_{tot}^{DFT}	E_b	E_{exc}	E_{stab}	M_{tot}	ε_{HOMO}	ε_{LUMO}	E_{gap}	N_b	σ_{av}	d_{av}	ECN_{av}	R_{av}
5	1659	−1.94	0.47	−0.29	8	−3.24	−2.96	0.28	5	−0.60	2.23	2.24	1.53
2	1658	−1.94	0.47	−0.29	8	−3.24	−2.96	0.28	5	−0.60	2.23	2.24	1.53
3	1	−2.35	0.06	−0.70	4	−3.29	−2.97	0.32	6	−0.33	2.20	2.14	1.49
4	1	−2.35	0.06	−0.70	4	−3.29	−2.97	0.32	5	−0.20	2.20	2.13	1.49
1	0	−2.35	0.06	−0.70	4	−3.29	−2.97	0.31	6	−0.33	2.20	2.14	1.49

Table SI44: Structural, energetic and electronic properties for Mo$_3$Co$_2$ cluster, as follows: configuration number (i), relative DFT total energy (ΔE_{tot}^{DFT}, in meV), binding energy (E_b, in eV), excess energy (E_{exc}, in eV), stabilization energy (E_{stab}, in eV), total magnetic moment (M_{tot}, in μ_B), HOMO energy (ε_{HOMO}, in eV), LUMO energy (ε_{LUMO}, in eV), HOMO-LUMO energy difference, (E_{gap}, in eV), total number of bonds (N_b), average chemical order parameter (σ_{av}), average bond length (d_{av}, in Å), average effective coordination number (ECN_{av}, NNN), and average radius (R_{av}, in Å).

i	ΔE_{tot}^{DFT}	E_b	E_{exc}	E_{stab}	M_{tot}	ε_{HOMO}	ε_{LUMO}	E_{gap}	N_b	σ_{av}	d_{av}	ECN_{av}	R_{av}
6	292	−2.67	0.07	−0.85	6	−3.30	−2.89	0.40	9	−0.33	2.36	3.17	1.94
7	286	−2.67	0.07	−0.85	6	−3.20	−2.91	0.29	9	−0.11	2.28	2.56	1.80
0	285	−2.67	0.07	−0.85	6	−3.20	−2.91	0.28	9	−0.11	2.28	2.56	1.80
8	243	−2.68	0.06	−0.86	6	−3.20	−2.93	0.27	9	−0.11	2.33	3.00	1.88
1	243	−2.68	0.06	−0.86	6	−3.20	−2.93	0.27	9	−0.11	2.33	3.00	1.88
2	226	−2.68	0.05	−0.86	4	−3.20	−2.91	0.29	9	−0.33	2.28	2.75	1.62
3	1	−2.73	0.01	−0.91	4	−3.48	−2.89	0.59	8	0.00	2.29	2.84	1.69
5	0	−2.73	0.01	−0.91	4	−3.48	−2.89	0.59	8	0.00	2.29	2.84	1.69

Table SI45: Structural, energetic and electronic properties for Mo$_3$Co$_3$ cluster, as follows: configuration number (i), relative DFT total energy (ΔE_{tot}^{DFT}, in meV), binding energy (E_b, in eV), excess energy (E_{exc}, in eV), stabilization energy (E_{stab}, in eV), total magnetic moment (M_{tot}, in μ_B), HOMO energy (ε_{HOMO}, in eV), LUMO energy (ε_{LUMO}, in eV), HOMO-LUMO energy difference, (E_{gap}, in eV), total number of bonds (N_b), average chemical order parameter (σ_{av}), average bond length (d_{av}, in Å), average effective coordination number (ECN_{av}, NNN), and average radius (R_{av}, in Å).

i	ΔE_{tot}^{DFT}	E_b	E_{exc}	E_{stab}	M_{tot}	ε_{HOMO}	ε_{LUMO}	E_{gap}	N_b	σ_{av}	d_{av}	ECN_{av}	R_{av}
6	787	−2.90	0.0613	−0.96	7	−3.25	−3.13	0.11	12	−0.33	2.35	3.68	1.78
5	786	−2.90	0.0612	−0.96	7	−3.25	−3.13	0.11	12	−0.33	2.35	3.68	1.78
11	683	−2.92	0.0439	−0.98	7	−3.28	−3.16	0.11	12	−0.33	2.36	3.97	1.75
18	683	−2.92	0.0438	−0.98	7	−3.28	−3.16	0.11	12	−0.33	2.36	3.97	1.75
3	680	−2.92	0.0435	−0.98	7	−3.28	−3.16	0.11	12	−0.33	2.36	3.97	1.75
10	680	−2.92	0.0435	−0.98	7	−3.28	−3.16	0.11	12	−0.33	2.36	3.97	1.75
13	605	−2.93	0.0310	−0.99	5	−3.12	−2.91	0.20	12	−0.33	2.35	3.87	1.77
16	603	−2.93	0.0306	−0.99	5	−3.12	−2.91	0.20	12	−0.33	2.35	3.87	1.77
15	591	−2.93	0.0286	−0.99	3	−3.07	−2.81	0.26	13	−0.23	2.34	3.86	1.76
12	0	−3.03	−0.0699	−1.09	7	−3.60	−3.31	0.29	12	0.00	2.35	3.78	1.68
20	0	−3.03	−0.0699	−1.09	7	−3.60	−3.31	0.29	12	0.00	2.35	3.78	1.68
19	0	−3.03	−0.0699	−1.09	7	−3.60	−3.31	0.29	12	0.00	2.35	3.78	1.68
9	0	−3.03	−0.0699	−1.09	7	−3.60	−3.31	0.29	12	0.00	2.35	3.78	1.68
14	0	−3.03	−0.0700	−1.09	7	−3.60	−3.31	0.29	12	0.00	2.35	3.78	1.68
1	0	−3.03	−0.0700	−1.09	7	−3.60	−3.31	0.29	12	0.00	2.35	3.78	1.68
7	0	−3.03	−0.0700	−1.09	7	−3.60	−3.31	0.29	12	0.00	2.35	3.78	1.68
2	0	−3.03	−0.0700	−1.09	7	−3.60	−3.31	0.29	12	0.00	2.35	3.78	1.68

Table SI46: Structural, energetic and electronic properties for Mo_4Co_3 cluster, as follows: configuration number (i), relative DFT total energy (ΔE_{tot}^{DFT}, in meV), binding energy (E_b, in eV), excess energy (E_{exc}, in eV), stabilization energy (E_{stab}, in eV), total magnetic moment (M_{tot}, in μ_B), HOMO energy (ε_{HOMO}, in eV), LUMO energy (ε_{LUMO}, in eV), HOMO-LUMO energy difference, (E_{gap}, in eV), total number of bonds (N_b), average chemical order parameter (σ_{av}), average bond length (d_{av}, in Å), average effective coordination number (ECN_{av}, NNN), and average radius (R_{av}, in Å).

i	ΔE_{tot}^{DFT}	E_b	E_{exc}	E_{stab}	M_{tot}	ε_{HOMO}	ε_{LUMO}	E_{gap}	N_b	σ_{av}	d_{av}	ECN_{av}	R_{av}
25	558	−3.10	−0.01	−0.83	9	−3.32	−3.14	0.18	16	0.00	2.37	3.51	2.00
28	558	−3.10	−0.01	−0.83	9	−3.32	−3.14	0.18	16	0.00	2.37	3.50	2.00
5	537	−3.10	−0.02	−0.83	7	−3.18	−3.09	0.09	16	−0.25	2.39	3.92	1.96
12	518	−3.11	−0.02	−0.83	7	−3.27	−3.08	0.20	16	−0.25	2.37	3.73	2.00
15	518	−3.11	−0.02	−0.83	7	−3.27	−3.08	0.20	16	−0.25	2.37	3.73	2.00
11	465	−3.11	−0.03	−0.84	7	−3.36	−3.20	0.16	16	−0.25	2.39	3.98	1.93
34	465	−3.11	−0.03	−0.84	7	−3.36	−3.20	0.16	16	−0.25	2.39	3.98	1.93
29	435	−3.12	−0.03	−0.85	7	−3.37	−3.03	0.34	14	−0.29	2.36	3.48	2.01
20	434	−3.12	−0.03	−0.85	7	−3.37	−3.03	0.34	14	−0.29	2.36	3.48	2.01
31	431	−3.12	−0.03	−0.85	7	−3.39	−3.09	0.30	16	−0.25	2.38	3.71	1.99
8	430	−3.12	−0.03	−0.85	7	−3.39	−3.09	0.29	16	−0.25	2.38	3.72	1.99
22	430	−3.12	−0.03	−0.85	7	−3.39	−3.09	0.30	16	−0.25	2.38	3.71	1.99
2	430	−3.12	−0.03	−0.85	7	−3.39	−3.09	0.30	16	−0.25	2.38	3.71	1.99
9	365	−3.13	−0.04	−0.86	5	−3.24	−2.94	0.30	16	−0.25	2.38	3.97	1.93
32	337	−3.13	−0.05	−0.86	7	−3.27	−3.08	0.19	16	0.00	2.38	3.83	2.01
1	303	−3.14	−0.05	−0.86	7	−3.36	−3.13	0.23	15	0.20	2.38	4.03	2.14
26	255	−3.14	−0.06	−0.87	7	−3.38	−3.04	0.34	14	0.00	2.35	3.45	2.01
23	254	−3.14	−0.06	−0.87	7	−3.38	−3.04	0.34	14	0.00	2.35	3.45	2.01
10	141	−3.16	−0.07	−0.89	7	−3.29	−2.93	0.36	15	−0.07	2.39	3.94	2.18
13	141	−3.16	−0.07	−0.89	7	−3.29	−2.93	0.36	15	−0.07	2.39	3.94	2.18
30	139	−3.16	−0.07	−0.89	7	−3.29	−2.93	0.36	15	−0.07	2.39	3.94	2.18
24	139	−3.16	−0.07	−0.89	7	−3.29	−2.92	0.36	15	−0.07	2.40	3.94	2.18
4	114	−3.16	−0.08	−0.89	7	−3.26	−2.96	0.30	14	0.14	2.35	3.57	1.98
6	114	−3.16	−0.08	−0.89	7	−3.26	−2.96	0.30	14	0.14	2.35	3.57	1.98
17	93	−3.17	−0.08	−0.89	7	−3.43	−3.14	0.29	15	−0.20	2.42	4.17	2.33
19	67	−3.17	−0.08	−0.90	7	−3.30	−3.02	0.28	16	0.00	2.38	3.84	2.00
35	66	−3.17	−0.09	−0.90	7	−3.33	−3.03	0.30	14	0.14	2.34	3.42	2.01
33	66	−3.17	−0.09	−0.90	7	−3.33	−3.03	0.30	14	0.14	2.34	3.43	2.01
7	50	−3.17	−0.09	−0.90	7	−3.39	−3.01	0.39	15	−0.20	2.42	4.05	2.25
3	50	−3.17	−0.09	−0.90	7	−3.39	−3.01	0.39	15	−0.20	2.42	4.05	2.25
21	1	−3.18	−0.09	−0.91	5	−3.30	−2.99	0.31	16	−0.25	2.38	3.81	2.15
27	0	−3.18	−0.09	−0.91	5	−3.30	−2.99	0.31	16	−0.25	2.38	3.81	2.15

Table SI47: Structural, energetic and electronic properties for Mo_4Co_4 cluster, as follows: configuration number (i), relative DFT total energy (ΔE_{tot}^{DFT}, in meV), binding energy (E_b, in eV), excess energy (E_{exc}, in eV), stabilization energy (E_{stab}, in eV), total magnetic moment (M_{tot}, in μ_B), HOMO energy (ε_{HOMO}, in eV), LUMO energy (ε_{LUMO}, in eV), HOMO-LUMO energy difference, (E_{gap}, in eV), total number of bonds (N_b), average chemical order parameter (σ_{av}), average bond length (d_{av}, in Å), average effective coordination number (ECN_{av}, NNN), and average radius (R_{av}, in Å).

i	ΔE_{tot}^{DFT}	E_b	E_{exc}	E_{stab}	M_{tot}	ε_{HOMO}	ε_{LUMO}	E_{gap}	N_b	σ_{av}	d_{av}	ECN_{av}	R_{av}
48	991	−3.14	0.02	−0.69	6	−3.27	−3.03	0.23	19	−0.26	2.38	4.36	2.19
41	990	−3.14	0.02	−0.69	6	−3.27	−3.03	0.23	19	−0.26	2.38	4.36	2.19

62	855	−3.15	0.01	−0.71	10	−3.41	−3.24	0.16	17	−0.29	2.37	3.92	2.08
9	854	−3.15	0.01	−0.71	10	−3.40	−3.24	0.16	17	−0.29	2.37	3.92	2.08
29	804	−3.16	0.00	−0.72	6	−3.27	−2.99	0.28	20	−0.40	2.39	4.22	2.29
42	793	−3.16	0.00	−0.72	8	−3.44	−3.17	0.27	17	−0.41	2.37	4.04	2.11
52	725	−3.17	−0.00	−0.73	10	−3.47	−3.31	0.15	19	−0.26	2.37	3.92	2.22
57	725	−3.17	−0.00	−0.73	10	−3.47	−3.31	0.15	19	−0.26	2.37	3.92	2.22
6	725	−3.17	−0.00	−0.73	10	−3.47	−3.31	0.15	20	−0.20	2.37	3.92	2.22
51	725	−3.17	−0.00	−0.73	10	−3.47	−3.31	0.15	20	−0.20	2.37	3.92	2.22
43	686	−3.17	−0.00	−0.73	8	−3.41	−3.16	0.24	18	−0.33	2.36	3.79	2.17
28	686	−3.17	−0.00	−0.73	8	−3.41	−3.16	0.24	18	−0.33	2.36	3.79	2.17
31	652	−3.18	−0.01	−0.74	10	−3.43	−3.23	0.20	18	−0.11	2.37	3.86	2.18
59	651	−3.18	−0.01	−0.74	10	−3.43	−3.23	0.20	18	−0.11	2.37	3.86	2.18
15	644	−3.18	−0.01	−0.74	8	−3.46	−3.16	0.30	18	−0.33	2.39	4.14	2.19
26	643	−3.18	−0.01	−0.74	8	−3.46	−3.16	0.30	18	−0.33	2.39	4.14	2.19
13	643	−3.18	−0.01	−0.74	8	−3.46	−3.16	0.30	18	−0.33	2.39	4.14	2.19
56	641	−3.18	−0.01	−0.74	8	−3.46	−3.16	0.30	18	−0.33	2.39	4.14	2.19
49	638	−3.18	−0.01	−0.74	8	−3.39	−3.12	0.27	20	−0.20	2.35	3.98	2.23
68	638	−3.18	−0.01	−0.74	10	−3.36	−3.18	0.18	19	0.05	2.36	3.81	2.12
54	638	−3.18	−0.01	−0.74	8	−3.39	−3.12	0.27	20	−0.20	2.35	3.98	2.23
11	638	−3.18	−0.01	−0.74	10	−3.36	−3.18	0.18	19	0.05	2.36	3.81	2.12
27	638	−3.18	−0.01	−0.74	8	−3.39	−3.12	0.27	20	−0.20	2.35	3.98	2.23
46	637	−3.18	−0.01	−0.74	10	−3.36	−3.18	0.18	19	0.05	2.36	3.81	2.12
36	637	−3.18	−0.01	−0.74	8	−3.39	−3.12	0.27	20	−0.20	2.35	3.98	2.23
38	637	−3.18	−0.01	−0.74	10	−3.36	−3.18	0.18	19	0.05	2.36	3.81	2.12
8	625	−3.18	−0.01	−0.74	8	−3.42	−3.11	0.31	19	−0.26	2.35	3.68	2.49
66	624	−3.18	−0.01	−0.74	8	−3.42	−3.11	0.31	19	−0.26	2.35	3.68	2.49
7	611	−3.18	−0.01	−0.74	8	−3.44	−3.16	0.28	18	−0.11	2.37	3.92	2.18
32	580	−3.19	−0.02	−0.74	6	−3.37	−3.06	0.31	20	−0.20	2.38	4.16	2.23
47	548	−3.19	−0.02	−0.75	10	−3.40	−3.11	0.29	20	−0.20	2.36	4.07	2.21
55	466	−3.20	−0.03	−0.76	8	−3.42	−3.16	0.25	18	−0.33	2.38	4.17	2.10
16	465	−3.20	−0.03	−0.76	8	−3.42	−3.16	0.25	18	−0.33	2.38	4.17	2.10
4	386	−3.21	−0.04	−0.77	10	−3.37	−3.19	0.17	18	0.11	2.39	4.05	2.10
67	386	−3.21	−0.04	−0.77	10	−3.37	−3.19	0.17	18	0.11	2.39	4.05	2.10
40	324	−3.22	−0.05	−0.78	8	−3.44	−3.22	0.21	17	−0.17	2.34	3.75	2.15
12	323	−3.22	−0.05	−0.78	8	−3.43	−3.22	0.21	17	−0.17	2.34	3.75	2.15
60	296	−3.22	−0.05	−0.78	10	−3.39	−3.28	0.11	18	0.00	2.38	3.89	2.27
25	296	−3.22	−0.05	−0.78	10	−3.39	−3.28	0.11	19	−0.05	2.38	3.90	2.27
53	182	−3.24	−0.07	−0.79	8	−3.15	−3.10	0.05	19	0.05	2.39	4.31	2.23
2	181	−3.24	−0.07	−0.79	8	−3.15	−3.10	0.05	20	0.00	2.39	4.31	2.23
39	140	−3.24	−0.07	−0.80	8	−3.40	−3.14	0.25	20	0.00	2.39	4.32	2.17
64	140	−3.24	−0.07	−0.80	8	−3.40	−3.14	0.25	20	0.00	2.39	4.32	2.17
65	131	−3.24	−0.07	−0.80	8	−3.40	−3.18	0.21	19	−0.15	2.42	4.44	2.26
20	130	−3.24	−0.07	−0.80	8	−3.40	−3.18	0.21	19	−0.15	2.42	4.44	2.26
45	129	−3.24	−0.07	−0.80	8	−3.40	−3.18	0.21	19	−0.15	2.42	4.44	2.26
44	129	−3.24	−0.07	−0.80	8	−3.40	−3.18	0.21	19	−0.15	2.42	4.44	2.26
14	129	−3.24	−0.07	−0.80	8	−3.40	−3.18	0.21	19	−0.15	2.42	4.44	2.26
17	129	−3.24	−0.07	−0.80	8	−3.40	−3.18	0.21	19	−0.15	2.42	4.44	2.26
58	129	−3.24	−0.07	−0.80	8	−3.40	−3.18	0.21	19	−0.15	2.42	4.44	2.26
22	128	−3.24	−0.07	−0.80	8	−3.40	−3.18	0.21	19	−0.15	2.42	4.44	2.26
35	128	−3.24	−0.07	−0.80	8	−3.40	−3.18	0.21	19	−0.15	2.42	4.44	2.26
3	118	−3.25	−0.08	−0.80	8	−3.37	−3.11	0.26	19	0.05	2.38	4.03	2.22
33	117	−3.25	−0.08	−0.80	8	−3.37	−3.11	0.26	20	0.00	2.38	4.03	2.22
10	75	−3.25	−0.08	−0.81	8	−3.23	−3.00	0.22	18	0.11	2.38	4.20	2.16
61	74	−3.25	−0.08	−0.81	8	−3.23	−3.00	0.22	18	0.11	2.38	4.20	2.16
37	73	−3.25	−0.08	−0.81	8	−3.23	−3.00	0.22	18	0.11	2.38	4.20	2.16
70	58	−3.25	−0.08	−0.81	8	−3.29	−3.02	0.26	19	0.05	2.37	4.04	2.21
21	58	−3.25	−0.08	−0.81	8	−3.29	−3.02	0.26	19	0.05	2.37	4.04	2.21
50	58	−3.25	−0.08	−0.81	8	−3.29	−3.02	0.26	19	0.05	2.37	4.04	2.21

i												
1	57	−3.25	−0.08	−0.81	8	−3.29	−3.02	0.26	19	0.05	2.37	4.04	2.21
23	23	−3.26	−0.09	−0.81	8	−3.43	−3.14	0.28	19	−0.15	2.41	4.36	2.34
5	23	−3.26	−0.09	−0.81	8	−3.43	−3.15	0.28	19	−0.15	2.41	4.36	2.34
63	22	−3.26	−0.09	−0.81	8	−3.43	−3.15	0.28	19	−0.15	2.41	4.36	2.34
30	22	−3.26	−0.09	−0.81	8	−3.43	−3.15	0.28	19	−0.15	2.41	4.36	2.34
18	12	−3.26	−0.09	−0.82	6	−3.26	−3.00	0.26	19	0.05	2.37	4.21	2.24
24	0	−3.26	−0.09	−0.82	8	−3.35	−3.18	0.17	20	−0.20	2.41	4.33	2.27

Table SI48: Structural, energetic and electronic properties for Mo_5Co_4 cluster, as follows: configuration number (i), relative DFT total energy (ΔE_{tot}^{DFT}, in meV), binding energy (E_b, in eV), excess energy (E_{exc}, in eV), stabilization energy (E_{stab}, in eV), total magnetic moment (M_{tot}, in μ_B), HOMO energy (ε_{HOMO}, in eV), LUMO energy (ε_{LUMO}, in eV), HOMO-LUMO energy difference, (E_{gap}, in eV), total number of bonds (N_b), average chemical order parameter (σ_{av}), average bond length (d_{av}, in Å), average effective coordination number (ECN_{av}, NNN), and average radius (R_{av}, in Å).

i	ΔE_{tot}^{DFT}	E_b	E_{exc}	E_{stab}	M_{tot}	ε_{HOMO}	ε_{LUMO}	E_{gap}	N_b	σ_{av}	d_{av}	ECN_{av}	R_{av}
20	1457	−3.26	0.07	−0.61	10	−3.30	−3.16	0.14	21	−0.14	2.41	4.29	2.17
17	1455	−3.26	0.07	−0.61	10	−3.30	−3.15	0.14	21	−0.14	2.41	4.29	2.17
59	877	−3.32	0.01	−0.67	10	−3.31	−3.14	0.17	21	−0.23	2.41	4.32	2.16
34	876	−3.32	0.01	−0.67	10	−3.31	−3.14	0.17	21	−0.23	2.41	4.32	2.17
93	876	−3.32	0.01	−0.67	10	−3.31	−3.14	0.17	21	−0.23	2.41	4.32	2.16
73	876	−3.32	0.01	−0.67	10	−3.31	−3.14	0.17	21	−0.23	2.41	4.32	2.16
8	876	−3.32	0.01	−0.67	10	−3.31	−3.14	0.17	21	−0.23	2.41	4.32	2.16
50	781	−3.34	0.00	−0.68	8	−3.38	−3.23	0.14	21	−0.14	2.38	4.22	2.09
91	780	−3.34	0.00	−0.68	8	−3.38	−3.24	0.14	21	−0.14	2.38	4.22	2.09
13	653	−3.35	−0.01	−0.70	10	−3.31	−3.11	0.19	21	0.23	2.40	4.15	2.14
16	652	−3.35	−0.01	−0.70	10	−3.30	−3.10	0.19	21	0.23	2.40	4.15	2.14
6	625	−3.35	−0.01	−0.70	8	−3.41	−3.08	0.32	21	−0.23	2.37	3.99	2.34
33	625	−3.35	−0.01	−0.70	8	−3.41	−3.08	0.32	21	−0.23	2.37	3.98	2.34
92	624	−3.35	−0.01	−0.70	8	−3.41	−3.08	0.32	21	−0.23	2.37	3.98	2.34
61	623	−3.35	−0.01	−0.70	8	−3.41	−3.08	0.33	21	−0.23	2.37	3.99	2.34
58	622	−3.35	−0.01	−0.70	8	−3.41	−3.08	0.33	21	−0.23	2.37	3.99	2.34
64	621	−3.35	−0.01	−0.70	8	−3.32	−3.03	0.28	20	−0.10	2.38	4.09	2.15
46	621	−3.35	−0.01	−0.70	8	−3.32	−3.03	0.28	20	−0.10	2.38	4.09	2.15
99	620	−3.35	−0.01	−0.70	8	−3.32	−3.03	0.29	20	−0.10	2.38	4.08	2.15
60	620	−3.35	−0.01	−0.70	8	−3.32	−3.03	0.28	20	−0.10	2.38	4.09	2.15
51	619	−3.35	−0.01	−0.70	8	−3.32	−3.03	0.29	20	−0.10	2.38	4.08	2.15
12	549	−3.36	−0.02	−0.71	10	−3.36	−3.18	0.18	21	−0.14	2.41	4.37	2.20
84	549	−3.36	−0.02	−0.71	10	−3.36	−3.18	0.18	21	−0.14	2.41	4.37	2.20
45	548	−3.36	−0.02	−0.71	10	−3.37	−3.18	0.18	21	−0.14	2.41	4.37	2.20
69	548	−3.36	−0.02	−0.71	10	−3.36	−3.18	0.18	21	−0.14	2.41	4.37	2.20
77	548	−3.36	−0.02	−0.71	10	−3.36	−3.18	0.18	21	−0.14	2.41	4.37	2.20
72	544	−3.36	−0.02	−0.71	10	−3.33	−3.21	0.11	21	−0.23	2.41	4.35	2.16
29	544	−3.36	−0.02	−0.71	10	−3.33	−3.22	0.11	21	−0.23	2.41	4.35	2.16
3	523	−3.36	−0.02	−0.71	8	−3.31	−3.04	0.27	21	−0.14	2.40	4.33	2.33
76	492	−3.37	−0.03	−0.72	8	−3.34	−3.10	0.24	21	−0.23	2.40	4.41	2.21
1	492	−3.37	−0.03	−0.72	8	−3.34	−3.10	0.24	21	−0.23	2.40	4.41	2.21
88	492	−3.37	−0.03	−0.72	8	−3.34	−3.09	0.24	21	−0.23	2.40	4.41	2.22
81	492	−3.37	−0.03	−0.72	8	−3.34	−3.10	0.24	21	−0.23	2.40	4.41	2.21
48	492	−3.37	−0.03	−0.72	8	−3.33	−3.10	0.23	21	−0.23	2.40	4.41	2.21
98	491	−3.37	−0.03	−0.72	8	−3.34	−3.10	0.24	21	−0.23	2.40	4.41	2.21
25	491	−3.37	−0.03	−0.72	8	−3.34	−3.09	0.24	21	−0.23	2.40	4.40	2.21
53	491	−3.37	−0.03	−0.72	8	−3.34	−3.10	0.24	21	−0.23	2.40	4.41	2.21
42	491	−3.37	−0.03	−0.72	8	−3.34	−3.09	0.24	21	−0.23	2.40	4.41	2.21

0	491	−3.37	−0.03	−0.72	10	−3.26	−3.06	0.19	20	0.20	2.39	4.17	2.13
95	491	−3.37	−0.03	−0.72	8	−3.34	−3.10	0.24	21	−0.23	2.40	4.41	2.21
79	491	−3.37	−0.03	−0.72	8	−3.34	−3.09	0.24	21	−0.23	2.40	4.41	2.21
30	491	−3.37	−0.03	−0.72	8	−3.34	−3.09	0.24	21	−0.23	2.40	4.41	2.21
54	490	−3.37	−0.03	−0.72	10	−3.26	−3.06	0.19	20	0.20	2.39	4.17	2.13
80	490	−3.37	−0.03	−0.72	8	−3.34	−3.10	0.24	21	−0.23	2.40	4.41	2.21
36	490	−3.37	−0.03	−0.72	8	−3.34	−3.09	0.24	21	−0.23	2.40	4.41	2.21
10	490	−3.37	−0.03	−0.72	10	−3.26	−3.07	0.19	20	0.20	2.39	4.17	2.13
62	486	−3.37	−0.03	−0.72	8	−3.35	−3.07	0.27	21	−0.04	2.38	4.18	2.27
97	486	−3.37	−0.03	−0.72	8	−3.35	−3.07	0.27	21	−0.04	2.38	4.18	2.27
63	486	−3.37	−0.03	−0.72	8	−3.35	−3.07	0.27	21	−0.04	2.38	4.18	2.27
18	484	−3.37	−0.03	−0.72	8	−3.35	−3.07	0.27	21	−0.04	2.38	4.18	2.27
96	477	−3.37	−0.03	−0.72	8	−3.38	−3.13	0.24	21	−0.04	2.37	4.07	2.29
21	476	−3.37	−0.03	−0.72	8	−3.38	−3.13	0.24	21	−0.04	2.37	4.06	2.29
41	476	−3.37	−0.03	−0.72	8	−3.38	−3.13	0.24	21	−0.04	2.37	4.07	2.29
15	475	−3.37	−0.03	−0.72	8	−3.38	−3.13	0.25	21	−0.04	2.37	4.07	2.29
26	460	−3.37	−0.03	−0.72	8	−3.35	−3.11	0.24	21	−0.23	2.41	4.26	2.19
5	459	−3.37	−0.03	−0.72	8	−3.36	−3.11	0.24	21	−0.23	2.41	4.26	2.19
66	459	−3.37	−0.03	−0.72	8	−3.36	−3.11	0.25	21	−0.23	2.41	4.25	2.19
27	453	−3.37	−0.03	−0.72	10	−3.27	−3.04	0.23	21	0.14	2.42	4.44	2.25
22	453	−3.37	−0.03	−0.72	10	−3.27	−3.04	0.23	21	0.14	2.42	4.44	2.25
78	452	−3.37	−0.03	−0.72	10	−3.27	−3.04	0.23	21	0.14	2.42	4.44	2.25
24	449	−3.37	−0.03	−0.72	6	−3.29	−2.98	0.30	21	−0.14	2.39	4.21	2.30
32	449	−3.37	−0.03	−0.72	6	−3.29	−2.98	0.30	21	−0.14	2.39	4.21	2.30
4	443	−3.37	−0.03	−0.72	8	−3.29	−2.99	0.30	20	−0.20	2.39	4.14	2.12
74	441	−3.37	−0.03	−0.72	8	−3.29	−2.99	0.30	20	−0.20	2.39	4.14	2.12
11	426	−3.37	−0.03	−0.72	4	−3.21	−2.88	0.32	21	−0.14	2.36	4.34	2.27
43	423	−3.37	−0.03	−0.72	6	−3.33	−3.09	0.23	21	−0.33	2.41	4.36	2.36
83	421	−3.38	−0.03	−0.72	6	−3.36	−3.10	0.26	21	−0.33	2.40	4.26	2.37
2	421	−3.38	−0.03	−0.72	6	−3.33	−3.10	0.23	21	−0.33	2.41	4.35	2.36
14	400	−3.38	−0.04	−0.73	8	−3.25	−3.07	0.17	21	−0.23	2.39	4.25	2.33
07	399	−3.38	−0.04	−0.73	8	−3.19	−3.00	0.18	21	−0.23	2.41	4.32	2.34
57	249	−3.39	−0.05	−0.74	8	−3.19	−3.00	0.19	21	0.14	2.39	4.23	2.26
94	249	−3.39	−0.05	−0.74	8	−3.19	−3.00	0.19	21	0.14	2.39	4.23	2.26
28	5	−3.42	−0.08	−0.77	6	−3.39	−2.99	0.40	21	−0.14	2.41	4.49	2.30
55	4	−3.42	−0.08	−0.77	6	−3.39	−2.99	0.40	21	−0.14	2.41	4.49	2.30
90	3	−3.42	−0.08	−0.77	6	−3.39	−2.99	0.40	21	−0.14	2.41	4.49	2.30
19	2	−3.42	−0.08	−0.77	6	−3.39	−2.99	0.40	21	−0.14	2.41	4.49	2.30
47	2	−3.42	−0.08	−0.77	6	−3.39	−2.99	0.40	21	−0.14	2.41	4.49	2.30
70	1	−3.42	−0.08	−0.77	8	−3.32	−3.04	0.28	21	0.04	2.40	4.35	2.28
9	1	−3.42	−0.08	−0.77	8	−3.32	−3.04	0.28	21	0.04	2.40	4.35	2.28
38	1	−3.42	−0.08	−0.77	8	−3.33	−3.04	0.28	21	0.04	2.40	4.35	2.28
68	1	−3.42	−0.08	−0.77	8	−3.32	−3.04	0.28	21	0.04	2.40	4.35	2.28
40	1	−3.42	−0.08	−0.77	8	−3.33	−3.04	0.28	21	0.04	2.40	4.35	2.28
89	0	−3.42	−0.08	−0.77	8	−3.32	−3.04	0.28	21	0.04	2.40	4.35	2.28
56	0	−3.42	−0.08	−0.77	8	−3.32	−3.04	0.28	21	0.04	2.40	4.35	2.28
44	0	−3.42	−0.08	−0.77	8	−3.33	−3.04	0.28	21	0.04	2.40	4.35	2.28
23	0	−3.42	−0.08	−0.77	8	−3.32	−3.04	0.28	21	0.04	2.40	4.35	2.28
82	0	−3.42	−0.08	−0.77	8	−3.32	−3.04	0.28	21	0.04	2.40	4.35	2.28
31	0	−3.42	−0.08	−0.77	8	−3.32	−3.04	0.28	21	0.04	2.40	4.35	2.28

Table SI49: Structural, energetic and electronic properties for Mo_5Co_5 cluster, as follows: configuration number (i), relative DFT total energy (ΔE_{tot}^{DFT}, in meV), binding energy (E_b, in eV), excess energy (E_{exc}, in eV), stabilization energy (E_{stab}, in eV), total magnetic moment (M_{tot}, in μ_B), HOMO energy (ε_{HOMO}, in eV), LUMO energy (ε_{LUMO}, in eV), HOMO-LUMO energy difference, (E_{gap}, in eV), total number of bonds (N_b), average chemical order parameter (σ_{av}), average bond length (d_{av}, in Å), average effective coordination number (ECN_{av}, NNN), and average radius (R_{av}, in Å).

i	ΔE_{tot}^{DFT}	E_b	E_{exc}	E_{stab}	M_{tot}	ε_{HOMO}	ε_{LUMO}	E_{gap}	N_b	σ_{av}	d_{av}	ECN_{av}	R_{av}
30	1262	−3.34	−0.07	−0.58	7	−3.32	−3.09	0.23	24	−0.25	2.37	4.23	2.54
85	1218	−3.34	−0.08	−0.59	9	−3.25	−3.07	0.18	24	−0.25	2.36	3.98	2.48
63	1199	−3.34	−0.08	−0.59	7	−3.23	−3.07	0.15	24	−0.08	2.35	4.07	2.54
87	1193	−3.34	−0.08	−0.59	11	−3.37	−3.21	0.16	24	−0.25	2.37	4.05	2.44
55	1042	−3.36	−0.10	−0.61	9	−3.35	−3.18	0.17	25	−0.28	2.39	4.44	2.46
47	1029	−3.36	−0.10	−0.61	9	−3.17	−3.06	0.11	25	−0.04	2.35	3.99	2.77
88	922	−3.37	−0.11	−0.62	9	−3.44	−3.20	0.24	25	−0.12	2.40	4.39	2.63
36	848	−3.38	−0.12	−0.62	11	−3.42	−3.19	0.24	23	−0.04	2.37	4.01	2.46
86	846	−3.38	−0.12	−0.62	11	−3.42	−3.19	0.24	23	−0.04	2.37	4.01	2.46
14	833	−3.38	−0.12	−0.63	13	−3.38	−3.30	0.08	24	−0.08	2.42	4.45	2.61
67	822	−3.38	−0.12	−0.63	7	−3.24	−3.06	0.19	22	−0.18	2.35	4.11	2.56
48	781	−3.39	−0.12	−0.63	11	−3.34	−3.21	0.13	25	−0.28	2.42	4.44	2.89
54	772	−3.39	−0.12	−0.63	11	−3.38	−3.22	0.16	24	0.00	2.39	4.34	2.68
80	772	−3.39	−0.12	−0.63	11	−3.38	−3.22	0.17	24	0.00	2.39	4.34	2.67
1	757	−3.39	−0.12	−0.63	9	−3.32	−3.12	0.21	24	−0.17	2.40	4.35	2.65
28	749	−3.39	−0.13	−0.63	9	−3.38	−3.11	0.27	24	−0.17	2.41	4.34	2.90
17	724	−3.39	−0.13	−0.64	11	−3.29	−3.23	0.06	24	−0.25	2.42	4.61	2.37
29	710	−3.39	−0.13	−0.64	11	−3.38	−3.18	0.20	24	−0.17	2.40	4.26	2.72
79	705	−3.39	−0.13	−0.64	9	−3.36	−3.19	0.17	24	0.00	2.36	3.94	2.43
15	701	−3.39	−0.13	−0.64	9	−3.36	−3.19	0.18	24	−0.17	2.40	4.43	2.49
4	683	−3.39	−0.13	−0.64	11	−3.25	−3.20	0.05	24	−0.17	2.40	4.38	2.71
91	680	−3.40	−0.13	−0.64	9	−3.40	−3.12	0.28	25	−0.28	2.40	4.27	2.73
75	661	−3.40	−0.13	−0.64	9	−3.52	−3.36	0.16	22	−0.18	2.34	3.84	2.17
83	649	−3.40	−0.14	−0.64	11	−3.38	−3.15	0.23	23	0.22	2.38	4.05	2.52
31	648	−3.40	−0.14	−0.64	11	−3.37	−3.15	0.22	23	0.22	2.38	4.05	2.52
89	636	−3.40	−0.14	−0.65	11	−3.36	−3.19	0.17	24	−0.25	2.41	4.46	2.58
25	630	−3.40	−0.14	−0.65	9	−3.36	−3.19	0.17	23	−0.13	2.38	4.13	2.58
78	624	−3.40	−0.14	−0.65	11	−3.37	−3.20	0.17	24	−0.08	2.40	4.24	2.50
10	605	−3.40	−0.14	−0.65	9	−3.36	−3.13	0.22	25	−0.12	2.42	4.41	2.57
60	598	−3.40	−0.14	−0.65	9	−3.40	−3.19	0.21	23	−0.22	2.36	3.94	2.34
93	597	−3.40	−0.14	−0.65	11	−3.36	−3.19	0.17	26	−0.15	2.43	4.54	2.54
38	576	−3.41	−0.14	−0.65	9	−3.40	−3.09	0.31	24	−0.25	2.39	4.26	2.81
76	574	−3.41	−0.14	−0.65	9	−3.40	−3.22	0.18	22	−0.18	2.36	4.01	2.28
7	560	−3.41	−0.14	−0.65	9	−3.28	−3.09	0.19	24	−0.17	2.39	4.33	2.72
50	560	−3.41	−0.14	−0.65	9	−3.28	−3.09	0.19	24	−0.17	2.39	4.33	2.72
72	560	−3.41	−0.14	−0.65	9	−3.28	−3.09	0.19	24	−0.17	2.39	4.33	2.72
24	559	−3.41	−0.14	−0.65	9	−3.28	−3.09	0.19	24	−0.17	2.39	4.33	2.72
81	558	−3.41	−0.14	−0.65	9	−3.28	−3.09	0.19	24	−0.17	2.39	4.33	2.72
45	551	−3.41	−0.15	−0.65	9	−3.32	−3.09	0.23	25	−0.12	2.42	4.59	2.73
20	548	−3.41	−0.15	−0.65	9	−3.32	−3.09	0.23	25	−0.12	2.42	4.59	2.73
26	546	−3.41	−0.15	−0.66	9	−3.44	−3.14	0.30	25	−0.20	2.40	4.37	2.48
53	537	−3.41	−0.15	−0.66	7	−3.43	−3.15	0.27	21	−0.05	2.33	3.73	2.33
34	534	−3.41	−0.15	−0.66	11	−3.44	−3.17	0.27	24	−0.25	2.42	4.41	2.63
90	534	−3.41	−0.15	−0.66	11	−3.44	−3.17	0.27	24	−0.25	2.42	4.41	2.63
61	533	−3.41	−0.15	−0.66	11	−3.44	−3.17	0.27	24	−0.25	2.42	4.41	2.63
65	532	−3.41	−0.15	−0.66	11	−3.44	−3.17	0.27	24	−0.25	2.42	4.40	2.63
11	532	−3.41	−0.15	−0.66	11	−3.44	−3.17	0.27	24	−0.25	2.42	4.41	2.63
40	531	−3.41	−0.15	−0.66	9	−3.35	−3.20	0.16	23	−0.22	2.35	3.89	2.24

i	ΔE_{tot}^{DFT}	E_b	E_{exc}	E_{stab}	M_{tot}	ε_{HOMO}	ε_{LUMO}	E_{gap}	N_b	σ_{av}	d_{av}	ECN_{av}	R_{av}
69	521	−3.41	−0.15	−0.66	11	−3.31	−3.06	0.25	24	0.17	2.39	4.31	2.69
37	521	−3.41	−0.15	−0.66	11	−3.31	−3.06	0.25	24	0.17	2.39	4.31	2.69
27	519	−3.41	−0.15	−0.66	11	−3.31	−3.06	0.25	24	0.17	2.39	4.31	2.69
62	500	−3.41	−0.15	−0.66	9	−3.47	−3.16	0.31	24	−0.25	2.39	4.19	2.45
46	469	−3.42	−0.15	−0.66	9	−3.44	−3.17	0.27	24	−0.25	2.39	4.30	2.60
92	467	−3.42	−0.15	−0.66	9	−3.36	−3.09	0.26	25	−0.04	2.41	4.37	2.98
13	456	−3.42	−0.15	−0.66	9	−3.43	−3.20	0.24	24	0.00	2.37	4.22	2.57
96	448	−3.42	−0.16	−0.66	11	−3.31	−3.01	0.30	24	0.25	2.41	4.45	2.37
66	446	−3.42	−0.16	−0.66	9	−3.47	−3.15	0.32	24	−0.25	2.41	4.47	2.58
21	397	−3.42	−0.16	−0.67	9	−3.42	−3.21	0.20	24	−0.17	2.42	4.52	2.51
18	369	−3.43	−0.16	−0.67	9	−3.37	−3.18	0.20	24	−0.33	2.43	4.63	2.45
39	368	−3.43	−0.16	−0.67	9	−3.37	−3.17	0.19	24	−0.33	2.43	4.63	2.45
97	344	−3.43	−0.17	−0.68	11	−3.33	−3.08	0.25	24	0.08	2.40	4.18	2.53
42	330	−3.43	−0.17	−0.68	11	−3.40	−3.22	0.17	22	0.27	2.38	4.24	2.44
52	330	−3.43	−0.17	−0.68	11	−3.40	−3.22	0.17	23	0.22	2.38	4.24	2.44
70	329	−3.43	−0.17	−0.68	11	−3.40	−3.22	0.17	22	0.27	2.38	4.24	2.45
77	301	−3.43	−0.17	−0.68	11	−3.34	−3.12	0.22	23	0.22	2.40	4.39	2.60
5	300	−3.43	−0.17	−0.68	11	−3.35	−3.13	0.22	23	0.22	2.40	4.39	2.60
8	300	−3.43	−0.17	−0.68	11	−3.34	−3.12	0.22	23	0.22	2.40	4.39	2.60
9	300	−3.43	−0.17	−0.68	11	−3.34	−3.12	0.22	23	0.22	2.40	4.39	2.60
23	294	−3.43	−0.17	−0.68	9	−3.28	−3.00	0.28	22	−0.09	2.38	4.29	2.48
32	290	−3.43	−0.17	−0.68	9	−3.28	−3.00	0.28	22	−0.09	2.38	4.29	2.48
6	270	−3.44	−0.17	−0.68	9	−3.39	−3.05	0.34	24	0.00	2.42	4.53	2.58
98	270	−3.44	−0.17	−0.68	9	−3.38	−3.05	0.34	24	0.00	2.42	4.53	2.58
58	268	−3.44	−0.17	−0.68	9	−3.35	−3.09	0.26	24	0.08	2.39	4.34	2.46
94	266	−3.44	−0.17	−0.68	9	−3.35	−3.09	0.26	24	0.08	2.39	4.34	2.46
19	254	−3.44	−0.18	−0.68	11	−3.36	−3.09	0.27	24	0.08	2.40	4.32	2.64
95	253	−3.44	−0.18	−0.68	11	−3.36	−3.09	0.27	24	0.08	2.40	4.32	2.64
2	16	−3.46	−0.20	−0.71	7	−3.35	−3.10	0.25	27	−0.04	2.45	4.89	2.56
12	1	−3.46	−0.20	−0.71	11	−3.28	−3.22	0.07	24	0.08	2.41	4.50	2.41
59	0	−3.46	−0.20	−0.71	11	−3.28	−3.22	0.06	24	0.08	2.41	4.51	2.40
22	0	−3.46	−0.20	−0.71	11	−3.28	−3.22	0.07	24	0.08	2.41	4.50	2.41

Table SI50: Structural, energetic and electronic properties for Mo_6Co_5 cluster, as follows: configuration number (i), relative DFT total energy (ΔE_{tot}^{DFT}, in meV), binding energy (E_b, in eV), excess energy (E_{exc}, in eV), stabilization energy (E_{stab}, in eV), total magnetic moment (M_{tot}, in μ_B), HOMO energy (ε_{HOMO}, in eV), LUMO energy (ε_{LUMO}, in eV), HOMO-LUMO energy difference, (E_{gap}, in eV), total number of bonds (N_b), average chemical order parameter (σ_{av}), average bond length (d_{av}, in Å), average effective coordination number (ECN_{av}, NNN), and average radius (R_{av}, in Å).

i	ΔE_{tot}^{DFT}	E_b	E_{exc}	E_{stab}	M_{tot}	ε_{HOMO}	ε_{LUMO}	E_{gap}	N_b	σ_{av}	d_{av}	ECN_{av}	R_{av}
78	1625	−3.43	0.02	−0.47	7	−3.28	−3.14	0.13	28	−0.28	2.38	4.66	2.74
71	1446	−3.44	0.01	−0.48	11	−3.36	−3.27	0.09	28	−0.21	2.40	4.39	2.80
87	1438	−3.44	0.00	−0.48	9	−3.42	−3.20	0.21	28	−0.14	2.39	4.36	2.78
84	1438	−3.44	0.00	−0.48	11	−3.44	−3.34	0.09	28	−0.21	2.42	4.48	2.81
28	1434	−3.45	0.00	−0.48	5	−3.13	−2.96	0.16	28	−0.28	2.37	4.73	2.85
10	1423	−3.45	0.00	−0.49	11	−3.44	−3.26	0.17	28	−0.07	2.42	4.64	2.81
65	1359	−3.45	0.00	−0.49	9	−3.37	−3.18	0.19	28	−0.21	2.41	4.58	2.77
82	1300	−3.46	−0.00	−0.50	7	−3.26	−3.08	0.18	29	−0.31	2.37	4.53	2.87
61	1296	−3.46	−0.00	−0.50	11	−3.34	−3.21	0.13	28	−0.14	2.41	4.36	2.85
69	1292	−3.46	−0.00	−0.50	9	−3.34	−3.07	0.26	28	−0.14	2.40	4.49	2.79
01	1231	−3.46	−0.00	−0.50	9	−3.30	−3.19	0.11	28	−0.14	2.38	4.36	2.74
94	1214	−3.46	−0.01	−0.50	7	−3.31	−3.11	0.19	28	−0.14	2.39	4.88	2.81
37	1207	−3.47	−0.01	−0.50	7	−3.30	−3.13	0.17	27	−0.25	2.40	4.46	3.06

54	1201	−3.47	−0.01	−0.51	9	−3.50	−3.21	0.28	29	−0.10	2.38	4.33	2.76
76	1197	−3.47	−0.01	−0.51	9	−3.39	−3.20	0.18	28	−0.21	2.37	4.35	2.88
14	1158	−3.47	−0.01	−0.51	7	−3.29	−3.09	0.20	28	−0.28	2.37	4.37	2.71
06	1147	−3.47	−0.01	−0.51	11	−3.38	−3.22	0.16	28	−0.21	2.42	4.73	2.79
64	1129	−3.47	−0.01	−0.51	11	−3.36	−3.18	0.17	28	−0.07	2.42	4.55	2.83
50	1112	−3.47	−0.02	−0.51	5	−3.18	−2.91	0.26	29	−0.31	2.36	4.53	2.84
25	1086	−3.48	−0.02	−0.52	5	−3.33	−3.03	0.29	28	−0.21	2.38	4.64	2.74
62	1052	−3.48	−0.02	−0.52	7	−3.35	−3.10	0.24	27	−0.11	2.37	4.45	2.81
44	1042	−3.48	−0.02	−0.52	7	−3.21	−3.00	0.20	28	−0.28	2.36	4.33	2.79
59	1038	−3.48	−0.02	−0.52	7	−3.30	−3.09	0.20	27	−0.25	2.36	4.41	2.83
67	1034	−3.48	−0.02	−0.52	9	−3.23	−3.12	0.10	28	−0.14	2.38	4.30	2.73
4	1020	−3.48	−0.02	−0.52	11	−3.37	−3.16	0.21	29	0.10	2.41	4.49	2.71
19	1016	−3.48	−0.02	−0.52	9	−3.40	−3.14	0.26	28	−0.21	2.41	4.57	2.80
92	1013	−3.48	−0.02	−0.52	9	−3.22	−3.09	0.13	28	−0.14	2.39	4.41	2.68
21	997	−3.48	−0.03	−0.52	9	−3.44	−3.18	0.26	28	−0.28	2.41	4.56	2.78
66	994	−3.48	−0.03	−0.52	7	−3.40	−3.10	0.29	29	−0.17	2.38	4.41	2.80
00	989	−3.49	−0.03	−0.52	7	−3.26	−3.09	0.16	28	−0.07	2.35	4.20	2.88
36	987	−3.49	−0.03	−0.52	7	−3.32	−2.96	0.35	28	−0.14	2.36	4.39	2.84
68	958	−3.49	−0.03	−0.53	9	−3.34	−3.11	0.22	28	0.07	2.39	4.54	2.79
09	929	−3.49	−0.03	−0.53	7	−3.22	−3.04	0.17	28	−0.14	2.39	4.42	2.72
05	919	−3.49	−0.03	−0.53	9	−3.32	−3.15	0.16	29	−0.31	2.38	4.59	2.80
34	918	−3.49	−0.03	−0.53	9	−3.45	−3.18	0.26	27	0.11	2.42	4.43	2.92
80	903	−3.49	−0.03	−0.53	11	−3.39	−3.17	0.21	30	0.00	2.41	4.52	2.76
70	898	−3.49	−0.03	−0.53	7	−3.31	−2.97	0.33	28	−0.21	2.36	4.36	2.78
58	867	−3.50	−0.04	−0.54	9	−3.35	−3.09	0.25	28	−0.21	2.42	4.60	2.79
30	863	−3.50	−0.04	−0.54	9	−3.40	−3.12	0.28	28	0.07	2.44	4.56	2.89
73	835	−3.50	−0.04	−0.54	9	−3.40	−3.13	0.27	28	−0.28	2.42	4.56	2.96
46	817	−3.50	−0.04	−0.54	9	−3.27	−3.13	0.14	27	−0.03	2.41	4.59	2.71
26	815	−3.50	−0.04	−0.54	9	−3.33	−3.21	0.12	28	−0.21	2.44	4.72	2.86
48	798	−3.50	−0.04	−0.54	7	−3.41	−3.17	0.23	28	−0.07	2.38	4.37	2.92
81	790	−3.50	−0.04	−0.54	7	−3.41	−3.13	0.28	28	−0.21	2.42	4.69	2.74
40	777	−3.50	−0.05	−0.54	11	−3.50	−3.24	0.25	27	−0.18	2.40	4.24	3.06
49	756	−3.51	−0.05	−0.55	11	−3.24	−3.13	0.10	28	0.14	2.42	4.63	2.72
11	752	−3.51	−0.05	−0.55	11	−3.36	−3.20	0.15	28	−0.14	2.43	4.64	2.84
55	741	−3.51	−0.05	−0.55	7	−3.26	−3.04	0.22	27	−0.03	2.41	4.55	2.82
22	732	−3.51	−0.05	−0.55	7	−3.27	−3.02	0.24	28	−0.14	2.38	4.58	2.86
97	708	−3.51	−0.05	−0.55	11	−3.39	−3.22	0.17	28	0.21	2.38	4.32	2.90
89	703	−3.51	−0.05	−0.55	9	−3.09	−2.86	0.22	28	0.14	2.37	4.30	2.84
90	702	−3.51	−0.05	−0.55	7	−3.32	−3.14	0.18	29	−0.17	2.36	4.47	2.80
91	684	−3.51	−0.05	−0.55	9	−3.35	−3.20	0.15	28	0.07	2.43	4.77	2.84
63	680	−3.51	−0.05	−0.55	11	−3.32	−3.19	0.12	28	−0.07	2.44	4.81	2.85
77	649	−3.52	−0.06	−0.56	13	−3.29	−3.24	0.05	28	0.14	2.43	4.67	2.79
72	641	−3.52	−0.06	−0.56	9	−3.30	−3.14	0.15	30	−0.06	2.39	4.55	2.83
93	632	−3.52	−0.06	−0.56	7	−3.39	−3.11	0.27	28	−0.14	2.41	4.59	2.74
3	581	−3.52	−0.06	−0.56	5	−3.20	−2.91	0.29	28	−0.07	2.39	4.66	2.72
56	570	−3.52	−0.06	−0.56	9	−3.37	−3.10	0.26	29	0.03	2.40	4.50	2.80
43	556	−3.52	−0.07	−0.56	9	−3.48	−3.19	0.28	28	−0.14	2.43	4.72	2.82
85	549	−3.53	−0.07	−0.56	11	−3.31	−3.11	0.19	28	−0.07	2.42	4.50	2.83
75	542	−3.53	−0.07	−0.57	9	−3.36	−3.22	0.13	28	−0.14	2.42	4.62	2.75
18	541	−3.53	−0.07	−0.57	9	−3.48	−3.15	0.32	27	0.03	2.42	4.47	2.88
47	537	−3.53	−0.07	−0.57	9	−3.15	−3.01	0.13	27	−0.03	2.37	4.45	2.75
88	495	−3.53	−0.07	−0.57	9	−3.48	−3.24	0.24	27	−0.03	2.41	4.44	2.78
27	477	−3.53	−0.07	−0.57	9	−3.40	−3.10	0.29	29	−0.17	2.46	4.85	2.60
12	456	−3.53	−0.07	−0.57	9	−3.41	−3.24	0.16	29	−0.10	2.43	4.48	2.74
31	454	−3.53	−0.07	−0.57	7	−3.42	−3.09	0.32	29	−0.17	2.42	4.63	2.79
32	449	−3.53	−0.08	−0.57	9	−3.42	−3.15	0.27	28	−0.21	2.44	4.75	2.81
16	419	−3.54	−0.08	−0.58	11	−3.46	−3.12	0.33	28	−0.14	2.45	4.78	2.90
13	363	−3.54	−0.08	−0.58	11	−3.20	−3.12	0.07	28	0.21	2.42	4.55	2.77

Table SI51: Structural, energetic and electronic properties for Mo_6Co_6 cluster, as follows: configuration number (i), relative DFT total energy (ΔE_{tot}^{DFT}, in meV), binding energy (E_b, in eV), excess energy (E_{exc}, in eV), stabilization energy (E_{stab}, in eV), total magnetic moment (M_{tot}, in μ_B), HOMO energy (ε_{HOMO}, in eV), LUMO energy (ε_{LUMO}, in eV), HOMO-LUMO energy difference, (E_{gap}, in eV), total number of bonds (N_b), average chemical order parameter (σ_{av}), average bond length (d_{av}, in Å), average effective coordination number (ECN_{av}, NNN), and average radius (R_{av}, in Å).

i	ΔE_{tot}^{DFT}	E_b	E_{exc}	E_{stab}	M_{tot}	ε_{HOMO}	ε_{LUMO}	E_{gap}	N_b	σ_{av}	d_{av}	ECN_{av}	R_{av}
60	1624	−3.47	0.02	−0.37	12	−3.24	−3.11	0.12	36	0.06	2.40	4.84	2.64
54	1431	−3.48	0.00	−0.39	12	−3.40	−3.22	0.18	35	−0.26	2.43	4.93	2.62
20	1271	−3.50	−0.01	−0.40	12	−3.30	−3.08	0.22	36	−0.11	2.43	5.12	2.53
30	1106	−3.51	−0.02	−0.42	12	−3.28	−3.05	0.23	36	−0.06	2.42	4.98	2.64
100	1079	−3.51	−0.03	−0.42	12	−3.19	−3.04	0.15	36	−0.22	2.41	4.92	2.56
50	1055	−3.52	−0.03	−0.42	10	−3.20	−2.97	0.24	36	−0.11	2.40	4.84	2.59
45	1053	−3.52	−0.03	−0.42	14	−3.27	−3.16	0.11	35	−0.20	2.44	4.90	2.64
73	1043	−3.52	−0.03	−0.42	10	−3.17	−2.98	0.18	35	−0.14	2.40	4.93	2.54
63	1032	−3.52	−0.03	−0.42	10	−3.26	−3.07	0.19	35	−0.20	2.39	4.79	2.66
56	1022	−3.52	−0.03	−0.42	12	−3.38	−3.18	0.20	35	−0.03	2.42	4.75	2.66
81	1006	−3.52	−0.03	−0.42	10	−3.50	−3.24	0.25	33	−0.09	2.37	4.34	2.72
13	1003	−3.52	−0.03	−0.42	12	−3.14	−3.07	0.08	36	−0.17	2.44	5.25	2.56
11	979	−3.52	−0.03	−0.43	10	−3.19	−3.02	0.17	36	−0.11	2.40	4.78	2.67
10	973	−3.52	−0.03	−0.43	12	−3.29	−3.14	0.15	35	−0.14	2.40	4.78	2.72
92	962	−3.52	−0.04	−0.43	10	−3.36	−3.14	0.22	35	−0.03	2.40	4.94	2.59
2	956	−3.52	−0.04	−0.43	10	−3.22	−3.00	0.23	36	0.11	2.38	4.64	2.64
16	952	−3.52	−0.04	−0.43	10	−3.46	−3.23	0.23	32	0.13	2.37	4.42	2.83
52	947	−3.53	−0.04	−0.43	12	−3.44	−3.23	0.21	34	−0.24	2.42	4.74	2.66
23	930	−3.53	−0.04	−0.43	12	−3.21	−3.08	0.13	36	−0.11	2.43	5.10	2.56
33	924	−3.53	−0.04	−0.43	12	−3.46	−3.26	0.20	35	−0.14	2.43	4.95	2.72
22	914	−3.53	−0.04	−0.43	10	−3.19	−2.97	0.22	36	−0.17	2.40	4.89	2.58
44	914	−3.53	−0.04	−0.43	12	−3.46	−3.17	0.29	36	−0.17	2.43	4.72	2.71
88	910	−3.53	−0.04	−0.43	12	−3.21	−3.08	0.13	36	−0.11	2.39	4.59	2.66
25	901	−3.53	−0.04	−0.43	12	−3.21	−3.09	0.12	36	−0.22	2.42	5.05	2.56
29	893	−3.53	−0.04	−0.43	12	−3.32	−3.03	0.29	36	−0.22	2.42	5.04	2.58
98	886	−3.53	−0.04	−0.43	12	−3.41	−3.18	0.23	36	−0.17	2.44	4.88	2.66
9	880	−3.53	−0.04	−0.43	10	−3.27	−2.99	0.28	36	0.00	2.39	4.74	2.63
14	853	−3.53	−0.04	−0.44	10	−3.34	−3.16	0.17	36	−0.28	2.41	4.80	2.63
84	841	−3.53	−0.05	−0.44	10	−3.33	−3.15	0.18	35	−0.26	2.41	4.67	2.64
47	821	−3.54	−0.05	−0.44	12	−3.20	−3.08	0.12	36	−0.06	2.40	4.75	2.58
43	815	−3.54	−0.05	−0.44	12	−3.25	−3.05	0.20	36	−0.11	2.42	5.01	2.55
58	762	−3.54	−0.05	−0.44	10	−3.20	−2.99	0.20	36	0.00	2.41	4.95	2.59
59	762	−3.54	−0.05	−0.44	10	−3.44	−3.19	0.25	34	−0.24	2.41	4.55	2.86
35	748	−3.54	−0.05	−0.45	10	−3.44	−3.21	0.23	33	−0.21	2.39	4.50	2.79
8	740	−3.54	−0.05	−0.45	12	−3.39	−3.23	0.17	35	−0.26	2.45	5.00	2.61
6	730	−3.54	−0.05	−0.45	12	−3.29	−3.14	0.15	36	−0.22	2.43	5.12	2.54
28	722	−3.54	−0.06	−0.45	12	−3.40	−3.22	0.18	35	−0.20	2.44	4.78	2.66
18	720	−3.54	−0.06	−0.45	10	−3.35	−3.10	0.24	34	0.06	2.39	4.52	2.79

i	ΔE_{tot}^{DFT}	E_b	E_{exc}	E_{stab}	M_{tot}	ε_{HOMO}	ε_{LUMO}	E_{gap}	N_b	σ_{av}	d_{av}	ECN_{av}	R_{av}
19	719	−3.54	−0.06	−0.45	12	−3.24	−3.12	0.11	36	−0.28	2.40	4.78	2.58
79	717	−3.54	−0.06	−0.45	10	−3.37	−3.17	0.20	35	−0.20	2.40	4.43	2.78
66	703	−3.55	−0.06	−0.45	10	−3.36	−3.11	0.25	36	0.11	2.41	4.62	2.67
87	701	−3.55	−0.06	−0.45	12	−3.44	−3.22	0.23	35	−0.14	2.43	4.76	2.68
89	660	−3.55	−0.06	−0.45	14	−3.28	−3.14	0.14	36	−0.11	2.44	5.12	2.55
70	644	−3.55	−0.06	−0.45	12	−3.45	−3.24	0.21	35	−0.20	2.43	4.68	2.74
77	643	−3.55	−0.06	−0.45	12	−3.33	−3.06	0.27	36	−0.11	2.42	4.97	2.57
12	640	−3.55	−0.06	−0.45	10	−3.36	−3.20	0.17	34	−0.12	2.42	4.79	2.71
21	627	−3.55	−0.06	−0.46	12	−3.41	−3.22	0.19	34	−0.06	2.42	4.73	2.73
37	622	−3.55	−0.06	−0.46	12	−3.23	−3.13	0.10	36	−0.06	2.40	4.61	2.60
26	589	−3.56	−0.07	−0.46	12	−3.44	−3.27	0.17	34	−0.18	2.42	4.71	2.78
53	588	−3.56	−0.07	−0.46	12	−3.25	−3.05	0.20	36	0.06	2.44	5.10	2.54
64	586	−3.56	−0.07	−0.46	12	−3.22	−3.00	0.22	36	0.17	2.43	5.19	2.59
85	584	−3.56	−0.07	−0.46	12	−3.22	−3.00	0.22	36	0.17	2.43	5.19	2.59
46	583	−3.56	−0.07	−0.46	12	−3.17	−3.04	0.13	36	0.00	2.42	5.00	2.55
80	576	−3.56	−0.07	−0.46	12	−3.32	−3.05	0.26	36	−0.17	2.42	4.96	2.57
71	569	−3.56	−0.07	−0.46	12	−3.21	−3.08	0.13	36	−0.06	2.45	5.30	2.52
40	553	−3.56	−0.07	−0.46	12	−3.29	−3.05	0.24	36	0.11	2.43	5.13	2.56
55	547	−3.56	−0.07	−0.46	14	−3.38	−3.29	0.08	36	0.00	2.45	4.85	2.63
36	525	−3.56	−0.07	−0.46	12	−3.42	−3.13	0.29	35	0.09	2.43	4.82	2.67
76	505	−3.56	−0.07	−0.47	14	−3.43	−3.31	0.13	35	−0.09	2.43	4.59	2.79
65	502	−3.56	−0.07	−0.47	10	−3.17	−2.97	0.19	35	0.03	2.40	4.97	2.57
83	497	−3.56	−0.07	−0.47	10	−3.25	−3.10	0.15	36	−0.11	2.44	4.88	2.74
86	492	−3.56	−0.07	−0.47	14	−3.47	−3.25	0.22	34	−0.06	2.45	4.81	2.79
34	477	−3.56	−0.08	−0.47	12	−3.18	−3.08	0.10	36	0.17	2.40	4.70	2.60
74	474	−3.56	−0.08	−0.47	10	−3.26	−2.98	0.28	36	−0.17	2.41	4.87	2.60
41	469	−3.57	−0.08	−0.47	14	−3.43	−3.32	0.12	35	−0.09	2.46	4.89	2.70
7	459	−3.57	−0.08	−0.47	12	−3.28	−3.10	0.18	36	−0.11	2.40	4.55	2.63
31	421	−3.57	−0.08	−0.47	14	−3.41	−3.23	0.18	35	−0.09	2.44	4.77	2.66
4	418	−3.57	−0.08	−0.47	12	−3.38	−3.16	0.22	35	−0.14	2.43	4.78	2.71
93	412	−3.57	−0.08	−0.47	12	−3.47	−3.33	0.14	34	−0.18	2.43	4.68	2.74
69	398	−3.57	−0.08	−0.47	10	−3.43	−3.22	0.21	35	−0.14	2.44	4.95	2.64
5	387	−3.57	−0.08	−0.48	10	−3.37	−3.09	0.28	35	−0.09	2.42	4.60	2.66
3	381	−3.57	−0.08	−0.48	10	−3.44	−3.23	0.21	35	−0.26	2.42	4.84	2.63
91	379	−3.57	−0.08	−0.48	12	−3.35	−3.15	0.20	36	−0.06	2.43	4.64	2.64
72	347	−3.58	−0.09	−0.48	12	−3.54	−3.30	0.24	35	−0.14	2.46	4.85	2.73
17	337	−3.58	−0.09	−0.48	12	−3.35	−3.15	0.20	36	−0.06	2.42	4.66	2.69
97	324	−3.58	−0.09	−0.48	14	−3.30	−3.22	0.08	35	0.03	2.49	5.10	2.64
94	306	−3.58	−0.09	−0.48	12	−3.32	−3.23	0.09	35	−0.03	2.44	4.72	2.67
90	288	−3.58	−0.09	−0.48	12	−3.47	−3.22	0.26	36	−0.06	2.45	4.80	2.69
96	242	−3.58	−0.10	−0.49	8	−3.19	−2.94	0.25	36	−0.22	2.41	5.20	2.48
51	128	−3.59	−0.11	−0.50	10	−3.36	−3.19	0.17	35	−0.14	2.41	4.53	2.65
1	112	−3.59	−0.11	−0.50	12	−3.29	−3.13	0.16	35	0.20	2.44	4.76	2.67
62	0	−3.60	−0.12	−0.51	14	−3.45	−3.28	0.17	36	0.11	2.46	4.91	2.63

Table SI52: Structural, energetic and electronic properties for Mo_7Co_6 cluster, as follows: configuration number (i), relative DFT total energy (ΔE_{tot}^{DFT}, in meV), binding energy (E_b, in eV), excess energy (E_{exc}, in eV), stabilization energy (E_{stab}, in eV), total magnetic moment (M_{tot}, in μ_B), HOMO energy (ε_{HOMO}, in eV), LUMO energy (ε_{LUMO}, in eV), HOMO-LUMO energy difference, (E_{gap}, in eV), total number of bonds (N_b), average chemical order parameter (σ_{av}), average bond length (d_{av}, in Å), average effective coordination number (ECN_{av}, NNN), and average radius (R_{av}, in Å).

i	ΔE_{tot}^{DFT}	E_b	E_{exc}	E_{stab}	M_{tot}	ε_{HOMO}	ε_{LUMO}	E_{gap}	N_b	σ_{av}	d_{av}	ECN_{av}	R_{av}
90	1337	−3.60	−0.02	−0.41	14	−3.36	−3.23	0.12	39	−0.02	2.44	4.82	2.67

67	1181	−3.61	−0.03	−0.42	12	−3.38	−3.26	0.12	37	−0.13	2.44	4.95	2.71
74	1071	−3.62	−0.04	−0.43	10	−3.42	−3.26	0.16	36	−0.22	2.41	4.64	2.68
13	1050	−3.62	−0.04	−0.43	10	−3.25	−3.11	0.14	38	−0.10	2.41	4.68	2.74
49	1048	−3.62	−0.04	−0.43	10	−3.53	−3.35	0.17	37	−0.13	2.40	4.51	2.71
80	997	−3.62	−0.05	−0.43	10	−3.38	−3.06	0.32	38	−0.05	2.39	4.60	2.80
82	982	−3.62	−0.05	−0.43	14	−3.42	−3.31	0.10	38	−0.21	2.43	4.69	2.73
75	963	−3.63	−0.05	−0.43	8	−3.50	−3.34	0.15	34	−0.29	2.39	4.54	2.71
21	893	−3.63	−0.06	−0.44	10	−3.44	−3.25	0.18	37	−0.08	2.41	4.70	2.77
40	892	−3.63	−0.06	−0.44	10	−3.43	−3.25	0.18	37	−0.08	2.41	4.70	2.77
4	854	−3.63	−0.06	−0.44	12	−3.36	−3.21	0.14	37	0.02	2.44	4.76	2.78
12	845	−3.63	−0.06	−0.44	12	−3.41	−3.22	0.18	38	0.00	2.44	5.00	2.70
37	839	−3.63	−0.06	−0.44	10	−3.41	−3.24	0.17	38	−0.21	2.44	4.81	2.65
30	766	−3.64	−0.07	−0.45	8	−3.35	−3.11	0.23	38	−0.15	2.41	5.17	2.50
87	731	−3.64	−0.07	−0.45	12	−3.38	−3.23	0.15	39	−0.02	2.44	4.94	2.71
99	701	−3.65	−0.07	−0.45	12	−3.44	−3.26	0.18	36	−0.05	2.41	4.57	2.82
45	699	−3.65	−0.07	−0.46	12	−3.46	−3.24	0.22	38	−0.10	2.42	4.52	2.68
1	698	−3.65	−0.07	−0.46	8	−3.49	−3.27	0.22	38	−0.21	2.42	4.82	2.70
3	682	−3.65	−0.07	−0.46	10	−3.26	−3.08	0.17	41	−0.07	2.42	5.20	2.56
29	676	−3.65	−0.07	−0.46	12	−3.53	−3.29	0.23	37	−0.02	2.46	5.10	2.90
58	671	−3.65	−0.07	−0.46	8	−3.32	−3.11	0.21	38	−0.26	2.42	4.74	2.72
32	670	−3.65	−0.07	−0.46	8	−3.48	−3.24	0.24	35	−0.14	2.39	4.40	2.63
20	670	−3.65	−0.07	−0.46	14	−3.37	−3.23	0.13	38	0.05	2.43	4.64	2.71
57	665	−3.65	−0.07	−0.46	12	−3.17	−3.01	0.15	42	−0.14	2.46	5.64	2.53
25	640	−3.65	−0.08	−0.46	8	−3.25	−3.04	0.20	42	−0.14	2.41	5.17	2.48
54	618	−3.65	−0.08	−0.46	10	−3.41	−3.14	0.26	37	0.02	2.41	4.61	2.74
33	617	−3.65	−0.08	−0.46	10	−3.28	−3.08	0.19	42	−0.14	2.44	5.41	2.57
35	598	−3.65	−0.08	−0.46	12	−3.43	−3.26	0.16	39	−0.12	2.43	4.59	2.62
19	592	−3.65	−0.08	−0.46	12	−3.36	−3.22	0.13	38	0.21	2.42	4.63	2.80
63	590	−3.65	−0.08	−0.46	8	−3.25	−3.05	0.20	40	−0.10	2.43	5.32	2.54
69	589	−3.65	−0.08	−0.46	8	−3.26	−3.08	0.17	41	−0.17	2.41	5.07	2.56
24	584	−3.65	−0.08	−0.46	12	−3.22	−3.10	0.11	42	−0.04	2.44	5.49	2.47
64	558	−3.66	−0.08	−0.47	10	−3.37	−3.21	0.16	38	−0.05	2.42	4.79	3.02
50	552	−3.66	−0.08	−0.47	12	−3.40	−3.16	0.24	39	−0.02	2.42	4.69	2.78
81	528	−3.66	−0.08	−0.47	12	−3.25	−3.01	0.24	42	−0.14	2.45	5.42	2.50
0	519	−3.66	−0.08	−0.47	14	−3.32	−3.23	0.08	38	0.21	2.43	4.72	2.76
42	518	−3.66	−0.08	−0.47	14	−3.42	−3.26	0.15	40	0.10	2.44	4.63	2.68
97	506	−3.66	−0.09	−0.47	12	−3.40	−3.26	0.14	37	−0.08	2.45	4.93	2.76
27	502	−3.66	−0.09	−0.47	14	−3.22	−3.12	0.10	41	−0.02	2.46	5.65	2.52
89	498	−3.66	−0.09	−0.47	10	−3.40	−3.23	0.16	39	−0.07	2.43	4.85	2.79
76	491	−3.66	−0.09	−0.47	8	−3.24	−3.03	0.20	41	−0.02	2.43	5.36	2.55
15	456	−3.66	−0.09	−0.47	10	−3.36	−3.16	0.20	37	0.02	2.42	4.74	2.78
48	440	−3.67	−0.09	−0.48	10	−3.20	−3.01	0.19	42	−0.23	2.46	5.92	2.48
23	437	−3.67	−0.09	−0.48	8	−3.26	−3.04	0.21	42	−0.23	2.41	5.29	2.50
96	425	−3.67	−0.09	−0.48	10	−3.16	−2.99	0.16	42	−0.04	2.44	5.35	2.64
94	421	−3.67	−0.09	−0.48	10	−3.13	−2.95	0.17	42	−0.04	2.44	5.27	2.65
36	403	−3.67	−0.09	−0.48	12	−3.35	−3.05	0.29	40	−0.05	2.45	5.56	2.51
43	398	−3.67	−0.09	−0.48	10	−3.28	−3.07	0.20	40	−0.10	2.43	5.28	2.54
65	397	−3.67	−0.09	−0.48	10	−3.28	−3.07	0.20	40	−0.10	2.43	5.28	2.54
56	386	−3.67	−0.10	−0.48	8	−3.25	−3.13	0.12	38	−0.15	2.41	5.15	2.49
59	375	−3.67	−0.10	−0.48	8	−3.23	−3.00	0.23	42	−0.23	2.44	5.56	2.48
95	371	−3.67	−0.10	−0.48	10	−3.23	−2.95	0.28	42	−0.04	2.43	5.32	2.53
26	367	−3.67	−0.10	−0.48	12	−3.53	−3.29	0.23	37	−0.18	2.43	4.63	2.74
5	361	−3.67	−0.10	−0.48	12	−3.23	−3.12	0.11	42	−0.04	2.46	5.73	2.48
14	356	−3.67	−0.10	−0.48	12	−3.29	−3.04	0.24	42	0.04	2.45	5.51	2.52
39	348	−3.67	−0.10	−0.48	8	−3.28	−3.04	0.23	42	−0.04	2.45	5.72	2.47
9	317	−3.68	−0.10	−0.48	12	−3.36	−3.24	0.11	37	−0.02	2.42	4.48	2.82
11	309	−3.68	−0.10	−0.49	8	−3.14	−3.02	0.12	42	−0.23	2.42	5.26	2.52
41	301	−3.68	−0.10	−0.49	12	−3.35	−3.19	0.15	38	0.10	2.41	4.54	2.75

i	ΔE_{tot}^{DFT}	E_b	E_{exc}	E_{stab}	M_{tot}	ε_{HOMO}	ε_{LUMO}	E_{gap}	N_b	σ_{av}	d_{av}	ECN_{av}	R_{av}
85	297	−3.68	−0.10	−0.49	8	−3.18	−2.96	0.22	42	−0.04	2.44	5.41	2.49
68	271	−3.68	−0.10	−0.49	10	−3.30	−3.06	0.23	42	−0.04	2.45	5.53	2.50
61	266	−3.68	−0.10	−0.49	10	−3.21	−3.13	0.08	37	−0.02	2.42	4.66	2.79
88	256	−3.68	−0.11	−0.49	10	−3.43	−3.19	0.23	35	0.14	2.39	4.37	2.76
47	253	−3.68	−0.11	−0.49	12	−3.17	−3.02	0.15	42	0.14	2.44	5.41	2.49
7	249	−3.68	−0.11	−0.49	10	−3.25	−2.99	0.26	42	−0.04	2.45	5.53	2.48
72	232	−3.68	−0.11	−0.49	6	−3.35	−3.07	0.27	38	−0.26	2.40	5.01	3.03
38	229	−3.68	−0.11	−0.49	10	−3.28	−3.06	0.21	42	−0.04	2.46	5.65	2.48
70	229	−3.68	−0.11	−0.49	10	−3.28	−3.06	0.21	42	−0.04	2.46	5.65	2.48
2	217	−3.68	−0.11	−0.49	10	−3.41	−3.19	0.21	39	−0.02	2.43	4.57	2.71
51	217	−3.68	−0.11	−0.49	10	−3.25	−3.02	0.23	42	0.14	2.47	5.77	2.48
92	201	−3.68	−0.11	−0.49	10	−3.29	−3.11	0.18	38	0.05	2.40	4.42	2.82
16	201	−3.68	−0.11	−0.49	12	−3.23	−3.08	0.14	42	0.14	2.44	5.37	2.52
28	200	−3.68	−0.11	−0.49	10	−3.16	−3.02	0.13	42	0.14	2.45	5.53	2.51
62	200	−3.68	−0.11	−0.49	12	−3.23	−3.08	0.14	42	0.14	2.44	5.37	2.52
6	175	−3.69	−0.11	−0.50	10	−3.37	−3.15	0.21	40	−0.05	2.42	4.59	2.78
46	167	−3.69	−0.11	−0.50	8	−3.35	−3.13	0.21	42	−0.14	2.44	5.43	2.49
60	144	−3.69	−0.11	−0.50	10	−3.14	−3.02	0.11	41	−0.17	2.46	5.64	2.53
73	143	−3.69	−0.11	−0.50	10	−3.14	−3.02	0.11	42	−0.14	2.46	5.64	2.53
79	82	−3.69	−0.12	−0.50	10	−3.24	−3.06	0.18	42	0.04	2.43	5.29	2.47
53	14	−3.70	−0.12	−0.51	12	−3.24	−3.10	0.13	42	−0.04	2.45	5.61	2.49
55	14	−3.70	−0.12	−0.51	12	−3.24	−3.10	0.13	42	−0.04	2.45	5.61	2.49
31	11	−3.70	−0.12	−0.51	12	−3.24	−3.10	0.13	42	−0.04	2.45	5.61	2.49
83	0	−3.70	−0.12	−0.51	8	−3.33	−3.08	0.25	38	0.10	2.41	4.80	2.96

Table SI53: Structural, energetic and electronic properties for Mo_7Co_7 cluster, as follows: configuration number (i), relative DFT total energy (ΔE_{tot}^{DFT}, in meV), binding energy (E_b, in eV), excess energy (E_{exc}, in eV), stabilization energy (E_{stab}, in eV), total magnetic moment (M_{tot}, in μ_B), HOMO energy (ε_{HOMO}, in eV), LUMO energy (ε_{LUMO}, in eV), HOMO-LUMO energy difference, (E_{gap}, in eV), total number of bonds (N_b), average chemical order parameter (σ_{av}), average bond length (d_{av}, in Å), average effective coordination number (ECN_{av}, NNN), and average radius (R_{av}, in Å).

i	ΔE_{tot}^{DFT}	E_b	E_{exc}	E_{stab}	M_{tot}	ε_{HOMO}	ε_{LUMO}	E_{gap}	N_b	σ_{av}	d_{av}	ECN_{av}	R_{av}
10	2070	−3.61	−0.12	−0.42	13	−3.46	−3.29	0.17	41	−0.12	2.38	4.54	3.06
11	1974	−3.62	−0.12	−0.43	15	−3.54	−3.43	0.11	41	−0.22	2.46	5.30	3.00
97	1874	−3.63	−0.13	−0.44	13	−3.47	−3.34	0.14	41	−0.22	2.44	5.15	2.89
42	1840	−3.63	−0.13	−0.44	15	−3.41	−3.32	0.09	41	−0.02	2.43	4.93	3.10
16	1812	−3.63	−0.14	−0.44	13	−3.45	−3.33	0.12	41	−0.07	2.41	5.05	2.89
69	1758	−3.64	−0.14	−0.44	11	−3.57	−3.34	0.22	41	−0.27	2.44	5.19	2.87
46	1737	−3.64	−0.14	−0.45	11	−3.54	−3.33	0.21	40	−0.15	2.45	5.28	2.92
24	1641	−3.64	−0.15	−0.45	11	−3.46	−3.24	0.21	42	−0.14	2.42	5.23	2.95
59	1604	−3.65	−0.15	−0.46	9	−3.44	−3.18	0.26	42	0.00	2.40	5.06	2.91
8	1537	−3.65	−0.15	−0.46	11	−3.40	−3.23	0.18	42	0.00	2.43	5.12	2.98
56	1528	−3.65	−0.16	−0.46	11	−3.39	−3.25	0.15	40	−0.10	2.42	5.07	3.03
82	1494	−3.66	−0.16	−0.46	11	−3.48	−3.32	0.16	43	−0.02	2.41	5.20	3.04
36	1493	−3.66	−0.16	−0.46	13	−3.55	−3.48	0.07	40	−0.15	2.43	4.80	2.95
45	1487	−3.66	−0.16	−0.46	11	−3.41	−3.23	0.18	40	−0.20	2.43	5.13	2.92
44	1457	−3.66	−0.16	−0.47	11	−3.38	−3.20	0.18	42	−0.19	2.41	5.01	3.02
68	1439	−3.66	−0.16	−0.47	15	−3.42	−3.33	0.09	40	0.00	2.41	4.83	3.10
87	1422	−3.66	−0.16	−0.47	7	−3.35	−3.20	0.14	44	−0.32	2.41	5.29	2.95
99	1421	−3.66	−0.16	−0.47	15	−3.48	−3.33	0.15	41	−0.17	2.44	4.92	2.98
75	1409	−3.66	−0.16	−0.47	11	−3.52	−3.28	0.24	42	−0.10	2.44	4.99	2.84
84	1408	−3.66	−0.16	−0.47	9	−3.36	−3.15	0.21	41	−0.17	2.39	5.06	2.90
52	1384	−3.66	−0.17	−0.47	11	−3.39	−3.26	0.13	40	−0.15	2.42	5.01	2.97

96	1381	−3.66	−0.17	−0.47	13	−3.47	−3.31	0.16	41	−0.07	2.42	5.05	2.98
6	1377	−3.66	−0.17	−0.47	13	−3.42	−3.26	0.16	40	−0.05	2.40	4.77	2.92
17	1350	−3.67	−0.17	−0.47	13	−3.34	−3.26	0.08	43	−0.07	2.42	4.90	3.15
62	1349	−3.67	−0.17	−0.47	11	−3.39	−3.30	0.09	40	−0.05	2.40	5.10	2.95
21	1334	−3.67	−0.17	−0.48	11	−3.32	−3.17	0.15	42	−0.10	2.43	5.22	2.93
64	1330	−3.67	−0.17	−0.48	13	−3.36	−3.30	0.06	40	0.15	2.42	5.12	3.20
49	1321	−3.67	−0.17	−0.48	9	−3.50	−3.37	0.13	41	−0.27	2.41	5.20	2.90
77	1275	−3.67	−0.17	−0.48	13	−3.45	−3.24	0.21	42	−0.05	2.42	4.91	2.91
66	1271	−3.67	−0.17	−0.48	13	−3.50	−3.39	0.11	41	−0.07	2.43	5.13	3.06
93	1259	−3.67	−0.17	−0.48	13	−3.37	−3.29	0.08	42	0.00	2.44	5.02	3.02
41	1253	−3.67	−0.18	−0.48	13	−3.41	−3.27	0.14	41	−0.12	2.43	5.07	3.09
90	1247	−3.67	−0.18	−0.48	9	−3.35	−3.15	0.20	44	−0.09	2.42	5.42	2.91
85	1242	−3.67	−0.18	−0.48	11	−3.54	−3.37	0.17	40	−0.25	2.46	5.34	2.97
50	1232	−3.67	−0.18	−0.48	13	−3.43	−3.33	0.10	41	0.07	2.44	5.12	2.89
100	1210	−3.68	−0.18	−0.48	11	−3.36	−3.16	0.21	40	0.25	2.42	5.10	2.96
18	1187	−3.68	−0.18	−0.49	11	−3.48	−3.26	0.22	43	−0.12	2.43	5.04	3.26
86	1167	−3.68	−0.18	−0.49	11	−3.42	−3.21	0.21	41	−0.12	2.42	4.94	2.87
89	1164	−3.68	−0.18	−0.49	11	−3.41	−3.20	0.21	40	0.00	2.43	5.19	3.28
73	1164	−3.68	−0.18	−0.49	11	−3.38	−3.25	0.13	41	−0.02	2.43	5.19	2.95
25	1163	−3.68	−0.18	−0.49	11	−3.40	−3.22	0.18	41	−0.02	2.40	4.96	2.88
4	1151	−3.68	−0.18	−0.49	11	−3.32	−3.19	0.13	44	0.23	2.42	5.21	2.90
7	1143	−3.68	−0.18	−0.49	9	−3.43	−3.27	0.16	41	−0.17	2.42	5.00	2.94
91	1124	−3.68	−0.18	−0.49	9	−3.31	−3.14	0.17	41	−0.02	2.41	5.03	2.98
26	1116	−3.68	−0.19	−0.49	11	−3.35	−3.22	0.12	42	−0.05	2.44	5.01	2.89
81	1059	−3.69	−0.19	−0.49	9	−3.41	−3.20	0.21	44	−0.05	2.42	5.34	2.79
28	1058	−3.69	−0.19	−0.50	11	−3.41	−3.21	0.20	40	−0.30	2.42	5.03	2.97
60	1036	−3.69	−0.19	−0.50	11	−3.45	−3.31	0.14	43	−0.21	2.42	5.18	2.95
30	1000	−3.69	−0.19	−0.50	9	−3.36	−3.14	0.22	41	−0.07	2.41	5.00	3.10
80	992	−3.69	−0.19	−0.50	13	−3.55	−3.36	0.19	40	−0.20	2.46	5.15	3.00
55	985	−3.69	−0.19	−0.50	13	−3.51	−3.30	0.21	41	−0.02	2.43	4.83	2.99
51	974	−3.69	−0.20	−0.50	9	−3.34	−3.14	0.20	43	−0.21	2.40	5.03	3.09
40	959	−3.69	−0.20	−0.50	13	−3.34	−3.24	0.10	44	0.00	2.44	5.30	2.99
57	936	−3.70	−0.20	−0.50	13	−3.44	−3.28	0.16	41	−0.07	2.44	5.14	3.11
72	906	−3.70	−0.20	−0.51	13	−3.42	−3.31	0.11	41	0.02	2.43	4.96	3.01
78	895	−3.70	−0.20	−0.51	13	−3.45	−3.33	0.12	42	0.05	2.42	4.92	3.02
2	857	−3.70	−0.20	−0.51	11	−3.37	−3.24	0.13	41	−0.07	2.42	5.19	3.05
61	853	−3.70	−0.20	−0.51	13	−3.44	−3.35	0.10	42	0.10	2.44	5.16	3.14
58	837	−3.70	−0.20	−0.51	9	−3.38	−3.16	0.22	42	−0.14	2.40	5.05	3.10
71	827	−3.70	−0.21	−0.51	13	−3.43	−3.14	0.29	41	0.17	2.42	4.98	3.04
79	805	−3.70	−0.21	−0.51	13	−3.41	−3.18	0.22	41	0.07	2.44	5.17	2.95
37	799	−3.71	−0.21	−0.51	13	−3.40	−3.19	0.21	44	−0.09	2.44	5.50	2.99
53	795	−3.71	−0.21	−0.51	13	−3.58	−3.36	0.21	40	0.00	2.45	5.07	2.99
12	737	−3.71	−0.21	−0.52	13	−3.61	−3.38	0.24	41	−0.07	2.47	5.29	3.01
9	700	−3.71	−0.21	−0.52	11	−3.54	−3.29	0.25	41	−0.22	2.44	5.27	3.17
19	697	−3.71	−0.21	−0.52	9	−3.33	−3.20	0.13	44	−0.05	2.41	5.18	2.98
63	693	−3.71	−0.22	−0.52	9	−3.40	−3.19	0.20	42	−0.24	2.46	5.30	3.10
88	684	−3.71	−0.22	−0.52	11	−3.39	−3.26	0.14	44	−0.09	2.43	5.42	2.61
67	665	−3.71	−0.22	−0.52	11	−3.52	−3.33	0.19	41	−0.12	2.41	4.75	3.36
38	658	−3.72	−0.22	−0.52	11	−3.48	−3.27	0.21	41	−0.17	2.41	5.08	3.12
65	633	−3.72	−0.22	−0.53	11	−3.45	−3.32	0.12	40	−0.10	2.44	5.01	3.18
76	625	−3.72	−0.22	−0.53	9	−3.45	−3.22	0.23	40	−0.05	2.44	5.01	3.07
5	573	−3.72	−0.22	−0.53	11	−3.38	−3.18	0.20	45	0.02	2.43	5.47	2.59
13	504	−3.73	−0.23	−0.53	13	−3.55	−3.34	0.21	41	0.12	2.47	5.34	3.06
34	465	−3.73	−0.23	−0.54	11	−3.41	−3.14	0.27	45	−0.07	2.46	5.59	3.11
92	261	−3.74	−0.25	−0.55	9	−3.50	−3.28	0.22	41	−0.02	2.45	5.17	3.14
15	0	−3.76	−0.26	−0.57	13	−3.51	−3.21	0.31	39	0.18	2.43	4.81	2.84

Table SI54: Structural, energetic and electronic properties for Mo_8Co_7 cluster, as follows: configuration number (i), relative DFT total energy (ΔE_{tot}^{DFT}, in meV), binding energy (E_b, in eV), excess energy (E_{exc}, in eV), stabilization energy (E_{stab}, in eV), total magnetic moment (M_{tot}, in μ_B), HOMO energy (ε_{HOMO}, in eV), LUMO energy (ε_{LUMO}, in eV), HOMO-LUMO energy difference, (E_{gap}, in eV), total number of bonds (N_b), average chemical order parameter (σ_{av}), average bond length (d_{av}, in Å), average effective coordination number (ECN_{av}, NNN), and average radius (R_{av}, in Å).

i	ΔE_{tot}^{DFT}	E_b	E_{exc}	E_{stab}	M_{tot}	ε_{HOMO}	ε_{LUMO}	E_{gap}	N_b	σ_{av}	d_{av}	ECN_{av}	R_{av}
58	1232	−3.75	−0.04	−0.45	13	−3.36	−3.20	0.15	50	−0.16	2.44	5.44	2.69
45	1139	−3.75	−0.05	−0.45	13	−3.33	−3.23	0.09	49	−0.06	2.44	5.61	3.11
56	1035	−3.76	−0.06	−0.46	13	−3.36	−3.27	0.08	47	−0.06	2.43	5.05	2.81
60	980	−3.77	−0.06	−0.46	15	−3.51	−3.36	0.14	48	−0.12	2.46	5.24	2.80
13	953	−3.77	−0.06	−0.47	9	−3.48	−3.31	0.17	49	−0.22	2.43	5.39	2.85
59	915	−3.77	−0.06	−0.47	10	−3.53	−3.32	0.20	47	−0.10	2.44	5.20	2.74
93	890	−3.77	−0.07	−0.47	13	−3.40	−3.28	0.12	46	−0.21	2.44	5.18	2.82
42	839	−3.77	−0.07	−0.47	13	−3.48	−3.33	0.15	47	−0.14	2.45	5.16	2.75
36	790	−3.78	−0.07	−0.48	12	−3.33	−3.19	0.13	48	−0.08	2.45	5.64	3.08
64	790	−3.78	−0.07	−0.48	11	−3.23	−3.09	0.13	47	−0.02	2.43	5.39	3.14
96	771	−3.78	−0.07	−0.48	11	−3.43	−3.23	0.19	49	−0.06	2.44	5.27	2.80
68	760	−3.78	−0.08	−0.48	13	−3.41	−3.24	0.17	49	−0.10	2.44	5.59	3.06
41	758	−3.78	−0.08	−0.48	11	−3.49	−3.30	0.18	45	−0.20	2.41	4.88	2.76
53	750	−3.78	−0.08	−0.48	9	−3.37	−3.20	0.16	48	−0.16	2.42	5.41	2.64
83	733	−3.78	−0.08	−0.48	7	−3.49	−3.35	0.14	48	−0.12	2.41	4.98	2.95
44	698	−3.78	−0.08	−0.48	11	−3.45	−3.32	0.13	47	−0.23	2.43	5.24	2.70
70	675	−3.79	−0.08	−0.48	11	−3.52	−3.33	0.18	46	−0.13	2.44	5.25	2.80
29	641	−3.79	−0.08	−0.49	11	−3.34	−3.23	0.11	49	−0.14	2.44	5.44	2.97
91	639	−3.79	−0.08	−0.49	11	−3.39	−3.17	0.21	49	−0.06	2.43	5.43	2.70
16	631	−3.79	−0.08	−0.49	13	−3.38	−3.23	0.15	47	−0.10	2.45	5.25	2.81
02	630	−3.79	−0.08	−0.49	15	−3.49	−3.31	0.17	49	0.02	2.46	5.29	2.75
77	617	−3.79	−0.08	−0.49	11	−3.40	−3.28	0.12	49	−0.06	2.42	5.23	2.98
14	616	−3.79	−0.08	−0.49	11	−3.39	−3.19	0.19	48	−0.12	2.44	5.25	2.84
50	599	−3.79	−0.09	−0.49	11	−3.54	−3.31	0.22	47	−0.14	2.44	5.22	2.72
51	578	−3.79	−0.09	−0.49	11	−3.39	−3.18	0.21	48	−0.08	2.43	5.41	3.16
8	576	−3.79	−0.09	−0.49	15	−3.38	−3.32	0.05	47	−0.02	2.45	5.14	2.76
98	563	−3.79	−0.09	−0.49	9	−3.47	−3.26	0.21	46	0.00	2.42	4.88	2.80
43	554	−3.79	−0.09	−0.49	11	−3.47	−3.34	0.13	48	0.04	2.45	5.64	3.15
1	551	−3.79	−0.09	−0.49	13	−3.56	−3.37	0.18	46	−0.13	2.46	5.33	2.80
92	542	−3.79	−0.09	−0.49	7	−3.38	−3.16	0.22	50	−0.20	2.43	5.17	2.91
82	538	−3.79	−0.09	−0.49	11	−3.28	−3.24	0.04	49	0.02	2.44	5.53	3.16
21	534	−3.79	−0.09	−0.49	11	−3.52	−3.35	0.17	45	−0.11	2.45	5.29	2.84
81	533	−3.79	−0.09	−0.49	15	−3.44	−3.24	0.19	48	−0.04	2.46	5.31	2.81
62	525	−3.80	−0.09	−0.49	9	−3.45	−3.24	0.20	48	−0.04	2.42	5.14	3.14
57	522	−3.80	−0.09	−0.49	11	−3.43	−3.22	0.21	49	0.06	2.43	5.43	2.81
35	517	−3.80	−0.09	−0.50	13	−3.32	−3.27	0.05	47	0.06	2.43	5.12	2.76
86	509	−3.80	−0.09	−0.50	13	−3.48	−3.32	0.15	48	0.00	2.45	5.24	2.79
49	500	−3.80	−0.09	−0.50	12	−3.55	−3.33	0.21	46	−0.17	2.47	5.38	2.84
3	498	−3.80	−0.09	−0.50	11	−3.53	−3.30	0.23	47	−0.06	2.45	5.24	3.03
10	493	−3.80	−0.09	−0.50	11	−3.40	−3.21	0.18	47	−0.06	2.44	5.54	3.09
19	484	−3.80	−0.09	−0.50	9	−3.41	−3.20	0.20	48	−0.08	2.43	5.50	3.08
63	476	−3.80	−0.09	−0.50	10	−3.49	−3.32	0.17	49	−0.18	2.44	5.43	3.20
78	475	−3.80	−0.09	−0.50	13	−3.40	−3.25	0.14	47	0.10	2.45	5.26	2.78
95	471	−3.80	−0.09	−0.50	11	−3.22	−3.15	0.06	46	−0.08	2.43	5.57	2.99
74	469	−3.80	−0.09	−0.50	11	−3.44	−3.23	0.20	48	−0.12	2.43	5.45	3.10
23	469	−3.80	−0.09	−0.50	13	−3.34	−3.23	0.11	48	0.00	2.45	5.18	2.78
34	459	−3.80	−0.10	−0.50	11	−3.44	−3.27	0.17	49	−0.06	2.45	5.30	2.73
52	441	−3.80	−0.10	−0.50	13	−3.46	−3.29	0.16	48	−0.16	2.46	5.62	3.14

6	437	−3.80	−0.10	−0.50	13	−3.47	−3.29	0.18	46	0.04	2.44	5.01	2.76
12	431	−3.80	−0.10	−0.50	11	−3.48	−3.28	0.20	47	−0.10	2.45	5.36	2.79
94	392	−3.80	−0.10	−0.50	11	−3.40	−3.25	0.14	49	−0.06	2.42	5.32	3.18
80	381	−3.81	−0.10	−0.50	13	−3.47	−3.29	0.17	48	−0.04	2.45	5.61	3.17
31	377	−3.81	−0.10	−0.50	9	−3.46	−3.25	0.20	49	0.02	2.43	5.00	2.83
88	373	−3.81	−0.10	−0.50	11	−3.34	−3.18	0.15	47	−0.02	2.43	5.41	3.03
32	368	−3.81	−0.10	−0.51	13	−3.54	−3.40	0.13	48	−0.04	2.45	5.22	3.17
40	343	−3.81	−0.10	−0.51	15	−3.40	−3.28	0.11	47	0.19	2.45	5.17	2.78
25	342	−3.81	−0.10	−0.51	8	−3.37	−3.23	0.13	47	−0.06	2.42	5.38	3.11
73	335	−3.81	−0.10	−0.51	11	−3.33	−3.22	0.10	48	−0.08	2.43	5.43	3.07
27	324	−3.81	−0.10	−0.51	9	−3.45	−3.20	0.25	49	−0.26	2.41	5.13	3.31
11	302	−3.81	−0.11	−0.51	9	−3.51	−3.26	0.25	47	−0.06	2.45	5.64	3.09
61	291	−3.81	−0.11	−0.51	11	−3.38	−3.27	0.11	48	−0.12	2.44	5.50	3.05
17	261	−3.81	−0.11	−0.51	13	−3.40	−3.28	0.11	46	0.17	2.46	5.35	2.85
69	244	−3.81	−0.11	−0.51	9	−3.47	−3.24	0.22	49	−0.14	2.44	5.20	2.92
22	237	−3.81	−0.11	−0.51	11	−3.34	−3.23	0.11	48	−0.12	2.43	5.51	3.16
85	222	−3.82	−0.11	−0.51	11	−3.31	−3.20	0.11	46	−0.04	2.42	4.93	3.13
39	185	−3.82	−0.11	−0.52	11	−3.34	−3.19	0.15	48	0.00	2.45	5.67	3.13
37	183	−3.82	−0.11	−0.52	9	−3.35	−3.22	0.13	48	−0.16	2.44	5.54	3.16
0	163	−3.82	−0.12	−0.52	7	−3.39	−3.18	0.20	46	−0.08	2.42	5.05	2.76
48	42	−3.83	−0.12	−0.53	11	−3.31	−3.24	0.06	47	0.14	2.43	5.50	3.05
24	33	−3.83	−0.12	−0.53	8	−3.42	−3.30	0.12	45	−0.02	2.43	4.95	3.01
47	24	−3.83	−0.12	−0.53	13	−3.42	−3.23	0.18	46	0.17	2.43	5.13	2.79
46	22	−3.83	−0.12	−0.53	13	−3.42	−3.23	0.18	46	0.17	2.43	5.14	2.78
89	0	−3.83	−0.13	−0.53	11	−3.40	−3.21	0.19	48	0.00	2.44	5.54	3.16

Table SI55: Lowest energy configurations for the near-equiatomic Mo_nCo_m subnanoalloys with $n+m = 2-15$.

MoCo

Mo_2Co

Mo_2Co_2

Mo_3Co_2

Mo_3Co_3

Mo_4Co_3

Mo_4Co_4

Mo_5Co_4

Mo_5Co_5

Mo_6Co_5

Mo_6Co_6

Mo_7Co_6

Mo_7Co_7

Mo_8Co_7
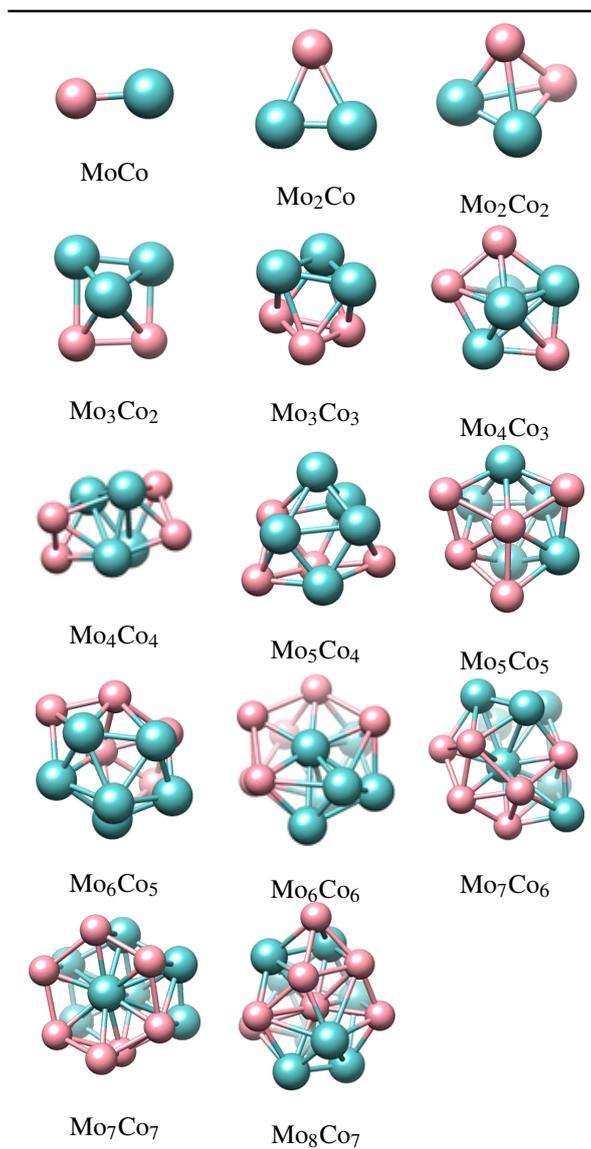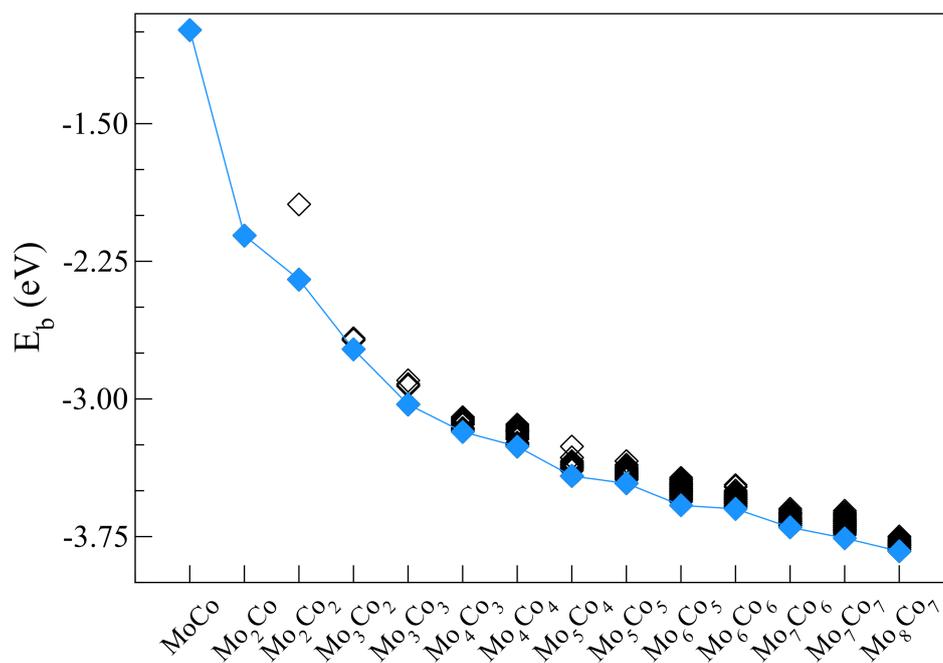
Figure SI33: Binding energy (E_b) for the near-equiatomic Mo_nCo_m subnanoalloys with $n + m = 2 - 15$.
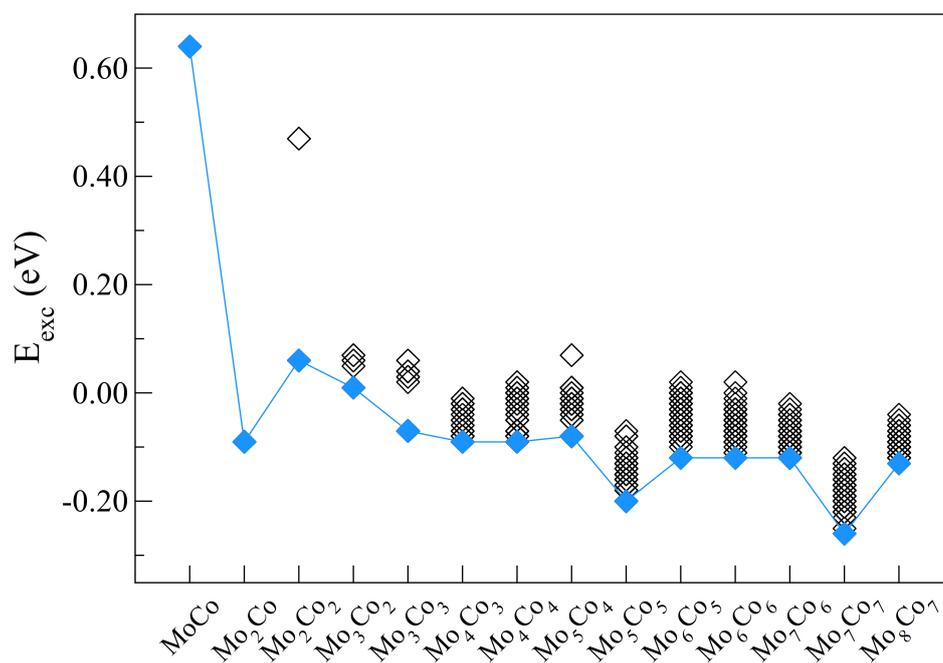
Figure SI34: Excess energy (E_{exc}) for the near-equiatomic Mo_nCo_m subnanoalloys with $n + m = 2 - 15$.
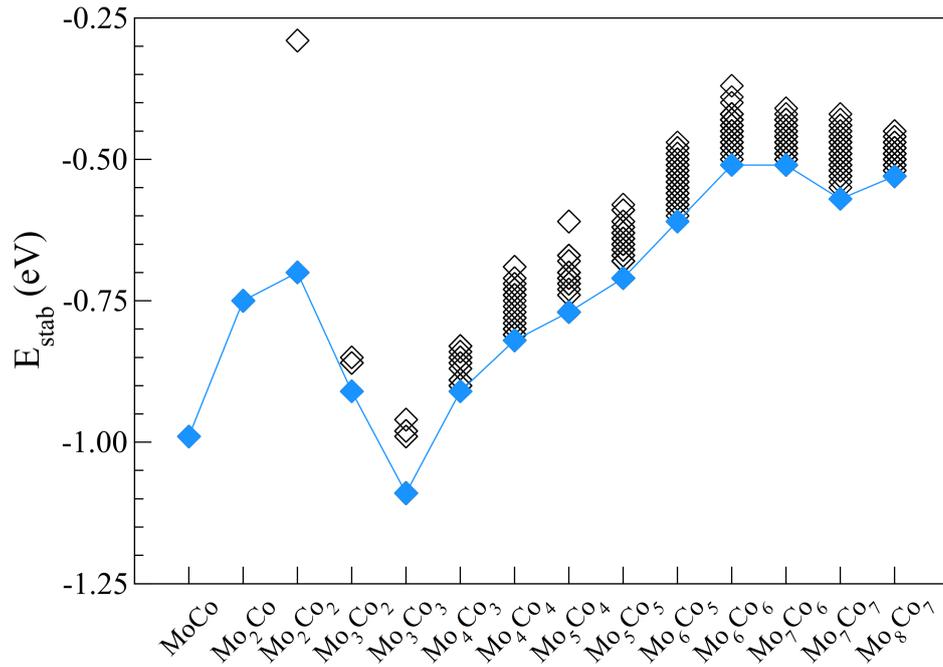
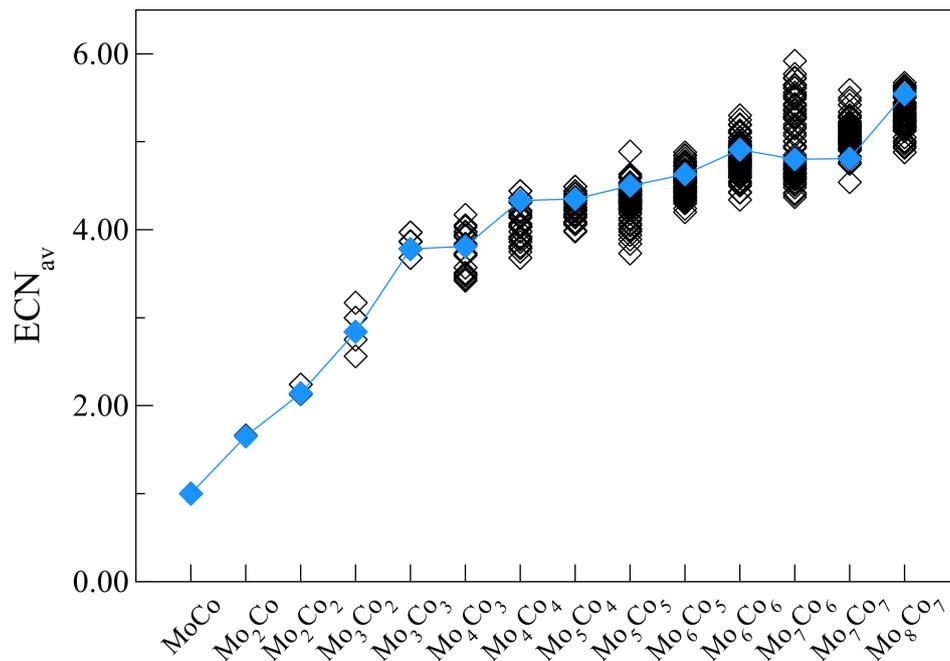Figure SI35: Stabilization energy (E_{stab}) for the near-equiatomic Mo_nCo_m subnanoalloys with $n+m=2-15$.
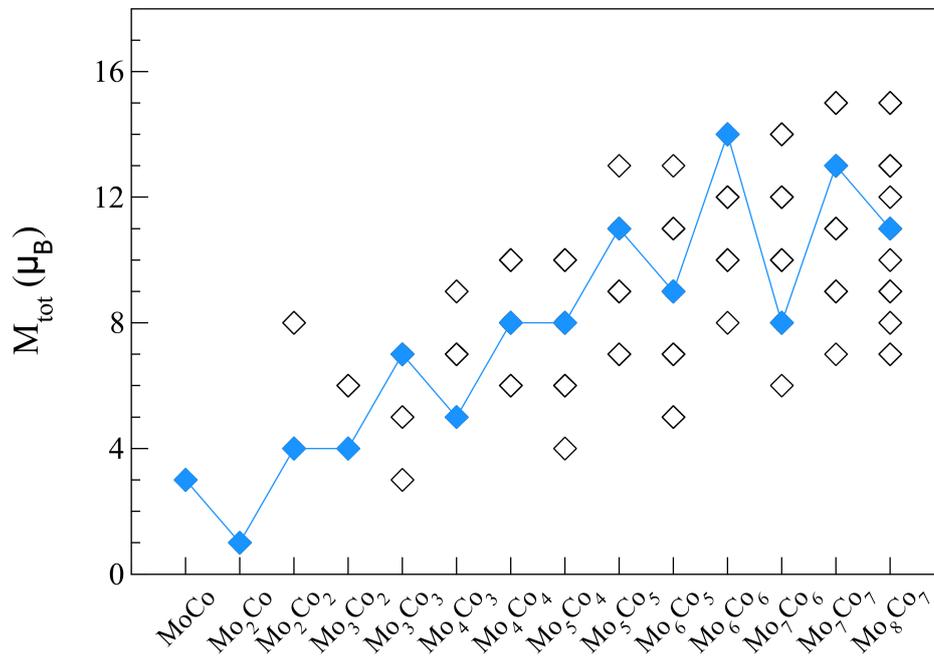
Figure SI36: Total magnetic moment (M_{tot}) for the near-equiatomic Mo_nCo_m subnanoalloys with $n+m=2-15$.
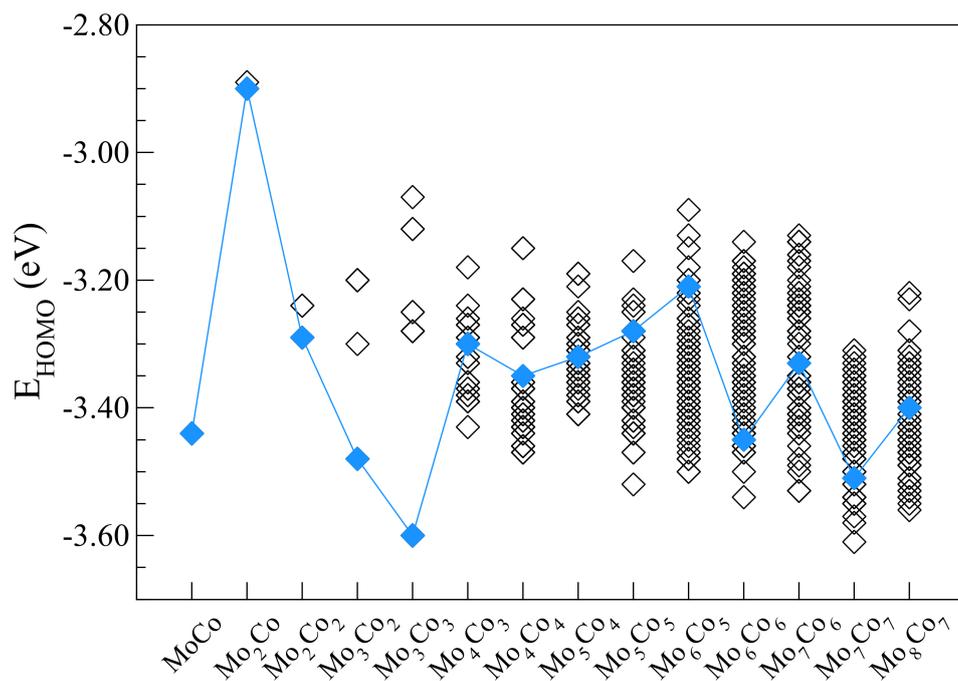
Figure SI37: HOMO energy (E_{HOMO}) for the near-equiatomic Mo$_n$Co$_m$ subnanoalloys with $n+m = 2-15$.
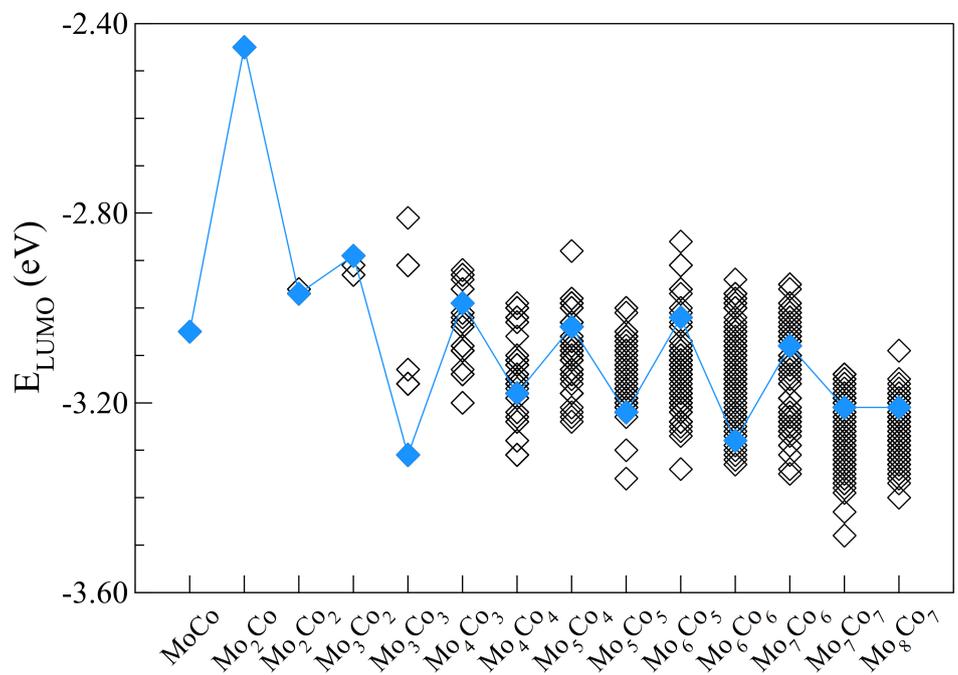
Figure SI38: LUMO energy (E_{LUMO}) for the near-equiatomic Mo$_n$Co$_m$ subnanoalloys with $n+m = 2-15$.
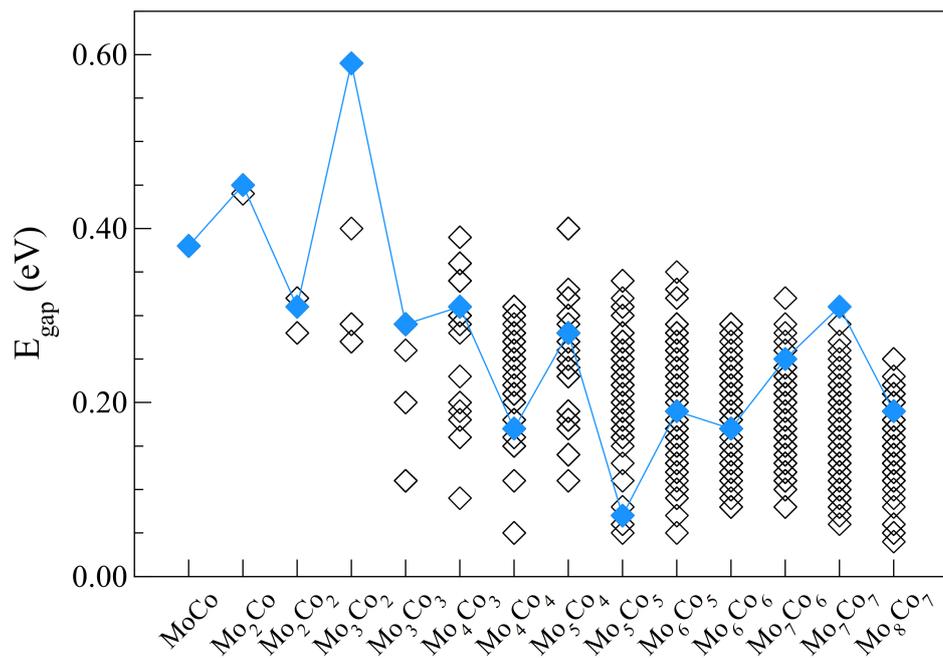
Figure SI39: HOMO-LUMO energy gap (E_{gap}) for the near-equiatomic Mo_nCo_m subnanoalloys with $n + m = 2 - 15$.
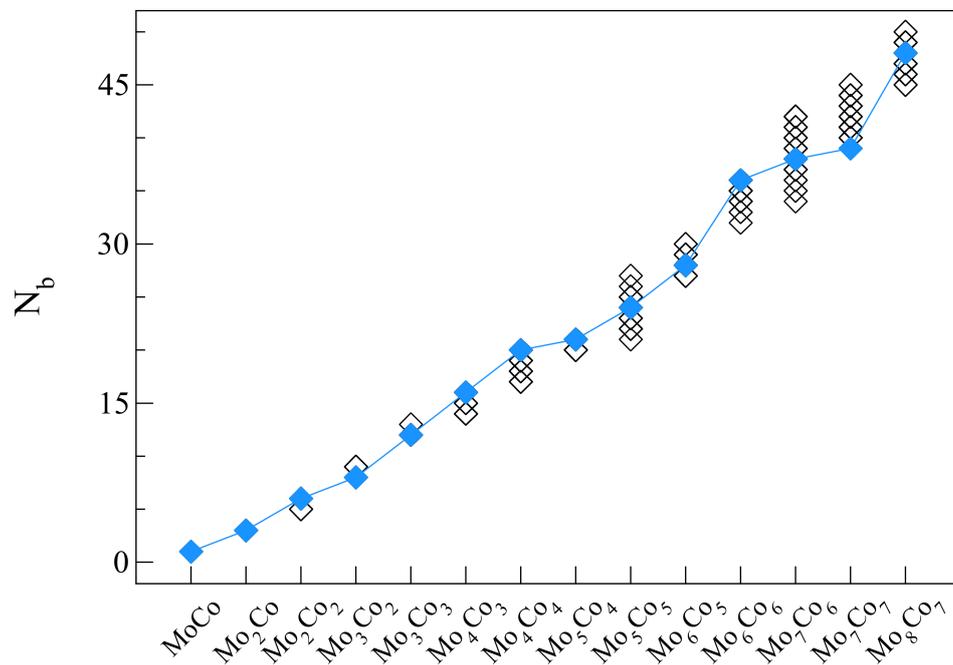
Figure SI40: Total number of bonds (N_b) for the near-equiatomic Mo_nCo_m subnanoalloys with $n + m = 2 - 15$.
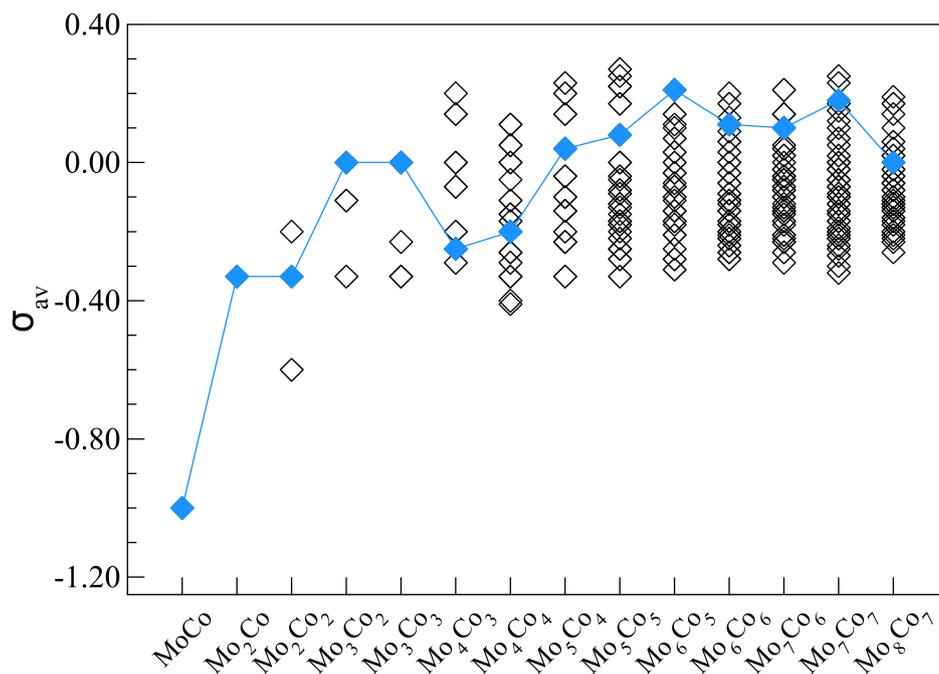
Figure SI41: Average chemical order parameter (σ_{av}) for the near-equiatomic Mo_nCo_m subnanoalloys with $n + m = 2 - 15$.
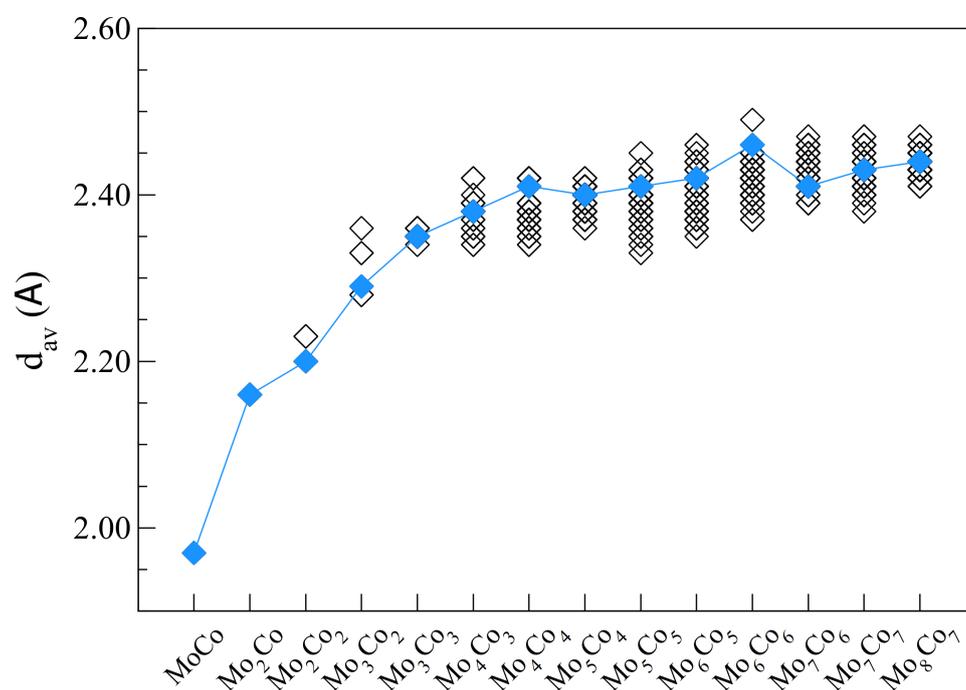
Figure SI42: Average bond length (d_{av}) for the near-equiatomic Mo_nCo_m subnanoalloys with $n + m = 2 - 15$.

Figure SI43: Average effective coordination number (ECN_{av}) for the near-equiatomic Mo_nCo_m subnanoalloys with $n + m = 2 - 15$.
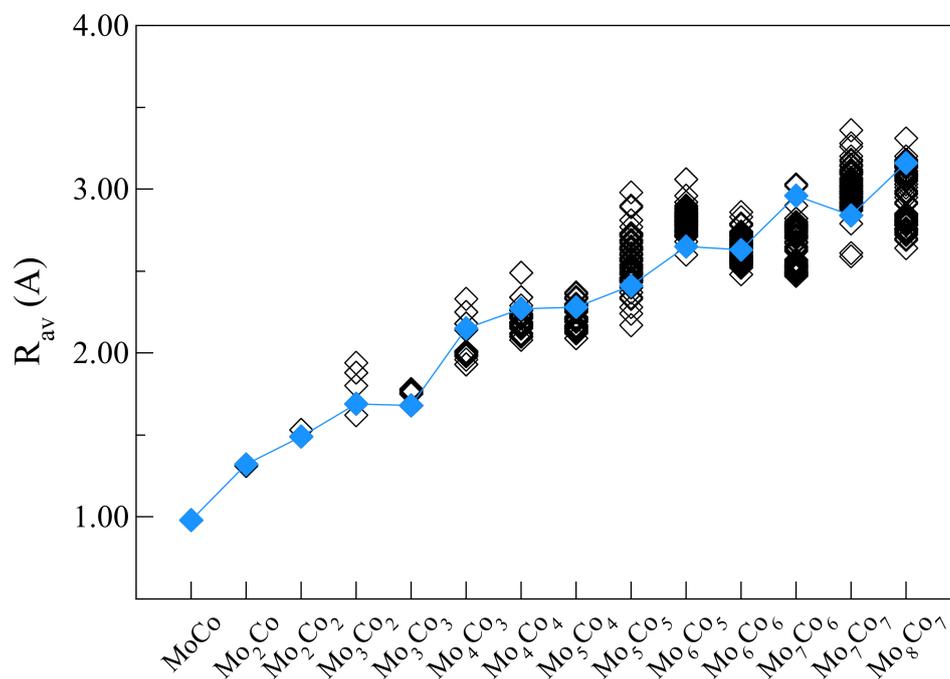
Figure SI44: Average radius (R_{av}) for the near-equiatomic Mo_nCo_m subnanoalloys with $n + m = 2 - 15$.

6 Data Availability

All DFT calculations were done using the FHI–aims package, which can be used under a non-free academic license. Additional details can be obtained from the link, `https://fhi-aims.org/`. Furthermore, additional details are provided within the supporting information, while raw (XYZ files) and processed data required to reproduce the above findings are available to download from `https://github.com/\karlandriani/ConMom.git`.

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