Supporting Information

The structural, magnetic and optical properties of $TM_n@(ZnO)_{42}$ (TM = Fe, Co and Ni) hetero-nanostructure

Yaowen Hu[a], Chuting Ji[a], Xiaoxu Wang[b, c, †], Jinrong Huo[b, †], Qing Liu[b], and Yipu Song[d, *]

[a]Department of Physics, Tsinghua University, Beijing 100084, China

[b]Department of Physics, University of Science and Technology Beijing, Beijing 100083, China.

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[d]Center for Quantum Information, IIIS, Tsinghua University, Beijing 100084, China

This file includes

Supporting Information I: Enlarged Picture of Core-Shell Structures

Supporting Information II: Electric Distribution and Coordination Number

Supporting Information III: Bond Length

Supporting Information I: Enlarged Picture of Core-shell Structures

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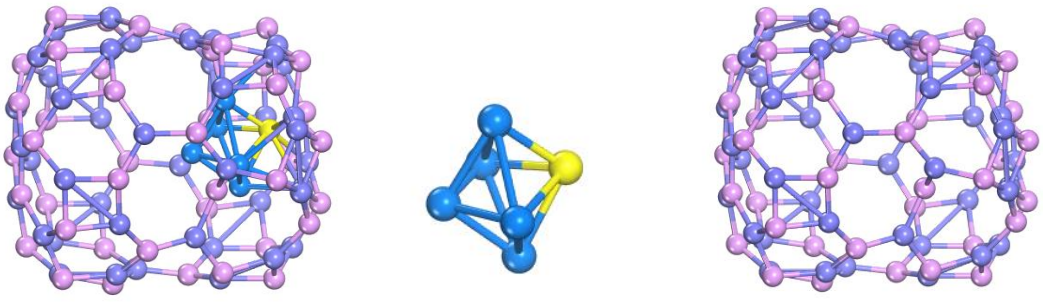
This file gives an enlarged picture of each optimized $TM_n@(ZnO)_{42}$ core-shell structure. The pink, purple and blue balls show the positions of O, Zn and TM atoms, respectively. The small or abnormal magnetic moment of TM atoms are shown by yellow balls.

The left column gives the core-shell structure of $TM_n@(ZnO)_{42}$. The center column is the core of $TM_n@(ZnO)_{42}$ and the right column shows the shell of $TM_n@(ZnO)_{42}$.

1. $Fe_n@(ZnO)_{42}$



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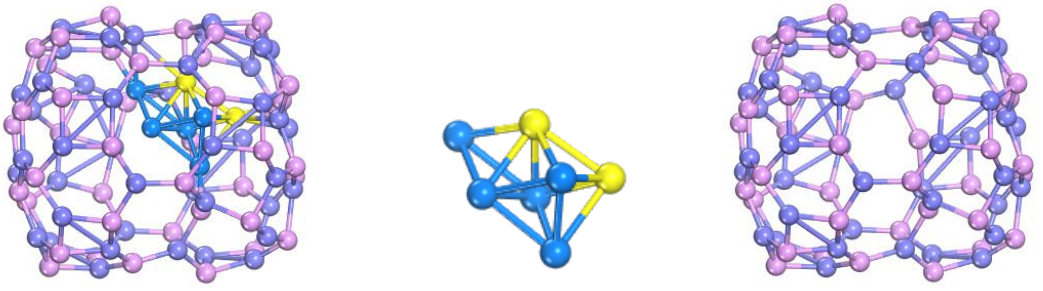

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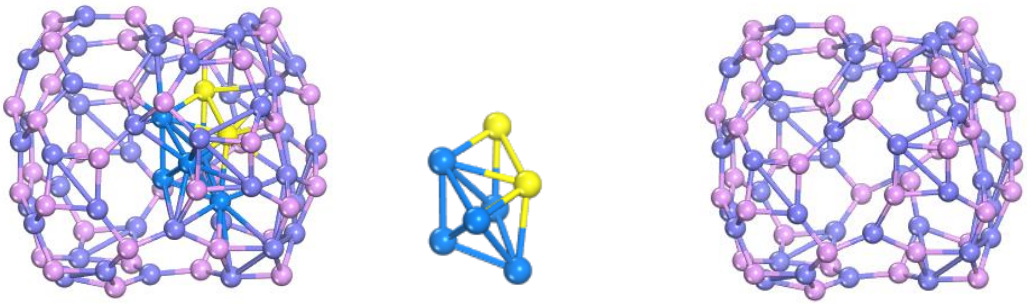
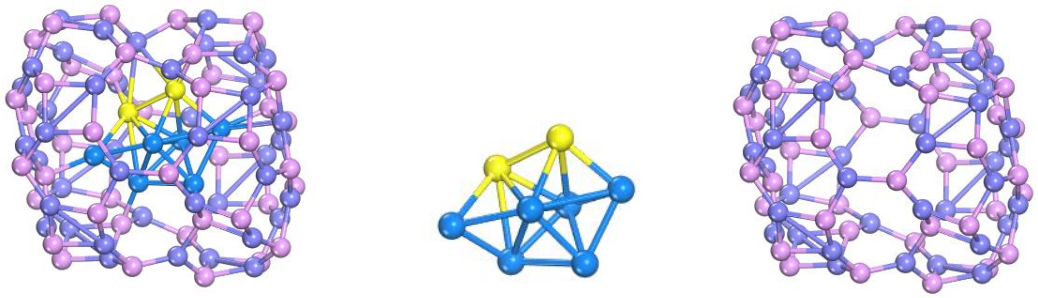


Fe7- the structure of the annealed + optimized $Fe_7@(ZnO)_{42}$



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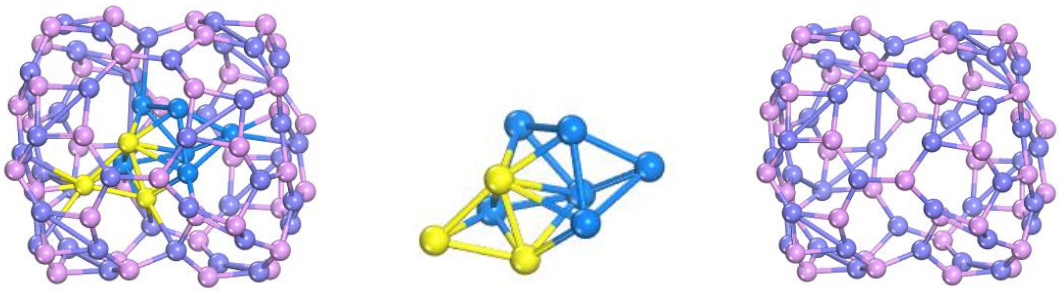

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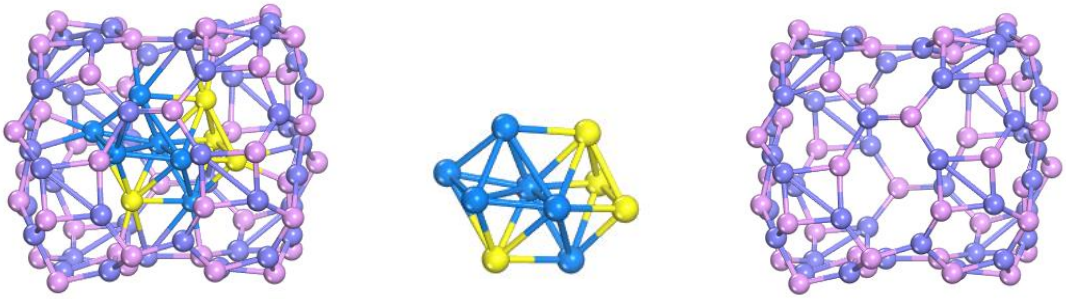

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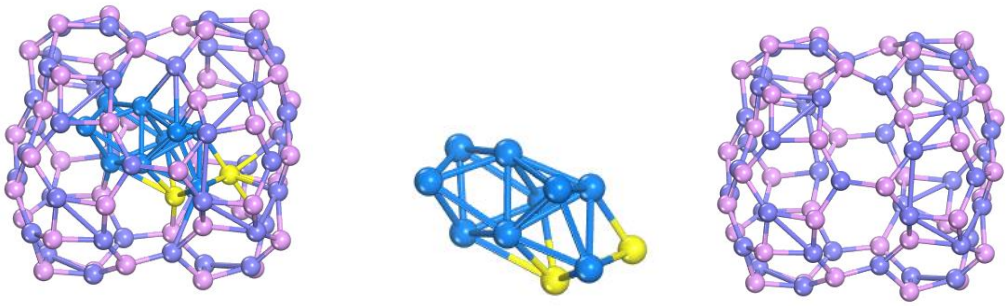

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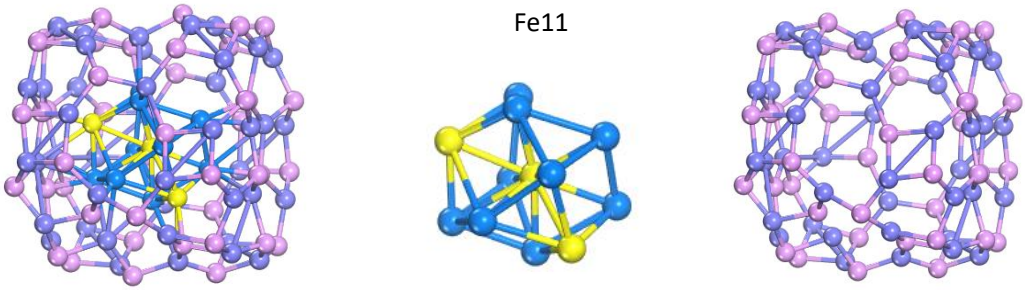

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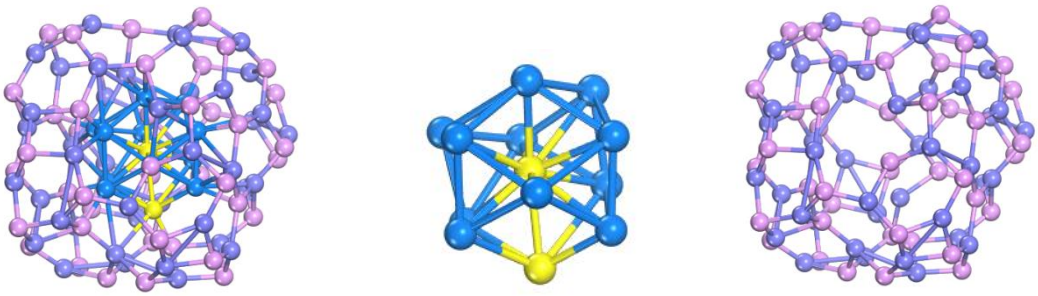

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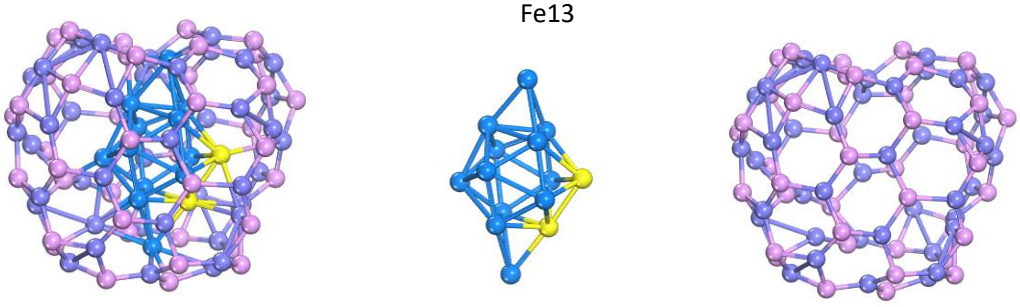

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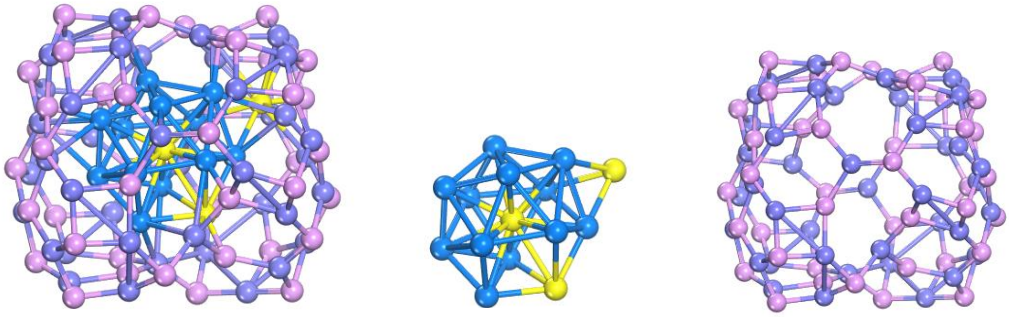

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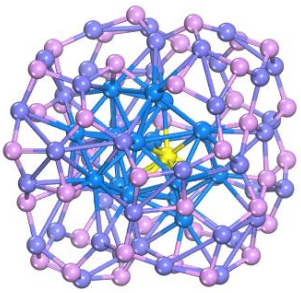
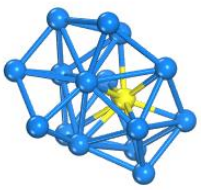
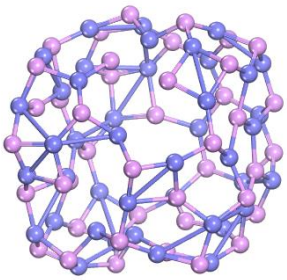
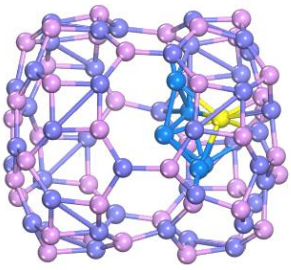
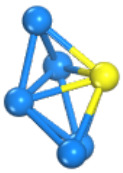
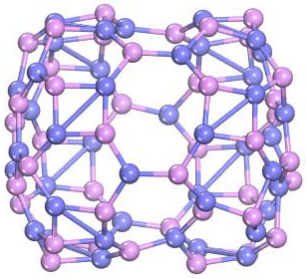




Fe16

2. $Co_n@(ZnO)_{42}$

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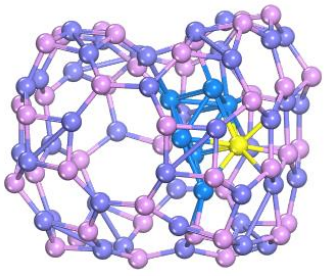
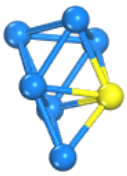
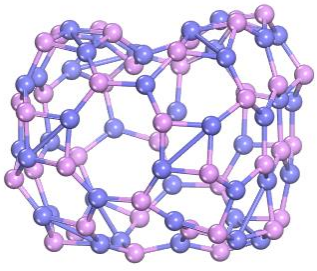

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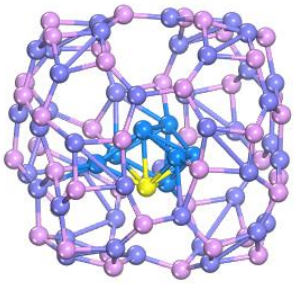
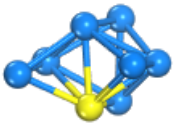
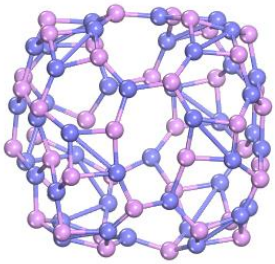

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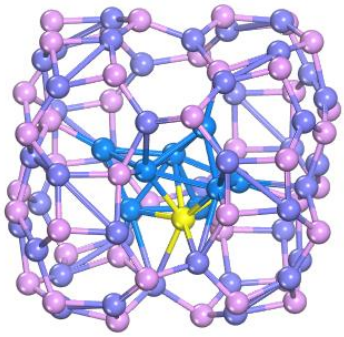
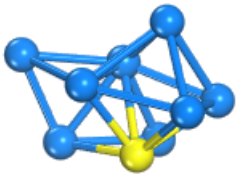
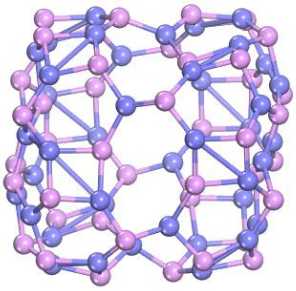

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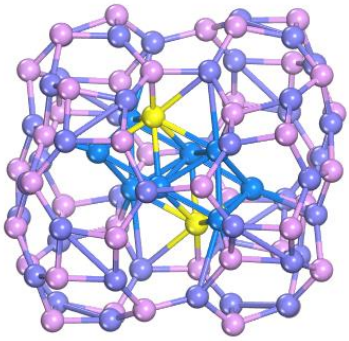
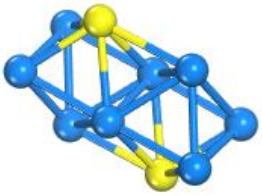
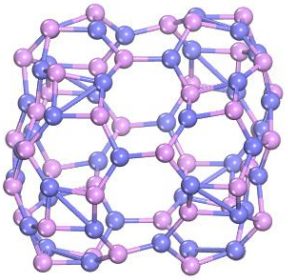

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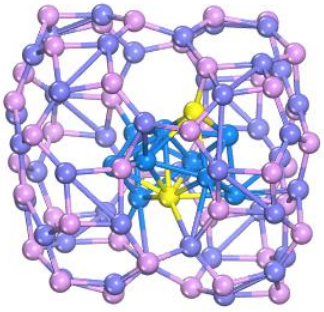
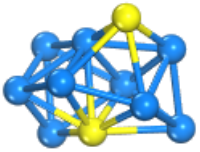
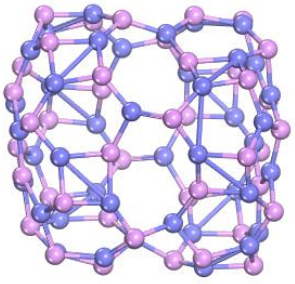

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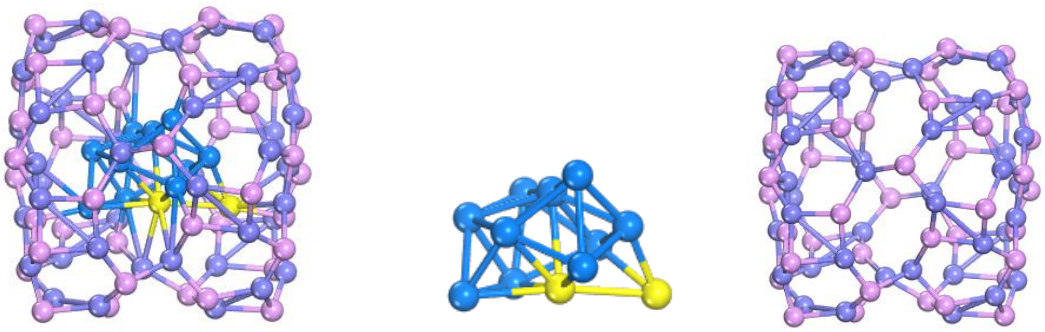

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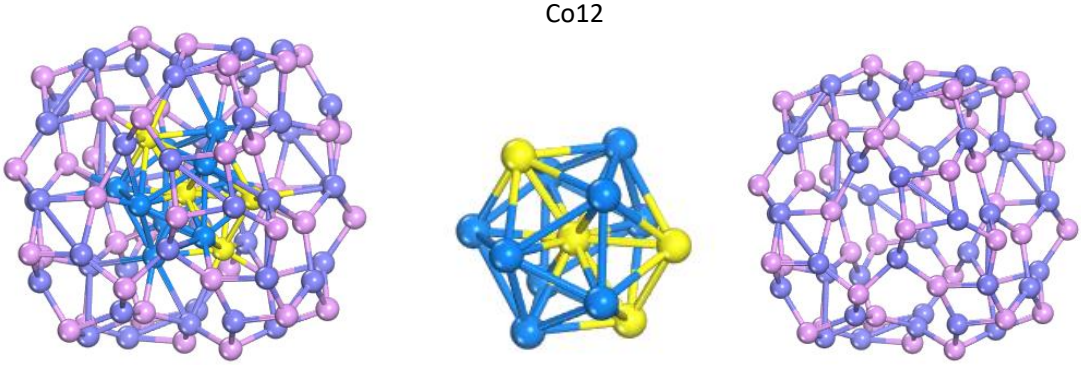

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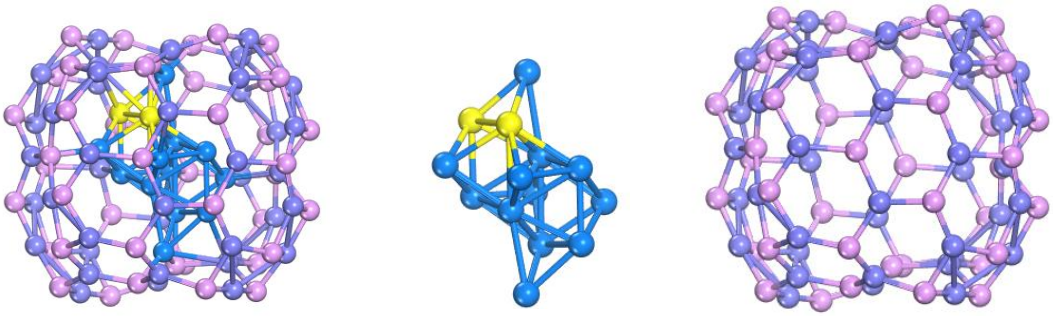

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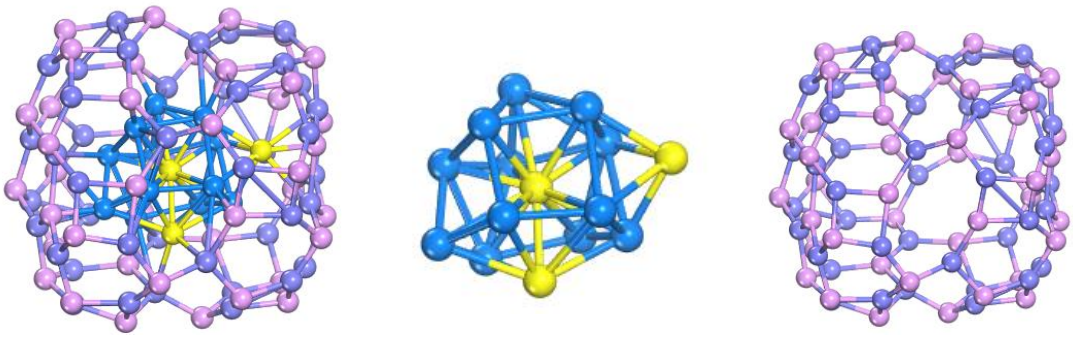

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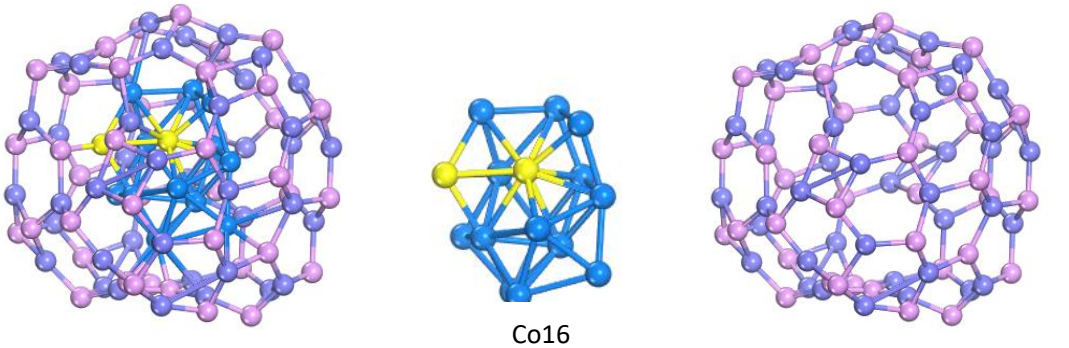

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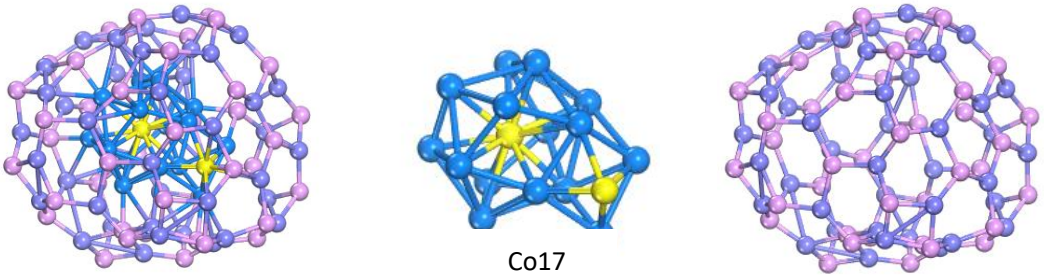

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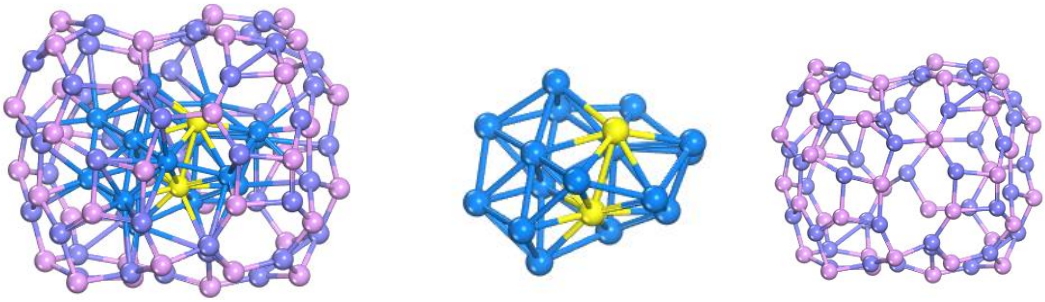
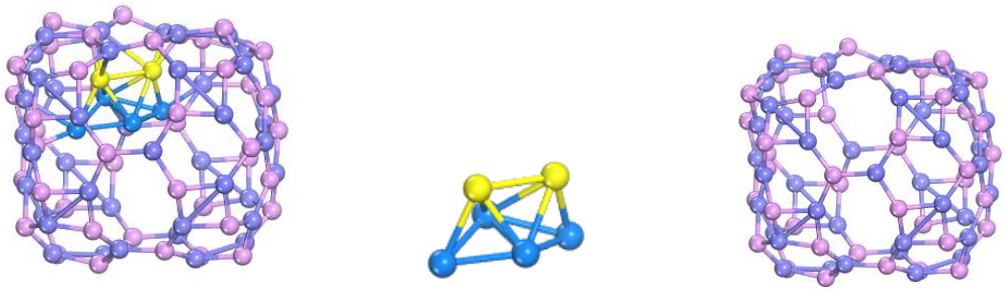


Co18

3. $Ni_n@(ZnO)_{42}$



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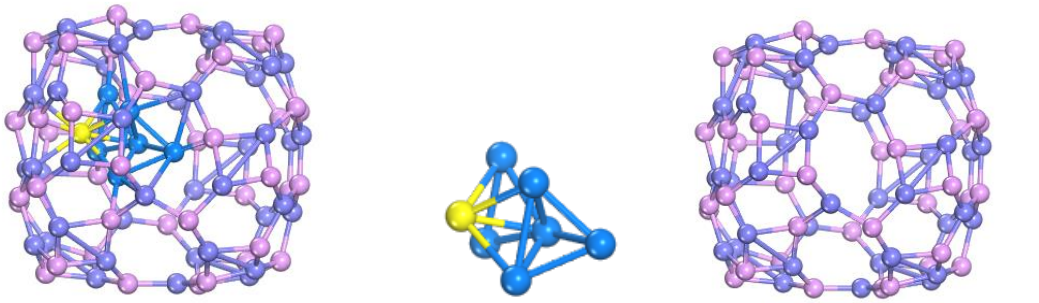

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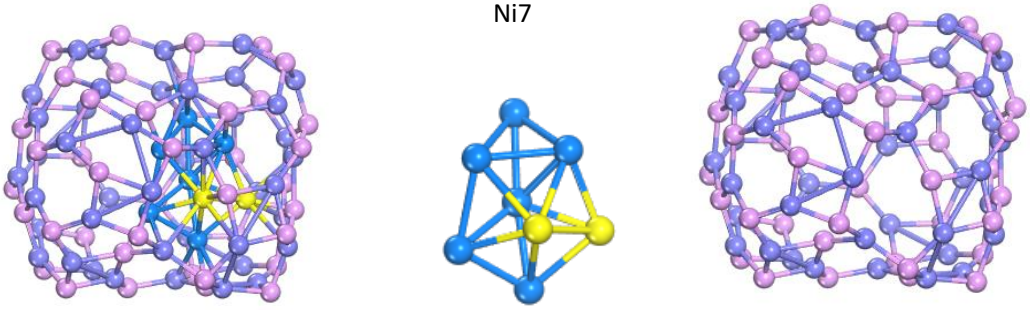

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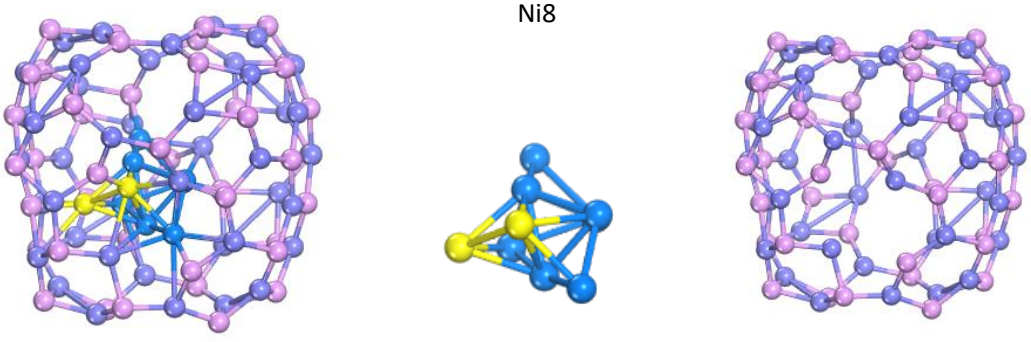

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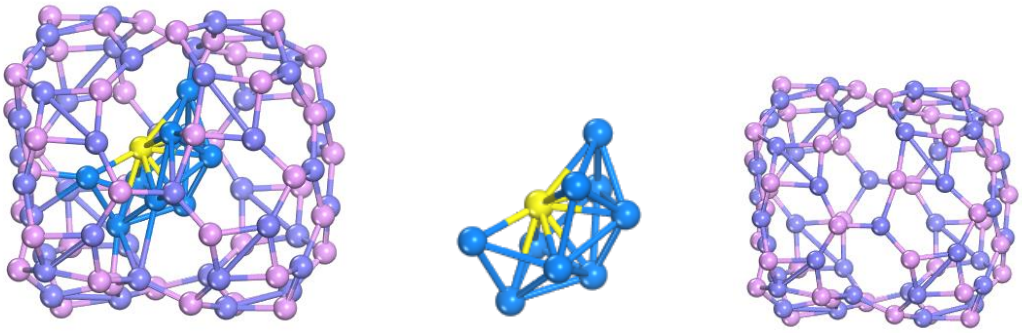

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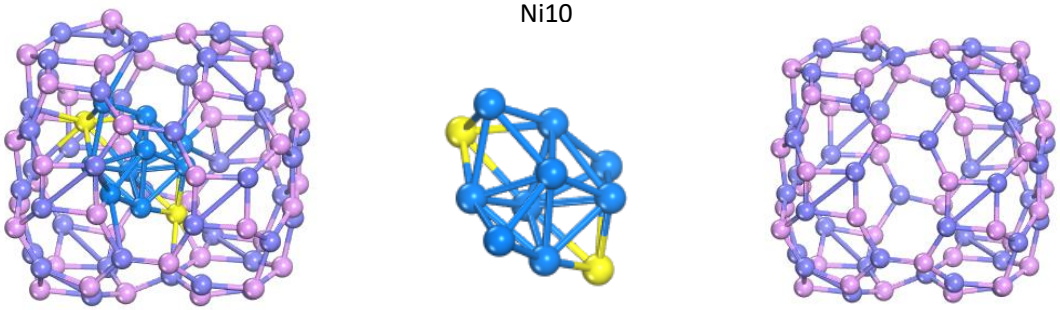

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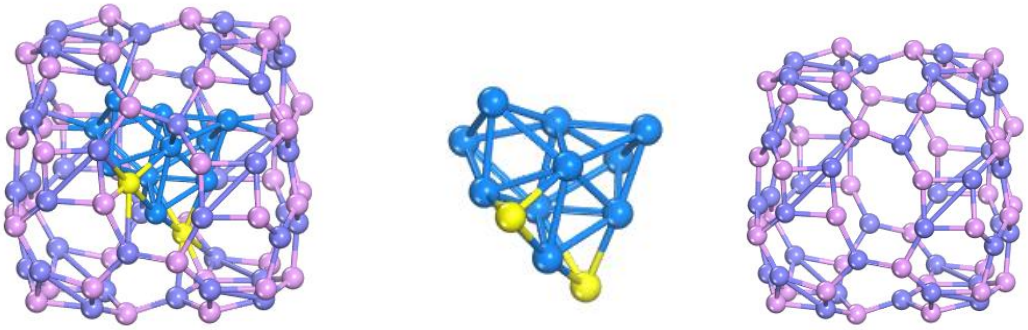

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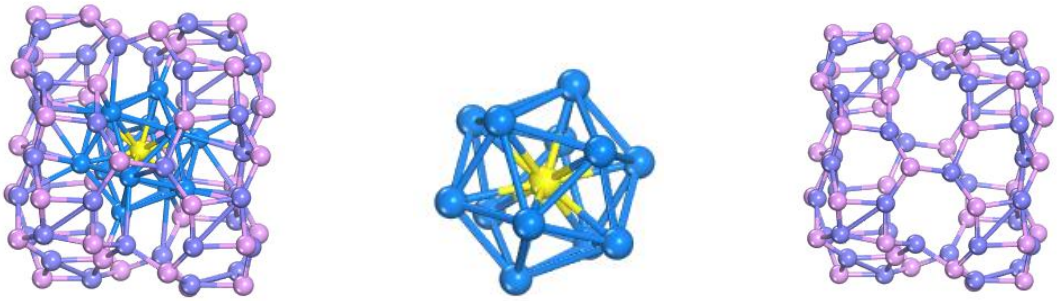

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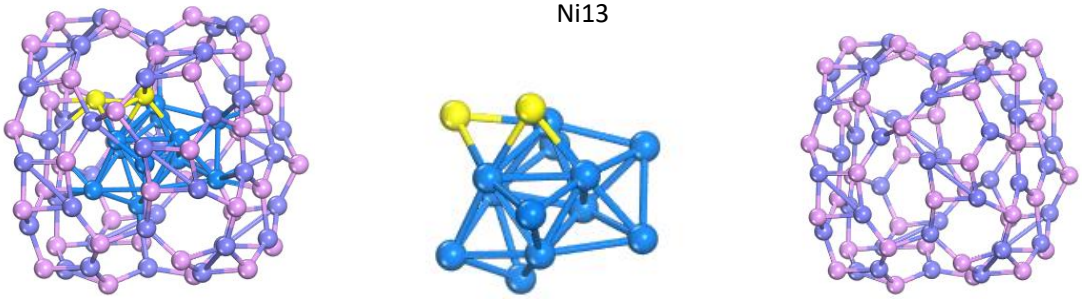

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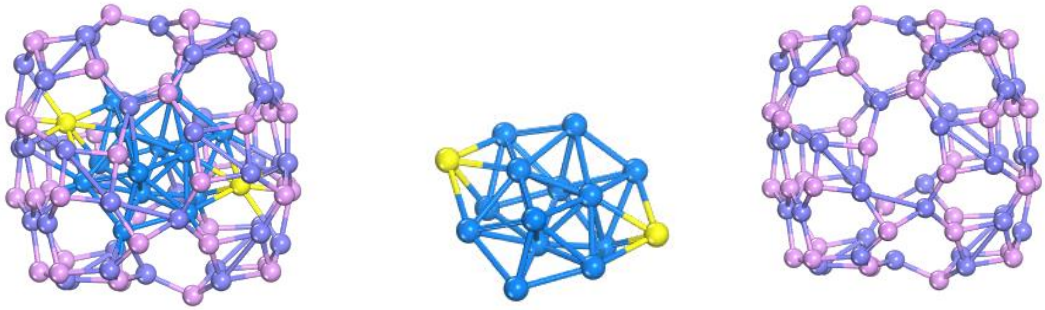

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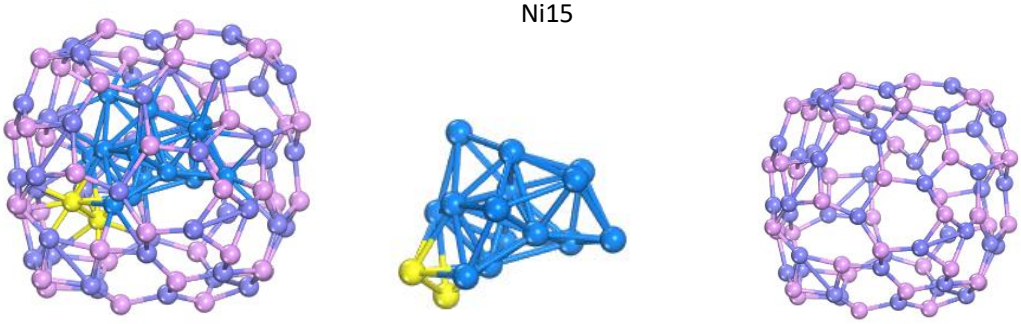

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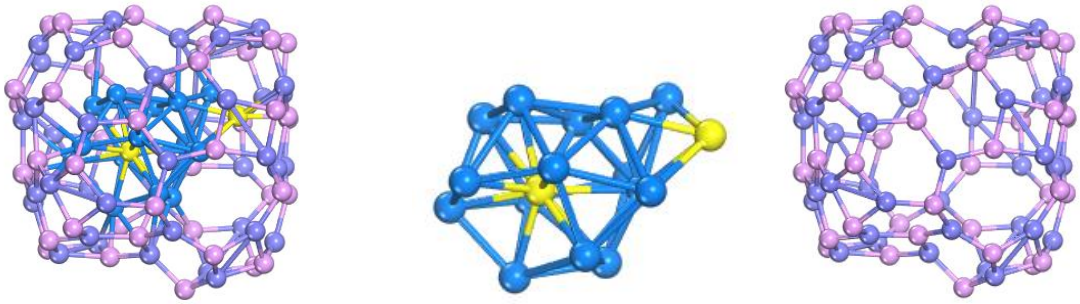

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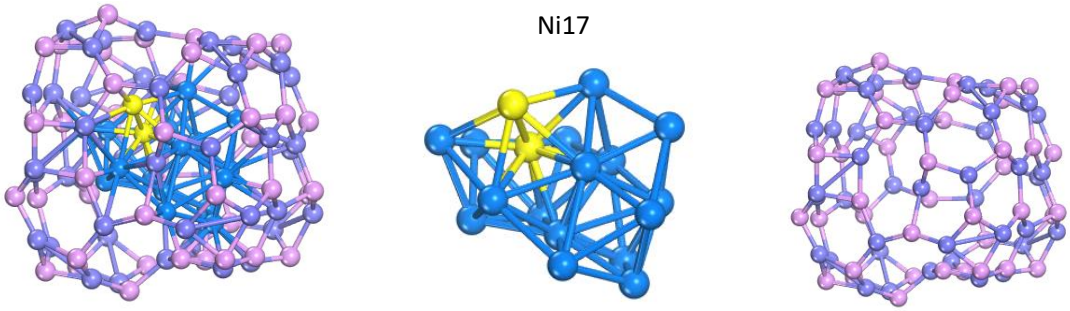
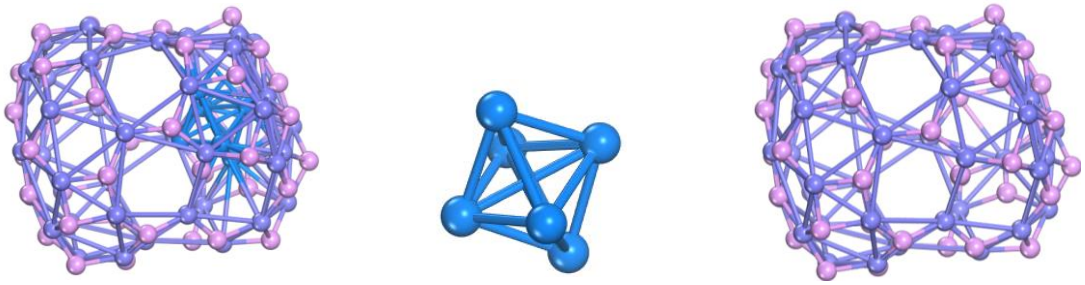


Ni18

4. Annealed $Fe_n@(ZnO)_{42}$



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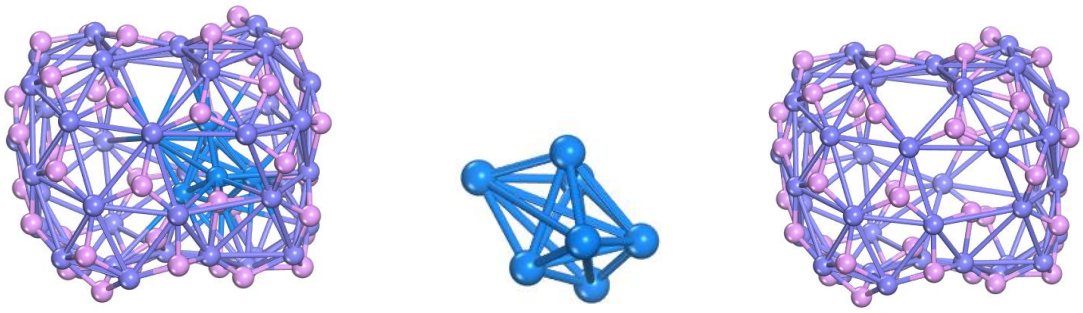
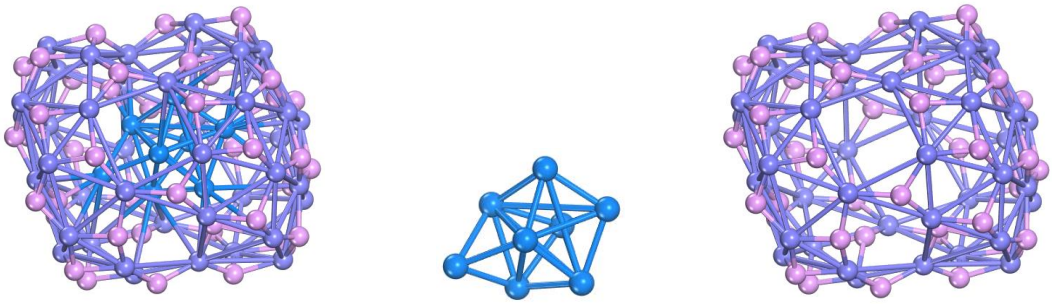
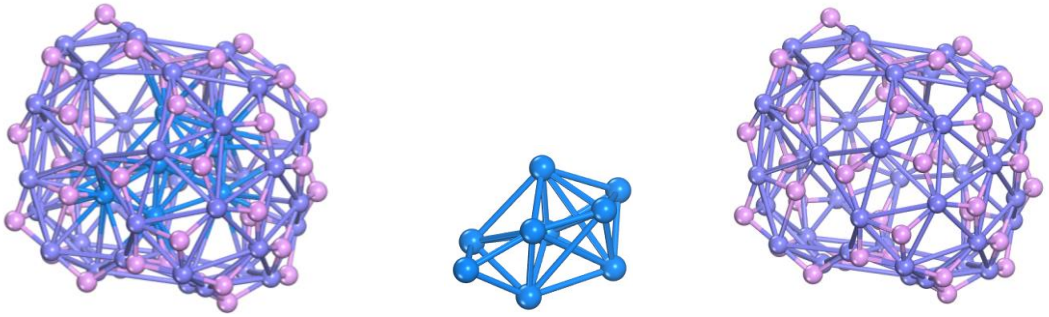


Fe7



Fe8



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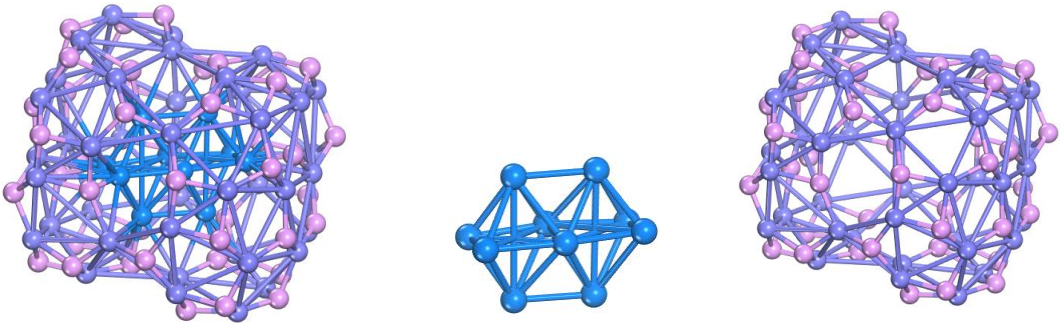

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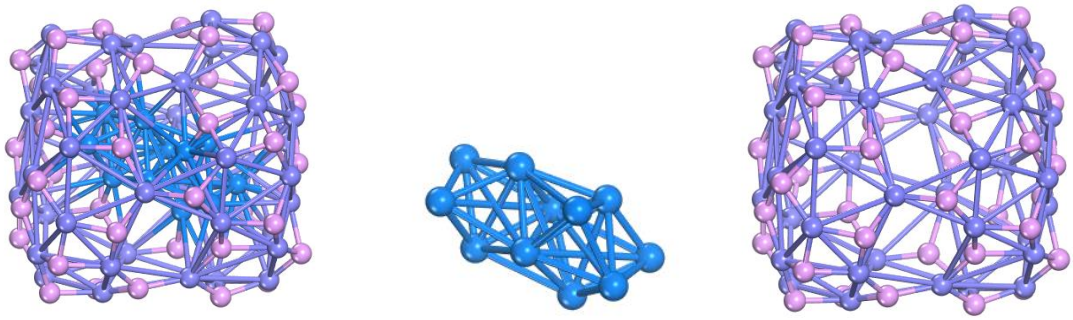

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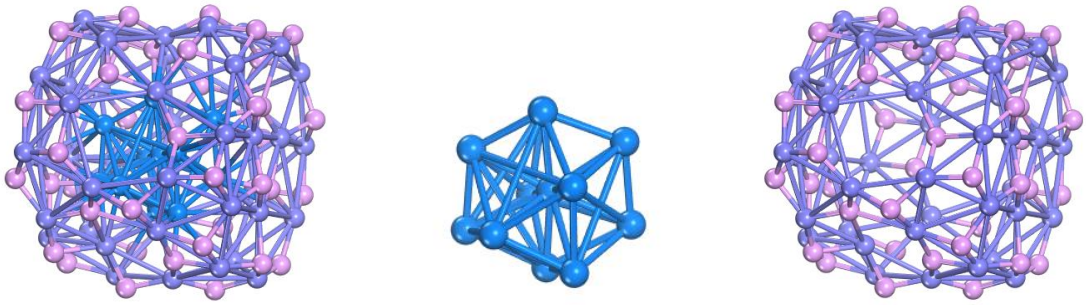
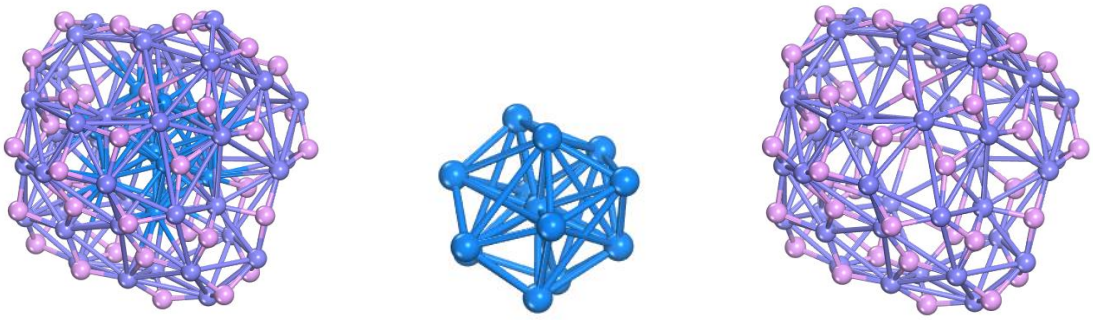
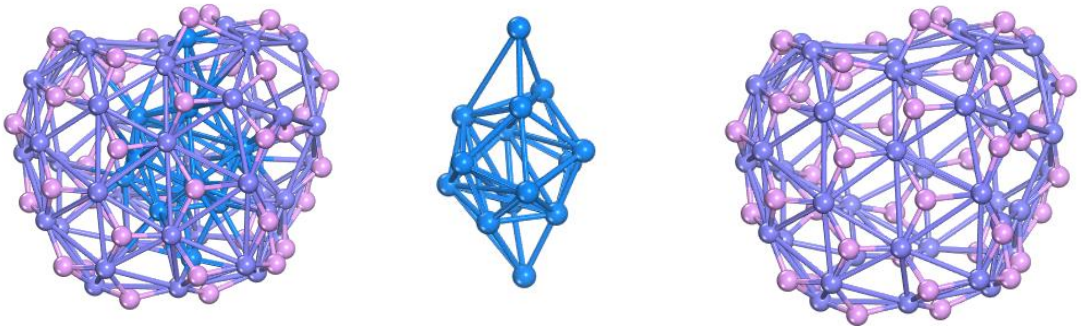


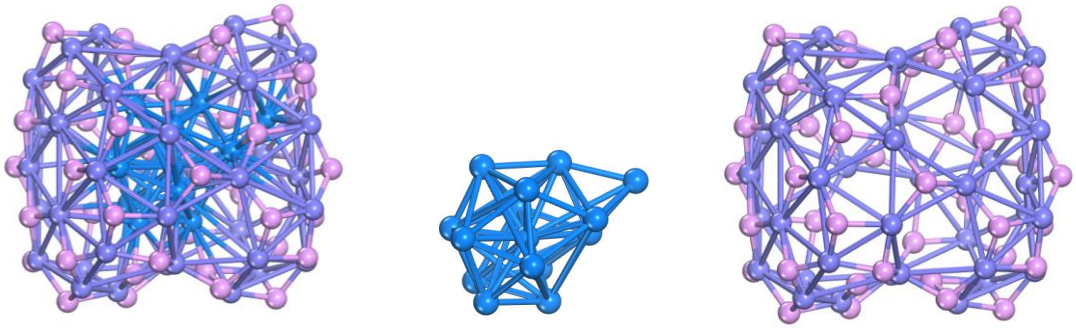
Fe12



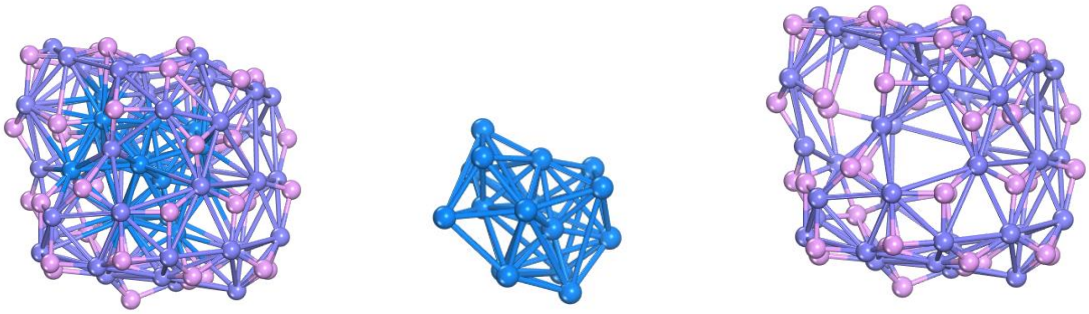
Fe13



Fe14



Fe15



Fe16

Supporting Information II: Electric Distribution and Coordination Number

The structural, magnetic and optical properties of $TM_n@(ZnO)_{42}$ (TM = Fe, Co and Ni) hetero-nanostructure

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This Supporting information II includes the detailed result of magnetic moment, charge transfer, coordination number and some related bond length. The result are displayed in table form.

1. Related information for magnetic analysis

	$Fe_{15}@(ZnO)_{42}$									
Number	Fe Charge Transfer (LSDA)	Fe Charge Transfer (LSDA+U)	Fe Magnetic Moment/μB (LSDA)	Fe Magnetic Moment/μB (LSDA+U)	O Charge Transfer (LSDA)	O Charge Transfer (LSDA+U)	O Magnetic Moment/μB (LSDA)	O Magnetic Moment/μB (LSDA+U)	Zn Charge Transfer (LSDA)	Zn Charge Transfer (LSDA+U)
1	-0.2779	-0.3179	2.676	3.143	0.0072	0.0086	0.004	0.001	0.0194	0.0241
2	0.0926	0.0810	2.603	2.884	0.0018	0.0030	-0.001	-0.006	0.0125	0.0198
3	-0.0445	-0.0501	2.710	2.976	0.0052	0.0081	0.034	0.008	0.0139	0.0171
4	-0.2108	-0.2826	2.619	3.020	0.0044	0.0070	0.045	0.012	0.0146	0.0169
5	0.1431	0.1855	1.996	2.718	0.0193	0.0182	-0.006	-0.012	0.2007	0.2106
6	-0.2029	-0.2449	2.616	3.079	0.0277	0.0268	0.013	-0.019	0.1766	0.1703
7	-0.2554	-0.3067	2.772	3.194	0.0089	0.0090	-0.007	-0.019	-0.0021	0.0049
8	-0.2273	-0.3291	2.332	3.073	0.0063	0.0082	0.001	-0.009	-0.0018	-5.00E-04
9	-0.3193	-0.3530	-2.176	3.093	-0.0166	-0.0015	0.035	0.025	0.1858	0.1959
10	-0.2649	-0.2994	2.778	3.174	0.0273	0.0342	-0.009	-0.020	0.1000	0.1087
11	0.0435	0.0611	2.784	3.058	-0.0378	-0.0284	0.077	0.044	-0.0029	9.00E-04
12	-0.3207	-0.3745	2.862	3.221	-0.0130	0.0027	0.057	0.041	0.0495	0.0583
13	0.0680	0.0541	2.340	2.996	6.00E-04	9.00E-04	1.50E-02	7.00E-03	-0.0049	4.00E-04
14	-0.2247	-0.3461	-0.767	3.093	0.0110	0.0117	-0.003	-0.005	0.0819	0.0824
15	-0.2009	-0.3048	2.577	3.123	0.0038	0.0080	0.017	-0.012	0.0249	0.0264
16	-2.2021	-0.188493333			0.0074	0.0083	0.000	-0.001	0.0148	0.0195
17					-0.0292	-0.0126	0.070	0.038	0.0040	0.0091
18					0.0148	0.0142	-0.004	-0.025	0.1998	0.2350
19					0.0065	0.0090	-0.004	-0.002	0.1218	0.1403
20					0.0051	0.0061	0.002	0.000	0.0208	0.0227
21					-0.0067	-0.0057	0.042	0.012	-0.0051	-0.0035
22					-0.0125	0.0029	0.052	0.024	0.1595	0.1732
23					0.0107	0.0105	0.002	-0.005	0.0131	0.0157
24					-0.0087	-0.0053	0.042	0.021	0.0190	0.0253
25					0.0193	0.0204	0.018	0.003	0.0741	0.0820
26					-0.0179	-6.00E-04	0.043	0.037	-0.0046	7.00E-04
27					0.0014	0.0028	0.001	0.003	0.0031	0.0077
28					0.0087	0.0091	0.006	-0.003	0.0556	0.0762
29					-0.0288	-0.0026	0.082	0.074	0.0028	0.0080
30					0.0110	0.0106	0.000	-0.003	0.0255	0.0230
31					-0.0428	0.0052	-0.064	0.075	0.2133	0.2855
32					0.0019	0.0058	0.001	0.002	0.0244	0.0249
33					0.0206	0.0614	-0.108	0.056	0.0188	0.0206
34					0.0055	0.0169	0.047	0.015	0.0113	0.0160
35					0.0034	0.0039	0.001	-0.003	-0.0160	-0.0142
36					0.0116	0.0133	0.022	0.002	0.0059	0.0090
37					0.0017	0.0018	0.003	0.000	-0.0055	-0.0060
38					0.0281	0.0278	0.011	-0.003	0.2330	0.3236
39					0.0390	0.0403	0.003	-0.001	0.0043	0.0041
40					0.0087	0.0084	0.004	0.006	0.0081	0.0081
41					0.0045	0.0044	0.003	-0.004	-5.00E-04	2.80E-03
42					0.0070	0.0058	0.000	0.001	0.0063	0.0034
					0.1264	0.009014286			2.0757	0.058307143

	$Co_{15}@(ZnO)_{42}$					$Ni_{13}@(ZnO)_{42}$				
Number	Co Charge Transfer	Co Magnetic Moment/μB	O Charge Transfer	O Magnetic Moment/μB	Zn Charge Transfer	Ni Charge Transfer	Ni Magnetic Moment/μB	O Charge Transfer	O Magnetic Moment/μB	Zn Charge Transfer
1	0.0045	1.861	0.0046	0.000	0.0057	-0.2049	0.750	0.0048	0.000	7.00E-04
2	-0.1379	1.704	0.0046	0.000	-9.00E-04	-0.1507	0.742	0.0049	0.001	0.0074
3	-0.2377	1.852	0.0045	-0.006	0.0039	0.2155	0.226	-0.0240	0.022	0.0073
4	-0.1892	1.745	0.0118	-0.005	0.0032	0.1263	0.664	0.0065	-0.005	-0.0085
5	-0.1871	1.790	0.0237	-0.007	0.1038	-0.1272	0.663	0.0156	-0.003	0.0659
6	-0.1772	1.792	0.0032	-0.008	0.1456	-0.1082	0.649	0.0068	-0.002	0.1302
7	-0.1319	1.700	0.0014	-0.001	0.0426	-0.1328	0.664	0.0044	-0.002	0.1118
8	0.2181	1.167	-0.0346	0.041	0.0059	-0.1046	0.651	0.0063	0.001	0.0051
9	-0.1834	1.802	-0.025	0.051	0.0137	0.1254	0.663	0.0146	-0.003	0.1016
10	0.0261	1.816	0.0032	-0.002	0.0176	-0.0987	0.655	-0.0026	0.009	0.0794
11	0.1668	1.701	-1.00E-04	1.00E-03	-0.0044	-0.1399	0.741	-0.0381	0.026	-0.0126
12	-0.2232	1.761	0.0042	-0.003	-0.0022	-0.0999	0.655	1.00E-03	-7.00E-03	0.0138
13	0.0577	1.798	0.004	-0.008	0.0086	-0.1983	0.750	0.0075	-0.006	-0.0094
14	-0.1803	1.785	-0.0405	0.059	0.0713	-0.8980		0.0059	-0.006	0.0139
15	-0.1895	1.800	0.018	-0.008	-0.0033			-0.0018	0.002	-0.0044
16	-1.3642		0.0013	-0.002	0.0144			-0.0284	0.012	3.00E-04

17			-0.0377	0.059	0.0228			0.0045	0.002	0.0771
18			0.0064	-0.008	0.0282			-0.0383	0.027	0.0403
19			-0.0299	0.036	0.118			-0.0018	0.009	-0.0024
20			0.0125	-0.020	0.1544			0.0061	-0.001	0.0056
21			0.0216	-0.011	-0.0085			0.0060	0.000	0.1186
22			0.0104	-0.002	0.1222			0.0069	0.002	-0.0217
23			0.0153	-0.012	0.0079			0.0158	-0.003	1.00E-04
24			-0.0284	0.037	0.0069			-0.0292	0.034	0.0656
25			0.0098	-0.015	0.1232			-0.0299	0.034	0.0019
26			0.0142	-0.015	1.00E-04			0.0060	0.002	-0.0222
27			0.0033	0.002	9.00E-04			0.0065	0.000	0.0063
28			-7.00E-04	6.00E-03	0.0115			0.0050	-0.001	-0.0019
29			0.0269	-0.002	0.0501			-0.0414	0.027	0.0420
30			-0.022	0.029	0.0041			0.0053	0.002	1.00E-03
31			0.0051	-0.002	0.0063			-0.0284	0.012	-0.0051
32			0.0089	-0.007	6.00E-04			-4.00E-04	2.00E-03	0.0147
33			0.0037	-0.002	-0.0029			-0.0410	0.026	-0.0118
34			0.0048	-0.007	0.0353			0.0128	-0.003	0.0142
35			-0.0248	0.039	0.0234			0.0063	0.001	-0.0117
36			-0.0464	0.054	-1.00E-03			9.00E-04	-7.00E-03	0.1019
37			0.0055	-0.004	0.2045			0.0052	-0.001	0.0054
38			0.0117	-0.008	0.0037			0.0073	-0.002	0.1131
39			-0.0231	0.046	0.0261			-0.0285	0.022	-0.0046
40			0.0096	-0.008	0.0249			0.0066	-0.005	0.0069
41			0.0037	-0.004	0.0057			0.0035	0.001	0.0073
42			0.0091	-0.001	0.0162			0.0055	0.000	2.00E-04
			-0.0462		1.4101			-0.1453		1.04E+00

2. Related information for optical properties

For charge transfer, negative value represents lossing electrons and positive value represents getting electrons

	$Co_{15}@(ZnO)_{42}$					$Fe_{13}@(ZnO)_{42}$					$Ni_{15}@(ZnO)_{42}$				
Number	Co Charge Transfer	Co Magnetic Moment/μB	O Charge Transfer	O Magnetic Moment/μB	Zn Charge Transfer	Fe Charge Transfer	Fe Magnetic Moment/μB	O Charge Transfer	O Magnetic Moment/μB	Zn Charge Transfer	Ni Charge Transfer	Ni Magnetic Moment/μB	O Charge Transfer	O Magnetic Moment/μB	Zn Charge Transfer
1	0.0045	1.861	0.0046	0.000	0.0057	-0.1998	2.758	0.0341	-0.006	0.003	0.0642	0.563	0.0024	0.000	0.0029
2	-0.1379	1.704	0.0046	0.000	-9.00E-04	-0.1645	2.619	0.0059	0.002	0.3526	-0.0893	0.507	0.0021	0.000	0.0026
3	-0.2377	1.852	0.0045	-0.006	0.0039	-0.3036	2.748	-0.0022	0.041	5.00E-04	-0.1483	0.713	9.00E-04	-0.003	-0.0038
4	-0.1892	1.745	0.0118	-0.005	0.0032	-0.2066	2.815	0.0148	0.056	0.0037	0.1607	0.439	5.00E-04	-0.004	-0.0082
5	-0.1871	1.790	0.0237	-0.007	0.1038	-0.2185	2.563	0.0485	0.004	0.0434	-0.1025	0.511	0.0169	-0.001	0.1580
6	-0.1772	1.792	0.0032	-0.008	0.1456	-0.2782	2.813	0.0077	0.002	0.0390	-0.1351	0.511	6.00E-04	-0.001	0.0495
7	-0.1319	1.700	0.0014	-0.001	0.0426	0.2096	1.537	0.0082	-0.001	0.0168	-0.0427	0.381	-0.0420	0.024	0.0034
8	0.2181	1.167	-0.0346	0.041	0.0059	-0.2061	2.665	0.0105	-0.001	0.0611	-0.1372	0.557	0.0013	-0.002	0.0171
9	-0.1834	1.802	-0.0250	0.051	0.0137	-0.2718	2.786	0.0125	-0.001	0.0734	0.0491	0.580	0.0022	-0.002	0.0054
10	0.0261	1.816	0.0032	-0.002	0.0176	-0.2146	2.459	0.0157	0.027	0.0116	-0.0962	0.574	0.0025	-0.001	-0.0044
11	0.1668	1.701	-1.00E-04	1.00E-03	-0.0044	-0.2106	2.770	-0.0249	0.058	0.1044	-0.0944	0.517	0.0083	-0.001	0.0326
12	-0.2232	1.761	0.0042	-0.003	-0.0022	-0.2507	2.816	0.0124	-0.002	0.0038	0.0908	0.618	-0.0385	0.032	0.0089
13	0.0577	1.798	0.0040	-0.008	0.0086	-0.1983	2.544	0.0045	0.001	0.0064	-0.0567	0.423	-0.0366	0.003	0.0719
14	-0.1803	1.785	-0.0405	0.059	0.0713			-0.0065	0.034	0.1252	-0.0993	0.594	0.0028	-0.008	0.0062
15	-0.1895	1.800	0.0180	-0.008	-0.0033			0.0114	0.001	-0.0022	0.0691	0.623	0.0011	-0.002	0.0101
16			0.0013	-0.002	0.0144			0.0119	0.002	0.0086			-0.0633	0.001	0.0230
17			-0.0377	0.059	0.0228			0.0366	-0.005	0.0094			0.0050	-0.003	-0.0047
18			0.0064	-0.008	0.0282			0.0244	0.032	0.3647			-0.0435	0.010	0.0720
19			-0.0299	0.036	0.1189			-0.0211	0.064	0.0647			0.0076	-0.009	0.0718
20			0.0125	-0.020	0.1544			0.0079	-0.009	0.0151			0.0074	-0.005	-0.0094
21			0.0216	-0.011	-0.0085			-5.00E-04	0.000	0.0113			0.0047	-0.002	0.0923
22			0.0104	-0.002	0.1222			-9.00E-04	0.005	0.1381			0.0113	-0.007	0.0091
23			0.0153	-0.012	0.0079			0.0070	-0.003	-0.0058			-0.0534	0.020	-0.0127
24			-0.0284	0.037	0.0069			0.0120	0.007	0.0027			0.0149	-0.001	0.0343
25			0.0098	-0.015	0.1232			0.0053	-0.006	0.0254			0.0119	-0.006	0.0068
26			0.0142	-0.015	1.00E-04			0.0033	0.039	0.0210			0.0230	0.000	-0.0243
27			0.0033	0.002	9.00E-04			-0.0082	0.046	0.0142			0.0061	-0.001	0.0072
28			-7.00E-04	6.00E-03	0.0115			0.0057	0.003	0.0561			0.0104	-0.003	0.0558
29			0.0269	-0.002	0.0501			0.0102	-0.002	0.0161			-0.0693	0.016	-0.0137
30			-0.0220	0.029	0.0041			0.0095	-0.003	0.0101			0.0073	0.000	0.0238
31			0.0051	-0.002	0.0063			0.0024	0.071	0.3247			-0.0644	0.008	0.0285
32			0.0089	-0.007	6.00E-04			0.0046	0.003	-0.0148			0.0051	-0.002	0.0039
33			0.0037	-0.002	-0.0029			-0.0078	0.040	0.0046			-0.0683	0.027	0.0377
34			0.0048	-0.007	0.0353			0.0245	-0.006	0.0055			0.0093	-0.004	0.0067
35			-0.0248	0.039	0.0234			0.0064	0.001	0.0197			0.0021	-0.003	0.0013
36			-0.0464	0.054	-1.00E-03			0.0246	-0.017	0.1270			-0.0364	0.006	0.0389
37			0.0055	-0.004	0.2045			0.0042	0.007	0.0072			0.0055	-0.004	0.0020
38			0.0117	-0.008	0.0037			0.0070	-0.002	0.0782			0.0093	-0.006	0.0589
39			-0.0231	0.046	0.0261			-0.0174	0.039	0.0038			0.0075	-0.008	0.0017
40			0.0096	-0.008	0.0249			0.0072	0.001	0.0201			0.0118	-0.003	0.0064
41			0.0037	-0.004	0.0057			0.0120	0.004	0.0056			0.0048	0.000	-0.0013
42			0.0091	-0.001	0.0162			0.0018	0.000	0.0121			0.0050	-0.001	0.0041
Total	-1.3642	26.074	-0.0462	0.282	1.4101	-2.5137	33.893	0.3252	0.526	2.1881	-0.5678	8.111	-0.3041	0.054	0.8723

It can be seen from this table that :

1) For $Co_{15}@ZnO_{42}$: Co loss electrons and the charges transfer to Zn. At the same time, O loss only a very small part of electrons, indicating that, with the introducing of Co atoms, the interaction between Co and Zn increase and the interaction between Zn and O decrease

2) For $Fe_{13}@ZnO_{42}$: Fe loss electrons. Most of the charges transfer to Zn and small part of electrons transfer to O. The interaction between Zn and O decrease.

3) For $Ni_{15}@ZnO_{42}$: A lot of electrons transfer to Zn from O. Compared with the case of Co and Fe, here the mount of electrons transfer to Zn from Ni is the smallest. So the interaction between Zn and O is much stronger in this case.

3. Coordination Number

$Co_{15}@(ZnO)_{42}$				$Fe_{15}@(ZnO)_{42}$				$Ni_{13}@(ZnO)_{42}$			
Atom1	Atom2	bond-length	coordination number	Atom1	Atom2	bond-length	coordination number	Atom1	Atom2	bond-length	coordination number
Co1	Co8	2.2585	7	Fe1	Fe4	2.3893	6	Ni1	Ni3	2.4549	6
	Co6	2.3671			Fe2	2.4290			Ni4	2.4682	
	Co7	2.4143			Fe3	2.4544			Ni5	2.4783	
	Co10	2.4768			Fe7	2.5451			Ni10	2.5122	
	Co2	2.5097			Fe5	2.5480			Ni8	2.5398	
	Co3	2.5345			Fe6	2.8609			Ni2	2.7532	
	Co4	2.6438		average-length		2.53778333		average-length		2.534433333	
average-length		2.457814286		Fe2	Fe5	2.2642	6	Ni2	Ni3	2.4485	6
Co2	Co14	2.3695	6		Fe1	2.4290			Ni4	2.4702	
	Co13	2.4350			Fe9	2.4992			Ni8	2.5134	
	Co8	2.4615			Fe7	2.5771			Ni12	2.5136	
	Co6	2.4667			Fe8	2.5963			Ni7	2.5441	
	Co4	2.4943			Fe3	2.6519			Ni1	2.7532	
	Co1	2.5097		average-length		2.50295		average-length		2.5405	
average-length		2.456116667		Fe3	Fe8	2.2564	6	Ni3	Ni4	2.3001	12
Co3	Co10	2.2490	5		Fe6	2.3295			Ni9	2.3017	
	Co4	2.3536			Fe1	2.4544			Ni10	2.3932	
	Co5	2.4177			Fe5	2.5277			Ni12	2.3936	
	Co1	2.5345			Fe2	2.6519			Ni8	2.4120	
	Co8	2.6136			Fe10	2.8701			Ni6	2.4147	
average-length		2.43368		average-length		2.515			Ni5	2.4428	
Co4	Co3	2.3536	6	Fe4	Fe1	2.3893	6		Ni7	2.4433	
	Co13	2.4071			Fe6	2.4317			Ni11	2.4470	
	Co5	2.4822			Fe15	2.4430			Ni2	2.4485	
	Co2	2.4943			Fe5	2.4746			Ni1	2.4549	
	Co8	2.5008			Fe11	2.5642			Ni13	2.4552	
	Co1	2.6438			Fe7	2.7598		average-length		2.408916667	
average-length		2.4803		average-length		2.51043333		Ni4	Ni3	2.3001	6
Co5	Co15	2.3685	6	Fe5	Fe2	2.2642	13		Ni12	2.4261	
	Co11	2.3773			Fe12	2.3673			Ni1	2.4682	
	Co3	2.4177			Fe11	2.4644			Ni5	2.4702	
	Co8	2.4761			Fe4	2.4746			Ni2	2.4702	
	Co4	2.4822			Fe10	2.5049			Ni6	2.6296	
	Co13	2.5596			Fe13	2.5254		average-length		2.460733333	
average-length		2.4469			Fe3	2.5277		Ni5	Ni3	2.4428	6
Co6	Co1	2.3671	6		Fe1	2.5480			Ni4	2.4702	
	Co7	2.3709			Fe6	2.5705			Ni1	2.4783	
	Co2	2.4667			Fe7	2.6108			Ni11	2.5458	
	Co14	2.4695			Fe15	2.6292			Ni6	2.5638	
	Co8	2.4833			Fe8	2.6618			Ni10	2.6754	
	Co9	2.6215			Fe9	2.6777		average-length		2.529383333	
average-length		2.463166667		average-length		2.52511538		Ni6	Ni3	2.4147	6
Co7	Co10	2.2748	4	Fe6	Fe3	2.3295	6		Ni12	2.4867	
	Co6	2.3709			Fe11	2.4189			Ni11	2.5132	
	Co1	2.4143			Fe4	2.4317			Ni13	2.5397	
	Co9	2.4590			Fe5	2.5705			Ni5	2.5638	
average-length		2.37975			Fe10	2.6066			Ni4	2.6296	
Co8	Co1	2.2585	13		Fe1	2.8609		average-length		2.524616667	
	Co11	2.2801		average-length		2.53635		Ni7	Ni3	2.4433	6
	Co13	2.3067		Fe7	Fe13	2.4375	7		Ni9	2.4723	
	Co14	2.4255			Fe14	2.4918			Ni13	2.4803	
	Co10	2.4262			Fe1	2.5451			Ni2	2.5441	
	Co2	2.4615			Fe2	2.5771			Ni8	2.5622	
	Co5	2.4761			Fe5	2.6108			Ni12	2.6654	
	Co12	2.4790			Fe4	2.7598		average-length		2.527933333	
	Co6	2.4833			Fe15	2.8131		Ni8	Ni3	2.4120	6
	Co4	2.5008		average-length		2.60502857			Ni10	2.4852	
	Co9	2.5463		Fe8	Fe3	2.2564	5		Ni2	2.5134	
	Co3	2.6136			Fe9	2.3254			Ni1	2.5398	
	Co15	2.7733			Fe10	2.5062			Ni7	2.5622	
average-length		2.463915385			Fe2	2.5963			Ni9	2.6247	
Co9	Co10	2.2815	6		Fe5	2.6618		average-length		2.522883333	
	Co12	2.3078		average-length		2.46922		Ni9	Ni3	2.3017	6
	Co7	2.4590		Fe9	Fe13	2.2915	5		Ni10	2.4225	
	Co8	2.5463			Fe8	2.3254			Ni13	2.4616	

	Co11	2.6037			Fe2	2.4992			Ni7	2.4723	
	Co6	2.6215			Fe5	2.6777			Ni11	2.4741	
average-length		2.469966667			Fe12	2.7466			Ni8	2.6247	
Co10	Co3	2.2490	6	average-length		2.50808		average-length		2.459483333	
	Co7	2.2748		Fe10	Fe11	2.4889	6	Ni10	Ni3	2.3932	6
	Co9	2.2815			Fe12	2.4997			Ni9	2.4225	
	Co8	2.4262			Fe5	2.5049			Ni8	2.4852	
	Co11	2.4325			Fe8	2.5062			Ni1	2.5122	
	Co1	2.4768			Fe6	2.6066			Ni11	2.5144	
average-length		2.3568			Fe3	2.8701			Ni5	2.6754	
Co11	Co8	2.2801	6	average-length		2.5794		average-length		2.500483333	
	Co5	2.3773		Fe11	Fe6	2.4189	6	Ni11	Ni3	2.4470	6
	Co12	2.4226			Fe15	2.4400			Ni9	2.4741	
	Co10	2.4325			Fe12	2.4642			Ni6	2.5132	
	Co15	2.5693			Fe5	2.4644			Ni10	2.5144	
	Co9	2.6037			Fe10	2.4889			Ni5	2.5458	
average-length		2.447583333			Fe4	2.5642			Ni13	2.7429	
Co12	Co15	2.3011	5	average-length		2.47343333		average-length		2.539566667	
	Co9	2.3078		Fe12	Fe5	2.3673	6	Ni12	Ni3	2.3936	6
	Co14	2.3826			Fe11	2.4642			Ni4	2.4261	
	Co11	2.4226			Fe10	2.4997			Ni6	2.4867	
	Co8	2.4790			Fe13	2.6182			Ni2	2.5136	
average-length		2.37862			Fe9	2.7466			Ni13	2.5181	
Co13	Co15	2.2507	6		Fe15	2.7717			Ni7	2.6654	
	Co8	2.3067		average-length		2.57795		average-length		2.500583333	
	Co4	2.4071		Fe13	Fe14	2.2202	6	Ni13	Ni3	2.4552	6
	Co14	2.4176			Fe9	2.2915			Ni9	2.4616	
	Co2	2.4350			Fe7	2.4375			Ni7	2.4803	
	Co5	2.5596			Fe5	2.5254			Ni12	2.5181	
average-length		2.396116667			Fe15	2.5408			Ni6	2.5397	
Co14	Co2	2.3695	5		Fe12	2.6182			Ni11	2.7429	
	Co12	2.3826		average-length		2.43893333		average-length		2.532966667	
	Co13	2.4176		Fe14	Fe13	2.2202	3				
	Co8	2.4255			Fe15	2.4614					
	Co6	2.4695			Fe7	2.4918					
average-length		2.41294		average-length		2.39113333					
Co15	Co13	2.2507	5	Fe15	Fe11	2.4400	7				
	Co12	2.3011			Fe4	2.4430					
	Co5	2.3685			Fe14	2.4614					
	Co11	2.5693			Fe13	2.5408					
	Co8	2.7733			Fe5	2.6292					
average-length		2.45258			Fe12	2.7717					
					Fe7	2.8131					
				average-length		2.5856					

Supporting Information III: Bond length of TM@ZnO

The structural, magnetic and optical properties of $TM_n@(ZnO)_{42}$ (TM = Fe, Co and Ni) hetero-nanostructure

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This Supporting information I includes the detailed result of bond length. The results are displayed in table form.

1. Bond Length information of $Fe_n@ZnO_{42}$

$Fe_6@(ZnO)_{42}$				$Fe_7@(ZnO)_{42}$				$Fe_8@(ZnO)_{42}$				$Fe_9@(ZnO)_{42}$				$Fe_{10}@(ZnO)_{42}$				$Fe_{11}@(ZnO)_{42}$				$Fe_{12}@(ZnO)_{42}$				$Fe_{13}@(ZnO)_{42}$				$Fe_{14}@(ZnO)_{42}$				$Fe_{15}@(ZnO)_{42}$				$Fe_{16}@(ZnO)_{42}$			
Number	Atom1	Atom2	Length	Number	Atom1	Atom2	Length	Number	Atom1	Atom2	Length	Number	Atom1	Atom2	Length	Number	Atom1	Atom2	Length	Number	Atom1	Atom2	Length	Number	Atom1	Atom2	Length	Number	Atom1	Atom2	Length	Number	Atom1	Atom2	Length	Number	Atom1	Atom2	Length	Number	Atom1	Atom2	Length
1	Fe1	Fe2	2.2967	1	Fe1	Fe2	2.3917	1	Fe1	Fe2	2.3692	1	Fe1	Fe2	2.3940	1	Fe1	Fe2	2.7955	1	Fe1	Fe2	2.4574	1	Fe1	Fe2	2.5667	1	Fe1	Fe3	2.4834	1	Fe1	Fe2	2.4239	1	Fe1	Fe2	2.4290	1	Fe1	Fe2	2.3747
2	Fe1	Fe3	2.5269	2	Fe1	Fe4	2.4380	2	Fe1	Fe3	2.5182	2	Fe1	Fe3	2.5375	2	Fe1	Fe3	2.7059	2	Fe1	Fe3	2.4386	2	Fe1	Fe3	2.4503	2	Fe1	Fe4	2.8531	2	Fe1	Fe4	2.3310	2	Fe1	Fe3	2.4544	2	Fe1	Fe3	2.4732
3	Fe1	Fe4	2.4935	3	Fe1	Fe6	2.3537	3	Fe1	Fe6	2.7262	3	Fe1	Fe4	2.4100	3	Fe1	Fe4	2.4200	3	Fe1	Fe4	2.7767	3	Fe1	Fe4	2.4621	3	Fe1	Fe5	2.4225	3	Fe1	Fe7	2.4915	3	Fe1	Fe4	2.3893	3	Fe1	Fe4	2.4318
4	Fe1	Fe5	2.3500	4	Fe2	Fe3	2.3168	4	Fe1	Fe7	2.5213	4	Fe1	Fe5	2.5565	4	Fe1	Fe5	2.8382	4	Fe1	Fe5	2.6443	4	Fe1	Fe6	2.4408	4	Fe1	Fe7	2.4348	4	Fe1	Fe8	2.3665	4	Fe1	Fe5	2.5480	4	Fe1	Fe5	2.8509
5	Fe2	Fe3	2.3043	5	Fe2	Fe4	2.4029	5	Fe1	Fe8	2.3165	5	Fe1	Fe6	2.4211	5	Fe1	Fe6	2.6503	5	Fe1	Fe6	2.4154	5	Fe2	Fe3	2.2657	5	Fe1	Fe8	2.4484	5	Fe1	Fe10	2.5690	5	Fe1	Fe6	2.8609	5	Fe1	Fe9	2.4392
6	Fe2	Fe4	2.2869	6	Fe2	Fe6	2.8223	6	Fe2	Fe3	2.5294	6	Fe1	Fe7	2.6579	6	Fe1	Fe8	2.3056	6	Fe1	Fe8	2.3046	6	Fe2	Fe4	2.4238	6	Fe1	Fe9	2.9846	6	Fe2	Fe3	2.6019	6	Fe1	Fe7	2.5451	6	Fe2	Fe3	2.9923
7	Fe2	Fe5	2.9573	7	Fe2	Fe7	2.6856	7	Fe2	Fe4	2.3091	7	Fe1	Fe8	2.5141	7	Fe1	Fe9	2.3992	7	Fe1	Fe9	2.5142	7	Fe2	Fe5	2.9354	7	Fe2	Fe3	2.4932	7	Fe2	Fe4	2.4696	7	Fe2	Fe3	2.6519	7	Fe2	Fe5	2.3621
8	Fe2	Fe6	2.3563	8	Fe3	Fe4	2.9526	8	Fe2	Fe5	2.6928	8	Fe2	Fe3	2.4259	8	Fe2	Fe3	2.5298	8	Fe1	Fe11	2.7030	8	Fe2	Fe10	2.4679	8	Fe2	Fe4	2.4091	8	Fe2	Fe6	2.4364	8	Fe2	Fe5	2.2642	8	Fe2	Fe6	2.3955
9	Fe3	Fe5	2.5533	9	Fe3	Fe5	2.3302	9	Fe2	Fe6	2.3465	9	Fe2	Fe7	2.3134	9	Fe2	Fe8	2.4393	9	Fe2	Fe3	2.8829	9	Fe2	Fe11	2.4090	9	Fe2	Fe7	2.6831	9	Fe2	Fe7	2.5560	9	Fe2	Fe7	2.5771	9	Fe2	Fe8	2.5264
10	Fe3	Fe6	2.4971	10	Fe3	Fe6	2.3159	10	Fe2	Fe7	2.6617	10	Fe2	Fe8	2.3086	10	Fe2	Fe9	2.4067	10	Fe2	Fe4	2.3663	10	Fe3	Fe4	2.5278	10	Fe2	Fe11	2.4354	10	Fe2	Fe13	2.4065	10	Fe2	Fe8	2.5963	10	Fe2	Fe9	2.7575
11	Fe4	Fe5	2.393	11	Fe3	Fe7	2.3137	11	Fe3	Fe4	2.3999	11	Fe2	Fe9	2.4205	11	Fe2	Fe10	2.4389	11	Fe2	Fe9	2.4165	11	Fe3	Fe5	2.3561	11	Fe2	Fe12	2.3993	11	Fe3	Fe4	2.5081	11	Fe2	Fe9	2.4992	11	Fe2	Fe13	2.4832
12	Fe4	Fe6	2.8084	12	Fe4	Fe5	2.2956	12	Fe3	Fe7	2.319	12	Fe3	Fe4	2.4288	12	Fe3	Fe4	2.4473	12	Fe2	Fe10	2.3011	12	Fe3	Fe6	2.4147	12	Fe3	Fe7	2.3610	12	Fe3	Fe6	2.8856	12	Fe2	Fe13	3.0486	12	Fe2	Fe15	2.6572
13	Fe5	Fe6	2.2696	13	Fe4	Fe6	2.5191	13	Fe4	Fe5	2.3229	13	Fe3	Fe5	2.5191	13	Fe3	Fe7	2.5377	13	Fe2	Fe11	2.9305	13	Fe3	Fe7	2.4734	13	Fe3	Fe8	2.5923	13	Fe4	Fe5	2.6307	13	Fe3	Fe5	2.5277	13	Fe3	Fe4	2.6788
average bond length			2.468715	14	Fe4	Fe7	2.4715	14	Fe4	Fe7	2.8033	14	Fe3	Fe7	2.6751	14	Fe3	Fe8	2.4040	14	Fe3	Fe4	2.3520	14	Fe3	Fe8	2.6956	14	Fe3	Fe12	2.4898	14	Fe4	Fe6	2.3502	14	Fe3	Fe6	2.3295	14	Fe3	Fe5	2.3414
				15	Fe5	Fe6	2.5148	15	Fe5	Fe6	2.4723	15	Fe4	Fe5	2.2919	15	Fe4	Fe5	2.3611	15	Fe3	Fe5	2.4284	15	Fe3	Fe9	2.2820	15	Fe4	Fe5	2.4023	15	Fe4	Fe10	2.3614	15	Fe3	Fe8	2.2564	15	Fe3	Fe13	2.366
				16	Fe5	Fe7	2.4684	16	Fe5	Fe6	2.5590	16	Fe4	Fe7	2.3292	16	Fe4	Fe7	2.3874	16	Fe3	Fe7	2.4233	16	Fe3	Fe10	2.4233	16	Fe4	Fe7	2.3845	16	Fe5	Fe6	2.5745	16	Fe3	Fe10	2.8701	16	Fe3	Fe14	2.6497
				average bond length			2.47455	17	Fe6	Fe7	2.5131	17	Fe5	Fe7	2.3186	17	Fe4	Fe8	2.9283	17	Fe3	Fe8	2.9482	17	Fe3	Fe11	2.7054	17	Fe4	Fe11	2.5494	17	Fe5	Fe10	2.3909	17	Fe4	Fe5	2.4746	17	Fe4	Fe5	2.3664
								18	Fe6	Fe8	2.4454	18	Fe6	Fe7	2.3484	18	Fe5	Fe6	2.4226	18	Fe4	Fe7	2.7165	18	Fe3	Fe12	2.5035	18	Fe5	Fe6	2.4426	18	Fe5	Fe12	2.4086	18	Fe4	Fe6	2.4317	18	Fe4	Fe9	2.4459
								19	Fe7	Fe8	2.4581	19	Fe6	Fe8	2.4343	19	Fe5	Fe7	2.5961	19	Fe4	Fe8	2.4647	19	Fe4	Fe5	2.5402	19	Fe5	Fe7	2.6197	19	Fe5	Fe14	2.6157	19	Fe4	Fe7	2.7598	19	Fe4	Fe11	3.0864
								average bond length			2.475863	20	Fe7	Fe8	2.5747	20	Fe5	Fe8	2.4229	20	Fe4	Fe10	2.9440	20	Fe4	Fe8	2.5333	20	Fe5	Fe9	2.4795	20	Fe6	Fe13	2.4851	20	Fe4	Fe11	2.5642	20	Fe5	Fe8	2.4686
												21	Fe7	Fe9	2.3833	21	Fe6	Fe8	2.4089	21	Fe4	Fe11	2.3223	21	Fe5	Fe8	2.5835	21	Fe6	Fe7	2.3838	21	Fe6	Fe14	2.3385	21	Fe4	Fe15	2.4430	21	Fe5	Fe9	2.3999
												22	Fe8	Fe9	2.5519	22	Fe6	Fe9	2.4324	22	Fe5	Fe7	2.4892	22	Fe5	Fe11	2.4895	22	Fe6	Fe9	2.5413	22	Fe7	Fe8	2.5333	22	Fe5	Fe6	2.5705	22	Fe5	Fe11	2.3321
												average bond length			2.456573	23	Fe6	Fe10	2.8813	23	Fe5	Fe8	2.3298	23	Fe5	Fe12	2.7828	23	Fe6	Fe11	2.6065	23	Fe7	Fe9	2.4146	23	Fe5	Fe7	2.6108	23	Fe5	Fe13	2.7708
																24	Fe7	Fe8	2.4349	24	Fe6	Fe8	2.7075	24	Fe6	Fe8	2.4667	24	Fe6	Fe13	2.5671	24	Fe7	Fe13	2.4623	24	Fe5	Fe8	2.6618	24	Fe5	Fe14	2.2687
																25	Fe8	Fe9	2.8857	25	Fe6	Fe9	2.5473	25	Fe6	Fe9	2.5314	25	Fe7	Fe8	2.5315	25	Fe8	Fe9	2.5838	25	Fe5	Fe9	2.6777	25	Fe5	Fe15	2.6208
																26	Fe8	Fe10	2.4314	26	Fe6	Fe11	2.3136	26	Fe7	Fe9	2.4303	26	Fe7	Fe9	2.4794	26	Fe8	Fe10	2.4648	26	Fe5	Fe10	2.5049	26	Fe5	Fe16	2.5228
																27	Fe9	Fe10	2.3018	27	Fe7	Fe8	2.4009	27	Fe7	Fe10	2.5410	27	Fe7	Fe10	2.4239	27	Fe8	Fe11	2.5868	27	Fe5	Fe11	2.4644	27	Fe6	Fe7	2.4144
																average bond length			2.524259	28	Fe8	Fe11	2.4839	28	Fe7	Fe12	2.4911	28	Fe7	Fe11	2.5137	28	Fe8	Fe12	2.3262	28	Fe5	Fe12	2.3673	28	Fe6	Fe8	2.3953
																				29	Fe9	Fe10	2.5843	29	Fe8	Fe9	2.4419	29	Fe7	Fe12	2.4081	29	Fe9	Fe11	2.6280	29	Fe5	Fe13	2.5254	29	Fe7	Fe8	2.6142
																				30	Fe9	Fe11	2.5091	30	Fe9	Fe12	2.4306	30	Fe7	Fe13	2.5817	30	Fe9	Fe12	2.3946	30	Fe5	Fe15	2.6292	30	Fe7	Fe9	2.3726
																				31	Fe10	Fe11	2.3129	31	Fe10	Fe11	2.4306	31	Fe8	Fe9	2.4310	31	Fe9	Fe13	2.5196	31	Fe6	Fe10	2.6066	31	Fe7	Fe12	2.3591
																				average bond length			2.528823	32	Fe10	Fe12	3.0398	32	Fe8	Fe10	2.4175	32	Fe9	Fe14	2.3074	32	Fe6	Fe11	2.4189	32	Fe8	Fe9	2.5147
																								33	Fe11	Fe12	2.3564	33	Fe9	Fe10	2.4961	33	Fe10	Fe12	2.5248	33	Fe7	Fe13	2.4375	33	Fe8	Fe10	2.3723
																								average bond length			2.511897	34	Fe10	Fe12	2.8468	34	Fe11	Fe12	2.4306	34	Fe7	Fe14	2.4917	34	Fe8	Fe11	2.6278
																												35	Fe10	Fe13	2.2856	35	Fe12	Fe14	2.5117	35	Fe7	Fe15	2.8131	35	Fe8	Fe12	2.5528
																												36	Fe11	Fe12	2.8991	36	Fe13	Fe14	2.4981	36	Fe8	Fe9	2.3254	36	Fe8	Fe15	2.4529
																												37	Fe11	Fe13	2.3464	average bond length			2.483006	37	Fe8	Fe10	2.5062	37	Fe8	Fe16	2.8200
																												38	Fe12	Fe13	2.4992					38	Fe9	Fe12	2.7466	38	Fe9	Fe11	2.5966
																												average bond length			2.516492					39	Fe9	Fe13	2.2915	39	Fe9	Fe12	2.4694
																																				40	Fe10	Fe11	2.4889	40	Fe10	Fe11	2.6186
																																				41	Fe10	Fe12	2.4997	41	Fe10	Fe12	2.4748
																																				42	Fe11	Fe12	2.4642	42	Fe10	Fe16	2.8125
																																				43	Fe11	Fe15	2.4400	43	Fe11	Fe12	2.3787
																																				44	Fe12	Fe13	2.6182	44	Fe11	Fe16	2.4607
																																				45	Fe12	Fe15	2.7717	45	Fe13	Fe14	2.3872
																																				46	Fe13	Fe14	2.2202	46	Fe13	Fe15	2.2940
																																				47	Fe13	Fe15	2.5408	47	Fe14	Fe15	2.7320
																																				48	Fe14	Fe15	2.4614	48	Fe14	Fe16	2.4936
																																				average bond length			2.534908	49	Fe15	Fe16	2.4086
																																							average bond length			2.524186

2. Bond Length information of $Co_n@ZnO_{42}$

$Co_6@(ZnO)_{42}$			$Co_7@(ZnO)_{42}$			$Co_8@(ZnO)_{42}$			$Co_9@(ZnO)_{42}$			$Co_{10}@(ZnO)_{42}$			$Co_{11}@(ZnO)_{42}$			$Co_{12}@(ZnO)_{42}$			$Co_{13}@(ZnO)_{42}$			$Co_{14}@(ZnO)_{42}$			$Co_{15}@(ZnO)_{42}$			$Co_{16}@(ZnO)_{42}$			$Co_{17}@(ZnO)_{42}$			$Co_{18}@(ZnO)_{42}$		
Atom1	Atom2	Length	Atom1	Atom2	Length	Atom1	Atom2	Length	Atom1	Atom2	Length	Atom1	Atom2	Length	Atom1	Atom2	Length	Atom1	Atom2	Length	Atom1	Atom2	Length	Atom1	Atom2	Length	Atom1	Atom2	Length	Atom1	Atom2	Length	Atom1	Atom2	Length	Atom1	Atom2	Length
Co1	Co2	2.3259	Co1	Co2	2.3644	Co1	Co2	2.4038	Co1	Co2	2.3313	Co1	Co2	2.3796	Co1	Co2	2.4560	Co1	Co2	2.4668	Co1	Co2	2.6227	Co1	Co2	2.4394	Co1	Co2	2.5097	Co1	Co2	2.3384	Co1	Co2	2.3204	Co1	Co2	2.3860
Co1	Co3	2.2487	Co1	Co3	2.2848	Co1	Co3	2.3411	Co1	Co3	2.3050	Co1	Co3	2.3761	Co1	Co4	2.5240	Co1	Co3	2.4141	Co1	Co3	2.3645	Co1	Co4	2.3276	Co1	Co3	2.5345	Co1	Co3	2.3903	Co1	Co3	2.4064	Co1	Co3	2.3381
Co1	Co4	2.3431	Co1	Co4	2.6181	Co1	Co4	2.3900	Co1	Co4	2.4067	Co1	Co4	2.4461	Co1	Co6	2.3651	Co1	Co4	2.4057	Co1	Co4	2.4706	Co1	Co5	2.4933	Co1	Co4	2.6438	Co1	Co4	2.3881	Co1	Co4	2.4301	Co1	Co4	2.4102
Co1	Co5	2.3700	Co1	Co6	2.3798	Co1	Co6	2.5118	Co1	Co7	2.3823	Co1	Co5	2.3841	Co1	Co7	2.5077	Co1	Co5	2.3512	Co1	Co5	2.4455	Co1	Co8	2.4077	Co1	Co6	2.3671	Co1	Co9	2.3155	Co1	Co5	2.4052	Co1	Co6	2.4298
Co2	Co3	2.2566	Co1	Co7	2.2541	Co1	Co7	2.3122	Co1	Co8	2.3075	Co1	Co7	2.2571	Co1	Co9	2.3619	Co1	Co6	2.3541	Co1	Co7	2.4423	Co1	Co9	2.2930	Co1	Co7	2.4143	Co2	Co3	2.3270	Co1	Co8	2.8009	Co1	Co8	2.4078
Co2	Co4	2.3372	Co2	Co3	2.3484	Co1	Co8	2.2927	Co1	Co9	2.2984	Co1	Co8	2.4352	Co2	Co3	2.3721	Co1	Co7	2.5104	Co1	Co9	2.4653	Co1	Co12	2.4351	Co1	Co8	2.2585	Co2	Co5	2.3579	Co1	Co9	2.5768	Co1	Co9	2.3551
Co2	Co5	2.3925	Co2	Co5	2.3233	Co2	Co3	2.3477	Co2	Co3	2.9350	Co1	Co10	2.4032	Co2	Co4	2.3380	Co1	Co9	3.1042	Co2	Co3	2.3854	Co2	Co3	2.5639	Co1	Co10	2.4768	Co2	Co6	2.2515	Co2	Co3	2.3356	Co1	Co11	2.5741
Co2	Co6	2.2387	Co2	Co6	2.3301	Co2	Co5	2.3493	Co2	Co5	2.3084	Co2	Co3	2.5507	Co2	Co5	2.3773	Co1	Co11	2.5595	Co2	Co4	2.4872	Co2	Co5	2.3807	Co2	Co4	2.4943	Co2	Co8	2.4852	Co2	Co4	2.4022	Co1	Co13	2.4100
Co3	Co5	2.4409	Co3	Co4	2.3564	Co2	Co6	2.3868	Co2	Co6	2.4526	Co2	Co7	2.3873	Co2	Co6	2.4302	Co1	Co12	2.4332	Co2	Co8	2.4769	Co2	Co7	2.3667	Co2	Co6	2.4667	Co2	Co9	2.5446	Co2	Co6	2.5307	Co2	Co6	2.5998
Co4	Co5	2.3538	Co3	Co5	2.4908	Co3	Co4	2.2648	Co2	Co7	2.3867	Co2	Co8	2.3580	Co2	Co9	2.3270	Co2	Co3	2.3115	Co2	Co9	2.4153	Co2	Co8	2.3821	Co2	Co8	2.4615	Co2	Co13	2.3711	Co2	Co11	2.4902	Co2	Co8	2.5955
Co4	Co6	2.3549	Co3	Co7	2.3508	Co3	Co5	2.2843	Co2	Co8	2.5779	Co2	Co9	2.2754	Co2	Co10	2.4490	Co2	Co5	2.5322	Co2	Co12	2.5522	Co2	Co11	2.6156	Co2	Co13	2.4350	Co2	Co15	2.6522	Co3	Co4	2.4656	Co2	Co11	2.5162
Co5	Co6	2.3509	Co4	Co7	2.2449	Co3	Co7	2.3765	Co3	Co4	2.4161	Co3	Co4	2.4105	Co2	Co11	3.1075	Co2	Co9	2.2823	Co3	Co4	2.4003	Co2	Co12	2.3983	Co2	Co14	2.3695	Co3	Co4	2.3777	Co3	Co5	2.7881	Co2	Co16	2.3091
average bond length		2.334433	Co5	Co6	2.3475	Co4	Co7	2.3818	Co3	Co5	2.3712	Co3	Co6	2.3373	Co3	Co4	2.3024	Co3	Co4	2.3490	Co3	Co5	2.3751	Co2	Co13	2.4658	Co3	Co4	2.3536	Co3	Co5	2.2945	Co3	Co6	2.5201	Co3	Co4	2.4171
			Co5	Co7	2.3115	Co5	Co6	2.4628	Co3	Co7	2.3834	Co3	Co7	2.4006	Co3	Co5	2.3756	Co3	Co7	2.3169	Co3	Co6	2.4099	Co2	Co14	2.3168	Co3	Co5	2.4177	Co3	Co13	2.5972	Co3	Co7	2.4110	Co3	Co5	2.5356
			Co6	Co7	2.3423	Co5	Co7	2.3783	Co4	Co7	2.3476	Co4	Co5	2.2767	Co3	Co8	2.3602	Co3	Co8	2.4146	Co3	Co7	2.3647	Co3	Co5	2.4216	Co3	Co8	2.6136	Co4	Co5	2.4267	Co3	Co8	2.3856	Co3	Co9	2.4146
			average bond length		2.35648	Co6	Co7	2.3452	Co4	Co9	2.4374	Co4	Co6	2.3294	Co4	Co6	2.2878	Co3	Co9	2.5363	Co3	Co8	2.3741	Co3	Co7	2.2670	Co3	Co10	2.2490	Co4	Co9	2.3698	Co3	Co9	2.4178	Co3	Co13	2.3931
						Co6	Co8	2.4259	Co5	Co7	2.3903	Co5	Co6	2.3534	Co4	Co8	2.3333	Co4	Co8	2.3813	Co3	Co9	2.4087	Co4	Co5	2.2593	Co3	Co11	3.0252	Co4	Co11	2.5474	Co3	Co10	2.4951	Co4	Co5	2.3487
						Co7	Co8	2.3810	Co6	Co7	2.3198	Co5	Co7	2.3796	Co5	Co6	2.3178	Co4	Co12	2.3215	Co3	Co10	2.4017	Co4	Co6	2.9179	Co4	Co5	2.4822	Co5	Co8	2.6493	Co3	Co11	2.5219	Co4	Co6	2.4014
						average bond length		2.368667	Co6	Co8	2.2939	Co5	Co10	2.5493	Co5	Co8	2.4001	Co5	Co6	2.3644	Co3	Co11	2.3848	Co4	Co12	2.3334	Co4	Co8	2.5008	Co5	Co11	2.2977	Co3	Co12	2.3735	Co4	Co7	2.2494
									Co6	Co9	2.5489	Co6	Co7	2.4319	Co5	Co10	2.3462	Co5	Co7	3.0519	Co3	Co12	2.3640	Co5	Co6	2.3171	Co4	Co13	2.4071	Co5	Co13	2.4701	Co3	Co13	2.5461	Co5	Co6	2.6629
									Co7	Co9	2.3930	Co7	Co9	2.4434	Co5	Co11	2.5533	Co5	Co9	2.3049	Co3	Co13	2.3638	Co5	Co7	2.5924	Co5	Co8	2.4761	Co5	Co14	2.2941	Co3	Co14	2.7493	Co5	Co13	2.3151
									Co8	Co9	2.3572	Co7	Co10	2.3743	Co6	Co7	2.3704	Co5	Co10	2.4203	Co4	Co5	2.4845	Co5	Co12	2.7040	Co5	Co11	2.3773	Co5	Co15	2.5054	Co4	Co5	2.3711	Co5	Co14	2.6027
									average bond length		2.406845	Co8	Co9	2.3273	Co6	Co8	2.3816	Co6	Co7	2.3336	Co4	Co6	2.7126	Co6	Co7	2.3698	Co5	Co13	2.5596	Co5	Co16	2.4361	Co4	Co6	2.4365	Co6	Co7	2.3219
												Co8	Co10	2.3341	Co6	Co9	2.9517	Co6	Co10	2.4290	Co4	Co12	2.4358	Co6	Co12	2.3508	Co5	Co15	2.3685	Co6	Co7	2.3290	Co4	Co7	2.3530	Co6	Co11	2.4859
												Co9	Co10	2.4140	Co6	Co11	2.3299	Co6	Co11	2.3199	Co5	Co6	2.4820	Co6	Co13	2.4084	Co6	Co7	2.3709	Co6	Co8	2.4555	Co5	Co7	2.8072	Co6	Co13	2.8992
												average bond length		2.384584	Co7	Co9	2.4514	Co6	Co12	2.5649	Co5	Co7	2.6992	Co7	Co13	2.2751	Co6	Co8	2.4833	Co6	Co9	2.5760	Co5	Co9	2.2893	Co6	Co14	2.2876
															Co7	Co11	2.2938	Co7	Co8	2.4178	Co5	Co11	2.4780	Co8	Co9	2.3423	Co6	Co9	2.6215	Co7	Co8	2.4216	Co5	Co14	2.3189	Co6	Co15	2.3481
															Co9	Co10	2.4847	Co7	Co9	2.3148	Co6	Co11	2.4140	Co8	Co11	2.3392	Co6	Co14	2.4695	Co7	Co9	2.3075	Co6	Co7	2.3810	Co6	Co16	2.4472
															Co9	Co11	2.3044	Co7	Co10	2.3972	Co6	Co12	2.4313	Co9	Co10	2.2833	Co7	Co9	2.4590	Co7	Co12	2.3523	Co6	Co11	2.2826	Co6	Co18	2.6710
															Co10	Co11	2.2637	Co7	Co12	2.3304	Co6	Co13	2.4649	Co9	Co11	2.5867	Co7	Co10	2.2748	Co8	Co9	2.3298	Co6	Co12	2.6437	Co7	Co15	2.3405
															average bond length		2.424137	Co8	Co12	2.3004	Co7	Co9	2.4291	Co9	Co12	2.3477	Co8	Co9	2.5463	Co8	Co10	2.2619	Co7	Co12	2.5065	Co8	Co9	2.5219
																		Co9	Co10	2.3025	Co7	Co10	2.4335	Co10	Co11	2.4314	Co8	Co10	2.4262	Co8	Co11	2.4069	Co7	Co14	2.3149	Co8	Co10	2.3325
																		Co11	Co12	2.2110	Co7	Co11	2.5580	Co10	Co12	2.5447	Co8	Co11	2.2801	Co8	Co12	2.6067	Co7	Co15	2.3028	Co8	Co11	2.3262
																		average bond length		2.427509	Co8	Co9	2.4827	Co11	Co12	2.3978	Co8	Co12	2.4790	Co8	Co15	2.3018	Co7	Co16	2.3447	Co9	Co10	2.2789
																					Co8	Co10	2.4867	Co11	Co13	2.4863	Co8	Co13	2.3067	Co8	Co16	2.5026	Co8	Co9	2.2910	Co9	Co13	2.3470
																					Co8	Co12	2.6948	Co11	Co14	2.2614	Co8	Co14	2.4255	Co9	Co11	2.5546	Co8	Co10	2.6592	Co10	Co11	2.3413
																					Co8	Co13	2.4459	Co12	Co13	2.3826	Co8	Co15	2.7733	Co9	Co12	2.6838	Co8	Co13	2.4541	Co10	Co12	2.4323
																					Co9	Co10	2.7131	Co13	Co14	2.3688	Co9	Co10	2.2815	Co10	Co11	2.8271	Co9	Co10	2.3534	Co10	Co13	2.3813
																					Co10	Co11	2.4879	average bond length		2.417763	Co9	Co11	2.6037	Co10	Co12	2.3529	Co9	Co14	2.3446	Co11	Co12	2.4445
																					Co10	Co13	2.4728				Co9	Co12	2.3078	Co10	Co16	2.2963	Co10	Co12	2.6169	Co11	Co13	2.3912
																					Co11	Co13	2.6161				Co10	Co11	2.4325	Co11	Co12	2.2244	Co10	Co13	2.3194	Co11	Co14	2.5700
																					Co12	Co13	2.4435				Co11	Co12	2.4226	Co11	Co16	2.3795	Co10	Co14	2.4277	Co11	Co16	2.3510
																					average bond length		2.472414				Co11	Co15	2.5693	Co13	Co14	2.5135	Co10	Co17	2.4343	Co11	Co17	2.3229
																											Co12	Co14	2.3826	Co13	Co15	2.2786	Co11	Co12	2.5968	Co12	Co13	2.4623
																											Co12	Co15	2.3011	Co14	Co15	2.3608	Co11	Co13	2.2862	Co12	Co14	2.3501
																											Co13	Co14	2.4176	Co14	Co16	2.3773	Co12	Co13	2.4182	Co12	Co17	2.4539
																											Co13	Co15	2.2507	Co15	Co16	2.3731	Co12	Co16	2.2893	Co13	Co14	2.5010
																											average bond length		2.449955	average bond length		2.420453	Co12	Co17	2.5801	Co14	Co17	2.3652
																																	Co14	Co15	2.2737	Co14	Co18	2.3866
																																	Co14	Co17	2.3048	Co15	Co16	2.3434
																																	Co15	Co16	2.3031	Co15	Co18	2.3406
																																	Co15	Co17	2.5406	Co16	Co17	2.3788
																																	Co16	Co17	2.3917	Co16	Co18	2.2789
																																	average bond length		2.44547	Co17	Co18	2.4417
																																				average bond length		2.422541

3. Bond Length information of $Ni_n@ZnO_{42}$

$Ni_6@(ZnO)_{42}$			$Ni_7@(ZnO)_{42}$			$Ni_8@(ZnO)_{42}$			$Ni_9@(ZnO)_{42}$			$Ni_{10}@(ZnO)_{42}$			$Ni_{11}@(ZnO)_{42}$			$Ni_{12}@(ZnO)_{42}$			$Ni_{13}@(ZnO)_{42}$			$Ni_{14}@(ZnO)_{42}$			$Ni_{15}@(ZnO)_{42}$			$Ni_{16}@(ZnO)_{42}$			$Ni_{17}@(ZnO)_{42}$			$Ni_{18}@(ZnO)_{42}$		
Atom1	Atom2	Length	Atom1	Atom2	Length	Atom1	Atom2	Length	Atom1	Atom2	Length	Atom1	Atom2	Length	Atom1	Atom2	Length	Atom1	Atom2	Length	Atom1	Atom2	Length	Atom1	Atom2	Length	Atom1	Atom2	Length	Atom1	Atom2	Length	Atom1	Atom2	Length	Atom1	Atom2	Length
Ni1	Ni2	2.4181	Ni1	Ni3	2.3023	Ni1	Ni2	2.5448	Ni1	Ni2	2.6213	Ni1	Ni2	2.4761	Ni1	Ni2	2.4271	Ni1	Ni2	2.4738	Ni1	Ni2	2.7532	Ni1	Ni2	2.4455	Ni1	Ni2	2.5668	Ni1	Ni2	2.3786	Ni1	Ni2	2.2927	Ni1	Ni2	2.4231
Ni1	Ni3	2.3952	Ni1	Ni4	2.4598	Ni1	Ni3	2.5214	Ni1	Ni4	2.4860	Ni1	Ni4	2.3138	Ni1	Ni4	2.3253	Ni1	Ni3	2.3496	Ni1	Ni3	2.4549	Ni1	Ni3	2.3993	Ni1	Ni3	2.5205	Ni1	Ni3	2.4833	Ni1	Ni3	2.7278	Ni1	Ni4	2.4421
Ni1	Ni6	2.3851	Ni1	Ni5	2.5470	Ni1	Ni4	2.3350	Ni1	Ni6	2.3620	Ni1	Ni5	2.4624	Ni1	Ni5	3.1578	Ni1	Ni4	2.3506	Ni1	Ni4	2.4682	Ni1	Ni5	2.4325	Ni1	Ni4	2.4194	Ni1	Ni4	2.3979	Ni1	Ni4	2.5498	Ni1	Ni5	2.3613
Ni2	Ni3	2.3042	Ni1	Ni6	2.3848	Ni1	Ni6	2.5537	Ni1	Ni7	2.4358	Ni1	Ni6	2.3083	Ni1	Ni7	2.4258	Ni1	Ni5	2.3461	Ni1	Ni5	2.4783	Ni1	Ni10	2.3722	Ni1	Ni6	2.3961	Ni1	Ni5	2.5216	Ni1	Ni7	2.5487	Ni1	Ni9	2.4542
Ni2	Ni4	2.5702	Ni2	Ni3	2.3333	Ni1	Ni7	2.4700	Ni1	Ni8	2.4410	Ni1	Ni8	2.4978	Ni1	Ni8	2.3701	Ni1	Ni8	2.8439	Ni1	Ni8	2.5398	Ni2	Ni3	2.3907	Ni1	Ni7	2.4440	Ni1	Ni6	2.6200	Ni1	Ni8	2.6998	Ni1	Ni10	2.4164
Ni2	Ni5	2.4434	Ni2	Ni4	2.4967	Ni2	Ni3	2.3729	Ni2	Ni3	2.3866	Ni1	Ni9	2.3645	Ni1	Ni10	2.3311	Ni1	Ni10	2.3512	Ni1	Ni10	2.5122	Ni2	Ni4	2.3721	Ni1	Ni9	2.3844	Ni1	Ni7	2.5297	Ni1	Ni13	2.326	Ni1	Ni14	2.4111
Ni2	Ni6	2.5954	Ni2	Ni7	2.3808	Ni2	Ni4	2.4178	Ni2	Ni4	2.3351	Ni2	Ni3	2.4084	Ni1	Ni11	2.3335	Ni1	Ni11	2.4774	Ni2	Ni3	2.4485	Ni2	Ni6	3.2907	Ni1	Ni10	2.4534	Ni1	Ni8	2.5129	Ni2	Ni3	2.5381	Ni2	Ni3	2.4155
Ni3	Ni4	2.3397	Ni3	Ni4	2.3166	Ni2	Ni5	2.5388	Ni2	Ni5	2.4731	Ni2	Ni4	2.4888	Ni2	Ni3	2.4722	Ni1	Ni12	2.8380	Ni2	Ni4	2.4702	Ni2	Ni7	2.3809	Ni1	Ni11	2.3185	Ni1	Ni9	2.4473	Ni2	Ni4	2.5917	Ni2	Ni5	2.3989
Ni3	Ni5	2.3309	Ni3	Ni5	2.2965	Ni2	Ni7	2.4282	Ni2	Ni6	2.3683	Ni2	Ni8	2.3272	Ni2	Ni4	2.3898	Ni2	Ni3	2.5227	Ni2	Ni7	2.5441	Ni2	Ni8	2.4909	Ni1	Ni12	2.4598	Ni1	Ni11	2.4690	Ni2	Ni5	2.4081	Ni2	Ni7	2.3287
Ni3	Ni6	2.3247	Ni3	Ni6	2.5423	Ni2	Ni8	2.4408	Ni2	Ni8	2.3900	Ni2	Ni9	2.3857	Ni2	Ni5	2.3360	Ni2	Ni4	2.5222	Ni2	Ni8	2.5134	Ni2	Ni9	2.3531	Ni2	Ni4	2.4343	Ni2	Ni3	2.4279	Ni2	Ni6	3.3686	Ni2	Ni8	2.6860
Ni4	Ni5	2.3623	Ni3	Ni7	2.3892	Ni3	Ni4	2.3867	Ni2	Ni9	2.3844	Ni2	Ni10	2.4439	Ni2	Ni8	2.3678	Ni2	Ni8	2.2938	Ni2	Ni12	2.5136	Ni2	Ni10	2.4070	Ni2	Ni6	2.5727	Ni2	Ni6	2.5368	Ni2	Ni7	2.4552	Ni2	Ni9	2.4770
Ni5	Ni6	2.3912	Ni4	Ni5	2.4260	Ni3	Ni5	2.3757	Ni3	Ni4	2.3709	Ni3	Ni4	2.3079	Ni2	Ni9	2.3692	Ni3	Ni5	3.0489	Ni3	Ni4	2.3001	Ni2	Ni13	2.5298	Ni2	Ni8	2.3573	Ni2	Ni7	2.4365	Ni2	Ni9	2.5363	Ni2	Ni12	2.3988
average bond length		2.405033	Ni4	Ni7	2.3665	Ni4	Ni5	2.3629	Ni3	Ni5	2.3803	Ni3	Ni7	2.5331	Ni2	Ni11	2.9518	Ni3	Ni6	2.4814	Ni3	Ni5	2.4428	Ni3	Ni4	2.4538	Ni2	Ni9	2.4755	Ni2	Ni9	2.4258	Ni2	Ni10	2.3813	Ni2	Ni14	2.4089
			Ni5	Ni6	2.3421	Ni4	Ni6	2.3988	Ni4	Ni5	2.3638	Ni3	Ni8	2.5748	Ni3	Ni4	2.3002	Ni3	Ni7	2.3688	Ni3	Ni6	2.4147	Ni3	Ni5	2.3976	Ni2	Ni14	2.5231	Ni2	Ni14	2.3554	Ni2	Ni11	2.3395	Ni2	Ni15	2.4769
			Ni5	Ni7	2.9683	Ni4	Ni7	2.3713	Ni4	Ni6	2.3592	Ni3	Ni10	3.3818	Ni3	Ni5	2.3824	Ni3	Ni8	2.3890	Ni3	Ni7	2.4433	Ni3	Ni6	2.3654	Ni3	Ni4	2.4601	Ni2	Ni16	2.5079	Ni2	Ni12	2.5085	Ni2	Ni16	2.7001
			average bond length		2.436813	Ni4	Ni8	2.3642	Ni5	Ni6	2.4807	Ni4	Ni5	2.4407	Ni3	Ni6	2.6870	Ni3	Ni10	2.5672	Ni3	Ni8	2.4120	Ni3	Ni10	2.8519	Ni3	Ni5	2.4986	Ni3	Ni4	2.4818	Ni3	Ni4	2.3474	Ni3	Ni9	2.5749
						Ni5	Ni8	2.4466	Ni5	Ni9	2.6154	Ni4	Ni7	2.3300	Ni4	Ni5	2.4656	Ni3	Ni12	2.3686	Ni3	Ni9	2.3017	Ni3	Ni12	2.6710	Ni3	Ni11	2.4782	Ni3	Ni6	2.3283	Ni3	Ni6	2.4326	Ni3	Ni12	2.7023
						Ni6	Ni7	2.4004	Ni6	Ni7	2.3325	Ni4	Ni8	2.4173	Ni4	Ni6	2.3197	Ni4	Ni5	2.5482	Ni3	Ni10	2.3932	Ni3	Ni13	2.4319	Ni3	Ni12	2.3636	Ni3	Ni14	2.5877	Ni3	Ni7	3.4158	Ni3	Ni15	2.3288
						Ni7	Ni8	2.4784	Ni6	Ni8	2.3642	Ni5	Ni6	2.3896	Ni4	Ni7	2.3471	Ni4	Ni8	2.3321	Ni3	Ni11	2.4470	Ni4	Ni9	2.8558	Ni4	Ni5	2.3695	Ni4	Ni5	2.4684	Ni3	Ni8	2.4014	Ni3	Ni17	2.6256
						average bond length		2.432021	Ni6	Ni9	2.3729	Ni5	Ni7	2.4324	Ni5	Ni6	2.3932	Ni4	Ni9	3.4341	Ni3	Ni12	2.3936	Ni4	Ni13	2.3133	Ni4	Ni9	2.4663	Ni4	Ni6	2.5681	Ni3	Ni9	2.2990	Ni4	Ni5	2.5544
									Ni7	Ni8	2.4946	Ni5	Ni8	2.2960	Ni5	Ni7	2.3917	Ni5	Ni6	2.4822	Ni3	Ni13	2.4552	Ni5	Ni6	2.4887	Ni4	Ni12	2.5482	Ni4	Ni11	2.4341	Ni3	Ni11	2.8750	Ni4	Ni6	2.6931
									Ni8	Ni9	2.4791	Ni6	Ni8	2.5447	Ni5	Ni9	2.4960	Ni5	Ni8	2.3741	Ni4	Ni5	2.4702	Ni5	Ni10	2.3588	Ni4	Ni13	2.3804	Ni5	Ni8	2.5009	Ni3	Ni13	2.3825	Ni4	Ni10	2.6299
									average bond length		2.4226	Ni6	Ni9	2.5584	Ni5	Ni11	2.4198	Ni5	Ni9	2.3650	Ni4	Ni6	2.6296	Ni6	Ni8	2.4704	Ni4	Ni14	2.5269	Ni5	Ni11	2.3619	Ni3	Ni14	2.3540	Ni4	Ni14	2.3781
												Ni7	Ni8	2.5080	Ni6	Ni7	2.4646	Ni5	Ni11	2.5195	Ni4	Ni12	2.4261	Ni6	Ni10	2.3547	Ni4	Ni15	2.4471	Ni5	Ni12	2.4493	Ni3	Ni15	2.4425	Ni5	Ni6	2.3986
												Ni8	Ni9	2.7197	Ni7	Ni10	2.3773	Ni5	Ni12	2.3882	Ni5	Ni6	2.5638	Ni6	Ni11	2.3823	Ni5	Ni12	2.4488	Ni6	Ni9	2.4835	Ni3	Ni16	2.5992	Ni5	Ni7	2.5467
												Ni8	Ni10	2.3307	Ni7	Ni11	2.4051	Ni6	Ni7	2.4150	Ni5	Ni10	2.6754	Ni6	Ni12	2.3828	Ni5	Ni13	2.4189	Ni6	Ni11	2.2940	Ni3	Ni17	2.4287	Ni5	Ni8	2.4695
												Ni9	Ni10	2.3826	Ni8	Ni9	2.4662	Ni6	Ni8	2.3410	Ni5	Ni11	2.5458	Ni6	Ni13	2.5461	Ni5	Ni15	2.3975	Ni6	Ni13	2.4496	Ni4	Ni5	2.4776	Ni5	Ni14	2.6775
												average bond length		2.467578	Ni8	Ni11	2.4767	Ni6	Ni9	2.4170	Ni6	Ni11	2.5132	Ni6	Ni14	2.3597	Ni6	Ni7	2.4671	Ni6	Ni14	2.3818	Ni4	Ni6	2.5618	Ni6	Ni8	2.5446
															Ni9	Ni11	2.3275	Ni6	Ni12	2.3430	Ni6	Ni12	2.4867	Ni7	Ni8	2.4031	Ni6	Ni8	2.5494	Ni6	Ni15	2.3139	Ni4	Ni13	2.7432	Ni6	Ni14	3.3736
															Ni10	Ni11	2.3427	Ni7	Ni12	2.3198	Ni6	Ni13	2.5397	Ni7	Ni9	3.2411	Ni6	Ni9	2.4099	Ni6	Ni16	2.5219	Ni5	Ni6	2.4687	Ni7	Ni8	2.6059
															average bond length		2.44401	Ni8	Ni9	2.3186	Ni7	Ni8	2.5622	Ni7	Ni10	2.3492	Ni6	Ni10	2.6468	Ni7	Ni8	2.7256	Ni5	Ni10	2.4489	Ni7	Ni15	2.4821
																		Ni10	Ni11	2.5156	Ni7	Ni9	2.4723	Ni7	Ni11	3.4075	Ni7	Ni10	2.3264	Ni7	Ni9	2.3147	Ni5	Ni11	2.4524	Ni7	Ni16	2.4238
																		Ni10	Ni12	2.3293	Ni7	Ni12	2.6654	Ni8	Ni9	2.4653	Ni7	Ni11	2.5681	Ni8	Ni9	2.3944	Ni6	Ni11	2.4365	Ni8	Ni12	2.9406
																		Ni11	Ni12	2.2957	Ni7	Ni13	2.4803	Ni8	Ni10	2.4731	Ni8	Ni9	2.3138	Ni8	Ni10	2.4324	Ni6	Ni14	2.4079	Ni8	Ni13	2.7344
																		average bond length		2.480341	Ni8	Ni9	2.6247	Ni8	Ni11	2.3820	Ni8	Ni14	2.4937	Ni8	Ni11	2.4750	Ni6	Ni17	2.3982	Ni8	Ni14	2.3516
																					Ni8	Ni10	2.4852	Ni8	Ni13	2.3633	Ni9	Ni10	2.4006	Ni8	Ni12	2.5366	Ni7	Ni8	2.5211	Ni8	Ni16	2.2803
																					Ni9	Ni10	2.4225	Ni8	Ni14	2.5671	Ni9	Ni12	2.4572	Ni9	Ni10	2.4276	Ni7	Ni9	2.3621	Ni8	Ni18	3.2858
																					Ni9	Ni11	2.4741	Ni9	Ni13	2.3370	Ni9	Ni14	2.4152	Ni9	Ni11	2.3733	Ni7	Ni12	2.6467	Ni9	Ni10	2.4612
																					Ni9	Ni13	2.4616	Ni10	Ni11	2.3488	Ni9	Ni15	2.3595	Ni9	Ni13	2.4038	Ni8	Ni9	2.5781	Ni9	Ni11	2.5043
																					Ni10	Ni11	2.5144	Ni11	Ni14	3.2975	Ni10	Ni11	2.6161	Ni9	Ni16	2.3809	Ni8	Ni13	2.5240	Ni9	Ni12	2.5365
																					Ni11	Ni13	2.7429	Ni12	Ni13	2.3311	Ni10	Ni12	2.3786	Ni10	Ni11	2.4056	Ni8	Ni15	2.4601	Ni9	Ni14	2.5092
																					Ni12	Ni13	2.5181	Ni12	Ni14	2.5302	Ni11	Ni12	2.5448	Ni10	Ni12	2.4382	Ni8	Ni16	2.5469	Ni10	Ni11	2.5849
																					average bond length		2.499386	Ni13	Ni14	2.3665	Ni12	Ni15	2.4008	Ni10	Ni13	2.5550	Ni9	Ni11	2.4111	Ni10	Ni14	2.3680
																								average bond length		2.521202	Ni13	Ni14	2.5668	Ni11	Ni12	2.3023	Ni9	Ni12	2.2810	Ni11	Ni12	2.4717
																											Ni13	Ni15	2.3280	Ni11	Ni13	2.6023	Ni9	Ni16	2.3384	Ni11	Ni13	2.4793
																											Ni14	Ni15	2.4719	Ni13	Ni15	2.5819	Ni9	Ni17	2.5511	Ni11	Ni14	2.3723
																											average bond length		2.453143	Ni13	Ni16	2.4130	Ni10	Ni11	2.4213	Ni12	Ni13	2.3763
																														Ni14	Ni15	2.4612	Ni10	Ni12	2.3966	Ni12	Ni14	2.4163
																														Ni14	Ni16	2.3750	Ni11	Ni12	2.5120	Ni12	Ni15	3.2854
																														Ni15	Ni16	2.4848	Ni11	Ni17	2.4003	Ni12	Ni16	2.4587
																														average bond length		2.455188	Ni13	Ni15	2.3658	Ni12	Ni17	2.3411
																																	Ni14	Ni15	2.4707	Ni12	Ni18	2.3933
																																	Ni14	Ni16	3.1821	Ni13	Ni14	2.4815
																																	Ni14	Ni17	2.4908	Ni13	Ni18	2.4266
																																	Ni15	Ni16	2.3857	Ni15	Ni16	2.2799
																																	Ni16	Ni17	2.3608	Ni15	Ni17	2.4779
																																	average bond length		2.515216	Ni16	Ni17	2.4288
																																				Ni16	Ni18	2.2980
																																				Ni17	Ni18	2.5837
																																				average bond length		2.524339