

Supplementary Information for:

**“Investigation of the interaction of CO, NO, and HCN gases with
Transition Metal-doped Ca₁₂O₁₂ nanocages: Theoretical Study”**

H. O. Taha ^{1,*}, A. M. El Mahdy ¹

¹ *Department of Physics, Faculty of Education, Ain Shams University, Roxy, 11575, Cairo, Egypt*

**Corresponding author. Emails: hyamosman@edu.asu.edu.eg; drhotaha@hotmail.com*

Table S1

Adsorption energies of CO, NO and HCN molecules on the $\text{Ca}_{12}\text{O}_{12}$ nanocage. Calculated at B3LYP/6-31+G(d), B3LYP/6-311+G(d), and PBEPBE/6-311+G(d) .

	CO/ $\text{Ca}_{12}\text{O}_{12}$	NO/ $\text{Ca}_{12}\text{O}_{12}$	HCN/ $\text{Ca}_{12}\text{O}_{12}$
B3LYP/6-31+G(d)	-0.282	-0.894	-0.456
B3LYP/6-311+G(d)	-0.404	-0.671	-0.423
PBEPBE/6-311+G(d)	-0.286	-0.985	-0.425

Table S2:

The obtained xyz coordinates for all studied systems, including $\text{Ca}_{12}\text{O}_{12}$ cluster CO, NO, and HCN, gases as well as CO / $\text{Ca}_{12}\text{O}_{12}$, NO / $\text{Ca}_{12}\text{O}_{12}$, HCN/ $\text{Ca}_{12}\text{O}_{12}$, as well as TM / $\text{Ca}_{11}\text{O}_{12}$ (TM=Sc-Zn), CO/TM $\text{Ca}_{11}\text{O}_{12}$, NO/TM $\text{Ca}_{11}\text{O}_{12}$, and HCN/TM $\text{Ca}_{11}\text{O}_{12}$ (TM=Sc-Zn) complex structures which have been calculated by DFT method and B3LYP/6-311+G(D)D3 level of theory.

CO

6	0.000000	0.000000	-0.644394
8	0.000000	0.000000	0.483296

NO

7	0.000000	0.000000	-0.612239
8	0.000000	0.000000	0.535709

HCN

1	0.000000	0.000000	0.650946
6	0.000000	0.000000	-0.498276
7	0.000000	0.000000	-1.566969

CO/ $\text{Ca}_{12}\text{O}_{12}$

8	3.217817	0.530189	0.19975
8	0.739952	3.165709	-0.956993
8	-2.414750	1.515323	-2.157595
8	0.711143	2.014760	2.603964
8	-2.091440	2.518212	1.441678
8	1.932771	-1.501940	2.141257
8	-1.22571	-3.165028	0.963179
8	-3.63184	-0.508917	-0.190209
8	1.600133	-2.506277	-1.433316
8	-1.19256	-2.014311	-2.619344
8	1.183245	0.888676	-2.959131
8	-1.65495	-0.886107	2.977335
20	-0.02207	-2.317128	2.600848
20	-3.30119	1.669339	-0.145978
20	-1.30793	1.250415	3.066573
20	2.347671	0.645077	2.251319
20	-0.08967	3.344423	1.040738
20	2.407199	1.805101	-1.388681
20	-0.45825	2.319381	-2.606009

NO / $\text{Ca}_{12}\text{O}_{12}$

8	-4.155800	-2.596710	-0.04843
8	1.367392	-3.036710	1.522345
8	3.787655	-0.392070	-0.03076
8	-1.26945	-0.629730	3.160429
8	1.723256	0.478281	3.161613
8	-3.17065	0.444831	0.027249
8	-0.86583	3.073571	-1.51856
8	2.687396	2.598456	0.049935
8	-1.30248	-0.483860	-3.17005
8	1.689602	0.629160	-3.15374
8	1.35133	-2.960880	-1.66879
8	-0.85071	2.999889	1.663771
20	-2.35946	2.531526	0.068125
20	3.212526	1.051429	1.618273
20	-0.32694	1.437045	3.162416
20	-2.75704	-1.191950	1.61245
20	0.788451	-1.583890	3.101079
20	-0.152200	-3.543650	-0.08001
20	2.857115	-2.408190	-0.06803

20	2.850004	-1.694156	0.140858	20	-2.77436	-1.122980	-1.63778
20	0.825764	-1.251291	-3.067615	20	0.758948	-1.436490	-3.16968
20	-2.83351	-0.648796	-2.240903	20	3.193366	1.126903	-1.59903
20	-0.40236	-3.332068	-1.036875	20	-0.36123	1.580129	-3.08973
20	-2.8921	-1.789241	1.393102	20	0.683728	3.543082	0.07727
8	6.072486	0.312024	-0.045471	7	-4.78346	-0.453710	0.050279
6	5.259731	-0.486609	0.021938	8	-5.71345	0.315358	-0.02743

HCN/Ca₁₂O₁₂

8	-2.670590	-1.949720	0.561662
8	0.8998180	-3.504160	0.136212
8	3.1933050	-1.003770	-1.781640
8	0.1010450	-1.359010	3.283487
8	3.0283600	-0.887450	2.110359
8	-2.642140	1.0015760	1.776060
8	-0.330260	3.5245480	-0.141970
8	3.2219430	1.9461010	-0.567880
8	-2.458100	0.8794040	-2.086440
8	0.4673390	1.3565420	-3.276310
8	-0.372370	-2.395770	-2.569900
8	0.9327150	2.378406	2.552131
20	-1.181050	2.668605	1.778306
20	3.8285230	-0.097420	0.195021
20	1.5578830	0.378334	3.281547
20	-1.952110	-1.025200	2.496273
20	1.5457420	-2.600370	2.057561
20	-1.215160	-3.146890	-0.605670
20	1.7401620	-2.685580	-1.803770
20	-3.360430	0.099644	-0.193710
20	-0.994380	-0.380220	-3.262920
20	2.5293190	1.0325130	-2.524800
20	-0.984290	2.5925670	-2.050140
20	1.7777070	3.1681570	0.601352
1	-8.124620	-0.230740	0.469780
6	-7.105350	-0.072690	0.182355
7	-6.007170	0.0986260	-0.130170

Sc /Ca₁₁O₁₂

8	1.50817	-2.85813	0.000000
8	2.93772	-0.22135	1.426390
8	1.63786	2.97977	0.000000
8	-0.07497	-1.53178	3.118640
8	-1.55877	-3.0186	0.000000
8	-3.05231	0.06753	-1.535620
8	-1.43634	3.09413	0.000000
8	-0.07497	-1.53178	-3.118640
8	0.05422	1.51788	-3.072840
8	2.93772	-0.22135	-1.426390
8	-3.05231	0.06753	1.535620
8	0.05422	1.51788	3.072840
20	-3.12678	-1.50674	0.000000
20	-1.60228	0.05727	3.140550
20	-0.05973	-3.05038	1.597950
20	1.5495	-0.07528	3.134590
20	3.17667	1.50024	0.000000
20	-0.05973	-3.05038	-1.597950
20	1.5495	-0.07528	-3.134590
20	0.09503	3.09041	-1.579120
20	-1.60228	0.05727	-3.140550
20	-3.05177	1.64769	0.000000
20	0.09503	3.09041	1.579120
21	2.93784	-1.55233	0.000000

V/Ca₁₁O₁₂

8	-1.29417	-2.98131	0.000000
8	1.58549	-2.4123	1.377520
8	3.3566	0.50709	0.000000
8	-1.25907	-0.88083	3.117080
8	-3.31237	-0.67076	0.000000
8	-1.8282	2.43688	-1.534990
8	1.55976	3.0068	0.000000
8	-1.25907	-0.88083	-3.117080
8	1.21897	0.89642	-3.085300
8	1.58549	-2.4123	-1.377520
8	-1.8282	2.43688	1.534990
8	1.21897	0.89642	3.085300
20	-0.94844	1.31225	3.154260
20	-2.45088	-1.84056	1.626930
20	0.89303	-1.24887	3.143270
20	3.22031	-1.60847	0.000000
20	-2.45088	-1.84056	-1.626930
20	0.89303	-1.24887	-3.143270
20	2.50052	1.79951	-1.581000
20	-0.94844	1.31225	-3.154260
20	-0.56988	3.40505	0.000000
20	2.50052	1.79951	1.581000
20	-3.09792	1.5115	0.000000
23	0.48813	-2.8953	0.000000

Ti /Ca₁₁O₁₂

8	-0.69566	-3.14557	0.000000
8	2.02078	-2.16979	1.419630
8	3.37384	1.16381	0.000000
8	-1.14798	-1.13994	3.317110
8	-3.27895	-1.32173	0.000000
8	-2.32309	2.12572	-1.595630
8	1.02796	3.3419	0.000000
8	-1.14798	-1.13994	-3.317110
8	1.09804	1.11387	-3.219540
8	2.02078	-2.16979	-1.419630
8	-2.32309	2.12572	1.595630
8	1.09804	1.11387	3.219540
20	-1.18319	1.13116	3.218520
20	-2.07629	-2.25149	1.655880
20	1.09279	-1.13216	3.219800
20	3.5167	-1.02375	0.000000
20	-2.07629	-2.25149	-1.655880
20	1.09279	-1.13216	-3.219800
20	2.15769	2.22453	-1.608590
20	-1.18319	1.13116	-3.218520
20	-1.19291	3.2735	0.000000
20	2.15769	2.22453	1.608590
20	-3.38345	0.91553	0.000000
22	1.08054	-2.78965	0.000000

Cr /Ca₁₁O₁₂

8	-1.69145	-2.90619	0.000000
8	1.31606	-2.56833	1.353790
8	3.47019	0.09425	0.000000
8	-1.39498	-0.68642	3.177690
8	-3.35928	-0.25922	0.000000
8	-1.51117	2.64908	-1.540980
8	1.92249	2.78158	0.000000
8	-1.39498	-0.68642	-3.177690
8	1.32608	0.74326	-3.078740
8	1.31606	-2.56833	-1.353790
8	-1.51117	2.64908	1.540980
8	1.32608	0.74326	3.078740
20	-0.77776	1.43039	3.172420
20	-2.57896	-1.52718	1.599450
20	0.68928	-1.34799	3.062890
20	2.94869	-1.99394	0.000000
20	-2.57896	-1.52718	-1.599450
20	0.68928	-1.34799	-3.062890
20	2.70797	1.46435	-1.573040
20	-0.77776	1.43039	-3.172420
20	-0.14591	3.43885	0.000000
20	2.70797	1.46435	1.573040
20	-2.87849	1.87009	0.000000
24	0.05756	-2.79029	0.000000

Mn/Ca₁₁O₁₂

8	-1.278510	-3.002700	0.000000
8	1.703460	-2.322610	1.376420
8	3.418790	0.609110	0.000000
8	-1.263670	-0.899050	3.132790
8	-3.340580	-0.705320	0.000000
8	-1.876860	2.412310	-1.538490
8	1.497300	3.032790	0.000000
8	-1.263670	-0.899050	-3.132790
8	1.205280	0.922690	-3.090100
8	1.703460	-2.322610	-1.376420
8	-1.876860	2.412310	1.538490
8	1.205280	0.922690	3.090100
20	-0.977510	1.289790	3.152550
20	-2.402010	-1.884300	1.593470
20	0.890550	-1.238830	3.106060
20	3.230850	-1.528420	0.000000
20	-2.402010	-1.884300	-1.593470
20	0.890550	-1.238830	-3.106060
20	2.462700	1.842940	-1.576960
20	-0.977510	1.289790	-3.152550
20	-0.641120	3.394590	0.000000
20	2.462700	1.842940	1.576960
20	-3.139060	1.465230	0.000000
25	0.534790	-2.731870	0.000000

Co/Ca₁₁O₁₂

8	0.70319	-3.12496	0.000000
8	2.76829	-0.86438	1.426350
8	2.34494	2.52715	0.000000
8	-0.50431	-1.44998	3.132750
8	-2.3005	-2.52118	0.000000
8	-2.95981	0.85211	-1.537910
8	-0.6215	3.36615	0.000000
8	-0.50431	-1.44998	-3.132750
8	0.40563	1.47703	-3.072370
8	2.76829	-0.86438	-1.426350
8	-2.95981	0.85211	1.537910
8	0.40563	1.47703	3.072370
20	-1.56265	0.47862	3.151040
20	-0.82862	-2.91477	1.585840
20	1.44691	-0.45734	3.099200
20	3.42002	0.64781	0.000000
20	-0.82862	-2.91477	-1.585840
20	1.44691	-0.45734	-3.099200
20	0.86554	2.97923	-1.576190
20	-1.56265	0.47862	-3.151040
20	-2.55025	2.37589	0.000000
20	0.86554	2.97923	1.576190
20	-3.42427	-0.65637	0.000000
27	2.14358	-1.96258	0.000000

Fe/Ca₁₁O₁₂

8	2.54335	-1.78218	0.000000
8	2.67498	1.1031	1.415530
8	0.08243	3.4241	0.000000
8	0.56008	-1.42403	3.152990
8	-0.05001	-3.39352	0.000000
8	-2.78854	-1.30646	-1.539630
8	-2.70629	2.11997	0.000000
8	0.56008	-1.42403	-3.152990
8	-0.66361	1.38239	-3.065650
8	2.67498	1.1031	-1.415530
8	-2.78854	-1.30646	1.539630
8	-0.66361	1.38239	3.065650
20	-1.50172	-0.65964	3.159310
20	1.29814	-2.69973	1.590020
20	1.39373	0.59858	3.091810
20	2.11097	2.67209	0.000000
20	1.29814	-2.69973	-1.590020
20	1.39373	0.59858	-3.091810
20	-1.3316	2.80802	-1.577220
20	-1.50172	-0.65964	-3.159310
20	-3.49779	0.10203	0.000000
20	-1.3316	2.80802	1.577220
20	-2.12765	-2.73917	0.000000
26	3.09481	-0.06212	0.000000

Ni/Ca₁₁O₁₂

8	-1.227570	-2.975320	0.000000
8	1.776790	-2.244460	1.366850
8	3.413210	0.714910	0.000000
8	-1.258940	-0.900180	3.120190
8	-3.345670	-0.754110	0.000000
8	-1.931530	2.393190	-1.538140
8	1.431830	3.085840	0.000000
8	-1.258940	-0.900180	-3.120190
8	1.175000	0.969710	-3.078250
8	1.776790	-2.244460	-1.366850
8	-1.931530	2.393190	1.538140
8	1.175000	0.969710	3.078250
20	-1.010810	1.287700	3.155010
20	-2.370830	-1.926700	1.582940
20	0.905490	-1.206480	3.067540
20	3.252250	-1.445060	0.000000
20	-2.370830	-1.926700	-1.582940
20	0.905490	-1.206480	-3.067540
20	2.426270	1.915380	-1.575450
20	-1.010810	1.287700	-3.155010
20	-0.714190	3.397500	0.000000
20	2.426270	1.915380	1.575450
20	-3.172890	1.416280	0.000000
28	0.583450	-2.651180	0.000000

Cu /Ca₁₁O₁₂

8	-0.665340	-3.141420	0.000000
8	2.182540	-1.865300	1.435220
8	3.200330	1.344150	0.000000
8	-1.067390	-1.107980	3.121600
8	-3.142550	-1.351360	0.000000
8	-2.353760	2.001780	-1.537460
8	0.819120	3.306890	0.000000
8	-1.067390	-1.107980	-3.121600
8	0.967280	1.191720	-3.088990
8	2.182540	-1.865300	-1.435220
8	-2.353760	2.001780	1.537460
8	0.967280	1.191720	3.088990
20	-1.240170	1.085740	3.151560
20	-1.972270	-2.326060	1.588360
20	1.123490	-0.997360	3.114770
20	3.433770	-0.809020	0.000000
20	-1.972270	-2.326060	-1.588360
20	1.123490	-0.997360	-3.114770
20	2.015990	2.346230	-1.577480
20	-1.240170	1.085740	-3.151560
20	-1.347950	3.217250	0.000000
20	2.015990	2.346230	1.577480
20	-3.393260	0.809990	0.000000
29	1.093650	-2.534330	0.000000

Zn /Ca₁₁O₁₂

8	0.663240	-3.119730	0.000000
8	2.753270	-0.807680	1.488670
8	2.356700	2.514710	0.000000
8	-0.529000	-1.433880	3.128710
8	-2.320170	-2.502130	0.000000
8	-2.979830	0.875180	-1.537440
8	-0.612870	3.349470	0.000000
8	-0.529000	-1.433880	-3.128710
8	0.379070	1.497580	-3.103640
8	2.753270	-0.807680	-1.488670
8	-2.979830	0.875180	1.537440
8	0.379070	1.497580	3.103640
20	-1.586850	0.497190	3.152260
20	-0.856900	-2.913010	1.593560
20	1.426470	-0.435660	3.155270
20	3.444340	0.645020	0.000000
20	-0.856900	-2.913010	-1.593560
20	1.426470	-0.435660	-3.155270
20	0.872760	2.960380	-1.577610
20	-1.586850	0.497190	-3.152260
20	-2.558910	2.396360	0.000000
20	0.872760	2.960380	1.577610
20	-3.440540	-0.636390	0.000000
30	2.073710	-1.883110	0.000000

CO/ScCa₁₁O₁₂

8	-2.438914	-0.093182	-1.655197
8	-2.410121	1.313755	1.345555
8	0.388271	-0.038407	3.428485
8	-0.560814	3.099149	-1.335495
8	0.072070	0.033598	-3.393968
8	2.981262	-1.424891	-1.499420
8	3.070535	0.080741	1.936463
8	-0.329778	-3.124512	-1.404323
8	1.074462	-3.035658	1.311332
8	-2.348263	-1.535471	1.310306
8	2.872123	1.647796	-1.464234
8	0.859972	3.076817	1.371248
20	1.549994	3.195925	-0.727000
20	-1.309835	1.561779	-2.634475
20	-1.245328	3.062355	0.743260
20	-1.680198	-0.111123	2.857985
20	-1.183019	-1.619577	-2.678337
20	-1.023790	-3.154140	0.671345
20	1.818644	-1.556269	2.707912
20	1.779798	-3.078472	-0.785685
20	3.734363	0.125592	-0.127602
20	1.691383	1.602635	2.725754
20	2.185500	0.101822	-2.877849
21	-3.170214	-0.109908	0.152176
8	-6.619030	-0.016891	-0.053067
6	-5.444986	-0.027537	0.019438

CO/TiCa₁₁O₁₂

8	-2.428357	0.640724	-1.474228
8	-2.161019	1.253959	1.601388
8	0.385054	-0.816686	3.325725
8	-0.120126	3.410665	-0.610635
8	0.007217	0.809468	-3.292589
8	2.714833	-1.395810	-1.877759
8	3.046264	-0.738157	1.786198
8	-0.795024	-2.623794	-2.011146
8	0.634494	-3.352104	0.585397
8	-2.519361	-1.429630	1.041400
8	3.047728	1.571376	-1.161220
8	1.264466	2.583735	1.983571
20	1.981589	3.091733	-0.046707
20	-1.105468	2.333720	-2.168989
20	-0.817978	2.969117	1.414124
20	-1.676212	-0.488764	2.854041
20	-1.431321	-0.786948	-2.907957
20	-1.458580	-3.067923	0.025173
20	1.587059	-2.319101	2.241842
20	1.313902	-2.994382	-1.489354
20	3.708544	-0.313283	-0.233239
20	1.900818	0.746227	2.941670
20	2.121687	0.493926	-2.841797
22	-3.031718	0.222041	0.204674
8	-6.245780	0.185257	0.019487
6	-5.071021	0.172773	0.066056

CO/VCa₁₁O₁₂

8	2.368547	-0.008630	-1.718934
8	2.469986	-1.373799	1.032128
8	-0.152475	0.014415	3.327476
8	0.401760	-3.151533	-1.356485
8	-0.197355	-0.014786	-3.373724
8	-2.958760	1.527915	-1.372326
8	-2.939538	0.008161	2.074858
8	0.399996	3.140015	-1.382995
8	-0.904562	3.081735	1.351584
8	2.468694	1.384302	1.017570
8	-2.957984	-1.541298	-1.359636
8	-0.902775	-3.070219	1.377722
80	1.850408	2.336689	0.006006
80	1.109781	2.139810	1.238621
80	1.145054	-0.084904	0.000000
80	1.890320	0.044630	3.828081
80	3.097024	10.600190	0.000007
80	1.178986	3.162362	0.661824
80	-2.137402	12.597498	0.000000
80	1.470580	0.146063	-0.626083
80	-3.688207	-0.060883	0.007560
80	-1.182694	2.139614	2.138101
80	-2.279781	-0.010452	12.590736
83	2.198810	0.086387	3.007582
80	0.661533	0.100396	3.145079
80	2.946812	0.060138	10.591827
20	-0.595003	1.181070	3.114692
20	-2.727723	1.944404	0.000000
20	2.746018	1.068525	-1.591014
20	-0.595003	1.181070	-3.114692
20	-2.820511	-1.502231	-1.577248
20	0.651533	-1.713960	-3.145207
20	-0.137729	-3.712801	0.000000
20	-2.820511	-1.502231	1.577248
20	2.720968	-2.374153	0.000000
25	0.089263	2.911732	0.000000
8	0.021097	5.814644	0.000000
6	0.085103	4.644075	0.000000

CO/CoCa₁₁O₁₂

8	2.462933	-0.131995	-1.651219
8	2.290266	-1.469517	1.355158
8	-0.389489	0.102608	3.409208
8	0.332311	-3.203783	-1.280453
8	-0.052206	-0.108439	-3.373492
8	-2.889127	1.569389	-1.545031
8	-3.084037	0.140893	1.922309
8	0.516897	3.077230	-1.460150
8	-0.925799	3.143149	1.240764
8	2.375158	1.422992	1.301074
8	-2.978198	-1.505192	-1.452590
8	-1.098459	-3.015030	1.421604

CO/CrCa₁₁O₁₂

8	1.668819	2.336999	0.000000
8	-1.162539	2.403231	1.408634
8	-3.432833	-0.218446	0.000000
8	1.401588	0.397029	3.149185
8	3.395690	-0.173439	0.000000
8	1.382704	-2.958228	-1.538515
8	-2.034090	-2.960557	0.000000
8	1.401588	0.397029	-3.149185
8	-1.367987	-0.899112	-3.067155
8	-1.162539	2.403231	-1.408634
8	1.382704	-2.958228	1.538515
8	-1.367987	-0.899112	3.067155
20	0.700071	2.188048	0.000000
20	2.470025	2.418880	1.500894
20	-0.345843	10.10508	0.000000
20	-2.768820	0.824337	0.000000
20	2.539863	10.138686	0.000004
20	-0.629881	13.104528	-3.528239
20	-2.270985	-2.810945	0.000000
20	0.700824	0.138847	-3.123182
20	-0.100747	-0.816031	0.000002
20	-2.170080	2.141089	11.588230
20	2.801788	-3.068013	0.000000
24	-0.658244	2.297387	0.000000
820	0.151320	5.192820	0.000000
620	0.724885	0.997684	0.000000
20	-0.56907	1.195456	3.098473
20	-2.68944	2.009246	0.000000
20	2.784875	0.994687	-1.596399
20	-0.56907	1.195456	-3.098473
20	-2.85519	-1.4386	-1.576847
20	0.613204	-1.72928	-3.148498
20	-0.21864	-3.70429	0.000000
20	-2.85519	-1.4386	1.576847
20	-1.40487	-0.83663	3.074322
26	0.191584	2.866544	0.000000
8	-0.03278	5.726031	0.000000
6	0.12292	4.575151	0.000000

CO
/M
nC
a₁₁
O₁₂
CO
/Fe
Ca₁
O₁
2CO/NiCa₁₁O₁₂

8	1.590538	3.148908	0.000000
8	-1.92307	2.031071	1.531643
8	-3.37607	-1.00042	0.000000
8	1.267122	0.72238	3.100136
8	3.25383	0.608064	0.000000
8	1.982953	-2.58274	-1.535705
8	-1.35019	-3.32229	0.000000
8	1.267122	0.72238	-3.100136
8	-1.13607	-1.20272	-3.084293
8	-1.92307	2.031071	-1.531643
8	1.982953	-2.58274	1.535705
8	-1.13607	-1.20272	3.084293

20	-1.781315	-3.136373	-0.675469	20	1.043796	-1.4765	3.142548	CO /Cu Ca ₁ O ₁ 2
20	1.207410	-1.715305	-2.561597	20	2.411538	1.762918	1.642192	
20	1.010552	-3.125211	0.801233	20	-0.93121	0.988692	3.130155	
20	1.693382	0.025981	2.824704	20	-3.31015	1.145358	0.000000	
20	1.297653	1.466763	-2.653139	20	2.411538	1.762918	-1.642192	
20	1.186629	3.101405	0.626573	20	-0.93121	0.988692	-3.130155	
20	-1.712680	1.699668	2.655316	20	-2.36566	-2.17415	-1.580646	
20	-1.598271	3.171366	-0.863347	20	1.043796	-1.4765	-3.142548	
20	-3.739871	0.096267	-0.143751	20	0.790428	-3.62825	0.000000	
20	-1.805591	-1.452279	2.749048	20	-2.36566	-2.17415	1.580646	
20	-2.171221	-0.031424	-2.878946	20	3.184231	-1.58056	0.000000	CO /Zn Ca ₁ O ₁ 2
27	2.957968	-0.065686	0.152837	28	-1.02902	2.684419	0.000000	
8	4.344359	-0.1336324	0.007006	8	0.412388	2.898638	0.000000	
6	5.2918400	-0.925518	-0.5109088	6	0.23827627	1.023907	0.490990	
8	-3.347561	-1.184439	0.000000	8	-3.195770	-1.525149	0.000000	
8	1.226872	0.765135	3.042198	8	1.078798	0.838685	3.132072	
8	3.296008	0.687019	0.000000	8	3.145915	1.055931	0.000000	
8	2.071916	-2.532236	-1.534803	8	2.322579	-2.287097	-1.536505	
8	-1.234743	-3.412969	0.000000	8	-0.863647	-3.539262	0.000000	
8	1.226872	0.765135	-3.042198	8	1.078798	0.838685	-3.132072	
8	-1.107787	-1.249103	-3.056059	8	-0.980957	-1.439467	-3.109140	
8	-2.084000	1.959821	-1.517402	8	-2.147127	1.653077	-1.490331	
8	2.071916	-2.532236	1.534803	8	2.322579	-2.287097	1.536505	
8	-1.107787	-1.249103	3.056059	8	-0.980957	-1.439467	3.109140	
20	1.073554	-1.442702	3.119166	20	1.225061	-1.358394	3.155268	
20	2.435666	1.812559	1.651587	20	1.997778	2.040798	1.596310	
20	-0.992640	0.953805	3.065550	20	-1.117269	0.753235	3.161850	
20	-3.342737	0.980832	0.000000	20	-3.389772	0.628794	0.000000	
20	2.435666	1.812559	-1.651587	20	1.997778	2.040798	-1.596310	
20	-0.992640	0.953805	-3.065550	20	-1.117269	0.753235	-3.161850	
20	-2.304706	-2.306261	-1.580528	20	-2.042686	-2.557827	-1.579061	
20	1.073554	-1.442702	-3.119166	20	1.225061	-1.358394	-3.155268	
20	0.914271	-3.623059	0.000000	20	1.303748	-3.493570	0.000000	
20	-2.304706	-2.306261	1.580528	20	-2.042686	-2.557827	1.579061	
20	3.250289	-1.507842	0.000000	20	3.374730	-1.109133	0.000000	
29	-1.190531	2.797111	0.000000	30	-1.089888	2.350156	0.000000	
8	0.430426	3.887914	0.000000	8	0.512933	6.172940	0.000000	
6	0.406694	5.100820	0.000000	6	-0.410408	5.518441	0.000000	

NO/ScCa₁₁O₁₂

8	-2.417607	-0.236312	-1.625542
8	-2.421283	1.374175	1.288764
8	0.421449	0.170704	3.422244
8	-0.596025	3.008768	-1.507899
8	0.065058	-0.176007	-3.405750
8	2.983043	-1.480799	-1.429714
8	3.092221	0.229570	1.912916
8	-0.297475	-3.230112	-1.207478
8	1.117767	-2.939276	1.486070
8	-2.316520	-1.475899	1.411180
8	2.847582	1.584770	-1.578443
8	0.839225	3.154796	1.185300
20	1.516544	3.161516	-0.918702
20	-1.321132	1.374491	-2.705848
20	-1.267851	3.087064	0.571783

NO/TiCa₁₁O₁₂

8	-2.368830	-0.010820	-1.646920
8	-2.453540	1.365670	1.036210
8	0.208040	0.015240	3.318860
8	-0.396280	3.131430	-1.382350
8	0.164670	-0.016130	-3.356260
8	2.966030	-1.542350	-1.391590
8	2.987870	0.010330	2.042400
8	-0.394570	-3.144520	-1.353600
8	0.936880	-3.056000	1.365210
8	-2.454990	-1.357600	1.051970
8	2.965170	1.530680	-1.405730
8	0.935660	3.069170	1.336670
20	1.719910	3.157510	-0.720840
20	-1.124470	1.605670	-2.677260
20	-1.123040	3.144650	0.670250

20	-1.649268	0.041018	2.860222	20	-1.839020	0.014140	2.851760	NO /V Ca ₁ O ₁ 2 NO /Cr Ca ₁ O ₁ 2
20	-1.151965	-1.799004	-2.566153	20	-1.123360	-1.633600	-2.665150	
20	-0.982192	-3.121746	0.868221	20	-1.121610	-3.137130	0.698880	
20	1.860630	-1.371519	2.786848	20	1.643570	-1.571120	2.780110	
20	1.813089	-3.107016	-0.604681	20	1.721550	-3.163130	-0.691290	
20	3.732037	0.154404	-0.158575	20	3.716000	0.000930	0.005390	
20	1.703385	1.779559	2.622900	20	1.642480	1.597820	2.765250	
20	2.178879	-0.047824	-2.896786	20	2.289340	-0.012520	-2.811280	
21	-3.169481	-0.122880	0.176341	22	-3.072150	-0.001370	0.025980	
7	-5.267209	0.029654	-0.007681	7	-5.038020	-0.000880	-0.084050	
8	-6.469125	-0.065126	-0.055895	8	-6.242800	0.001430	-0.127320	
8	-2.27038	0.014937	-1.70158	8	1.837446	2.284943	0.000000	
8	-2.40196	1.381334	1.136246	8	-1.072402	2.389987	1.373097	
8	0.160227	-0.03683	3.435223	8	-3.442855	-0.073773	0.000000	
8	-0.37402	3.162981	-1.37684	8	1.428237	0.318004	3.129453	
8	0.242921	0.035489	-3.40468	8	3.396515	-0.330758	0.000000	
8	2.985884	-1.51697	-1.34661	8	1.262434	-3.036295	-1.536997	
8	2.921931	-0.01706	2.087086	8	-2.157688	-2.873980	0.000000	
8	-0.36327	-3.13576	-1.43992	8	1.428237	0.318004	-3.129453	
8	0.87946	-3.08045	1.347954	8	-1.392017	-0.867995	-3.073136	
8	-2.40172	-1.41401	1.104954	8	-1.072402	2.389987	-1.373097	
8	2.981248	1.553488	-1.31653	8	1.262434	-3.036295	1.536997	
8	0.870321	3.055028	1.408954	8	-1.392017	-0.867995	3.073136	
20	1.697996	3.160648	-0.64038	20	0.638852	-1.737112	3.151839	
20	-1.09602	1.619829	-2.68898	20	2.751189	1.030875	1.594954	
20	-1.18223	3.130278	0.646107	20	-0.583341	1.169483	3.107023	
20	-1.86746	-0.0336	2.747756	20	-2.714040	1.953026	0.000000	
20	-1.09019	-1.56674	-2.71911	20	2.751189	1.030875	-1.594954	
20	-1.17226	-3.14691	0.582553	20	-0.583341	1.169483	-3.107023	
20	1.572413	-1.60645	2.779286	20	-2.830787	-1.496272	-1.577005	
20	1.708457	-3.14203	-0.70301	20	0.638852	-1.737112	-3.151839	
20	3.711736	0.005597	0.065983	20	-0.160807	-3.718448	0.000000	
20	1.564993	1.552444	2.809732	20	-2.830787	-1.496272	1.577005	
20	2.328335	0.031518	-2.76925	20	2.707183	-2.399939	0.000000	
23	-3.0155	-0.00403	0.001577	24	0.114715	2.987698	0.000000	
7	-4.67918	-0.00216	-0.08306	7	0.129378	4.691111	0.000000	
8	-5.90624	-0.00018	-0.14285	8	-0.003684	5.896882	0.000000	
NO/MnCa ₁₁ O ₁₂				NO/FeCa ₁₁ O ₁₂				
8	1.898230	2.248976	0.000000	8	1.493231	2.429489	0.0000000	
8	-0.974733	2.402323	1.366624	8	-1.3622	2.290604	1.4333680	
8	-3.425113	0.017329	0.000000	8	-3.40218	-0.48869	0.0000000	
8	1.443903	0.271549	3.135717	8	1.359815	0.441888	3.1508300	
8	3.378563	-0.409305	0.000000	8	3.371573	0.031	0.0000000	
8	1.184212	-3.068529	-1.537517	8	1.567316	-2.90016	-1.5377130	
8	-2.230321	-2.821995	0.000000	8	-1.84844	-3.14339	0.0000000	
8	1.443903	0.271549	-3.135717	8	1.359815	0.441888	-3.1508300	
8	-1.408808	-0.838709	-3.080561	8	-1.31071	-1.04707	-3.0716870	
8	-0.974733	2.402323	-1.366624	8	-1.3622	2.290604	-1.4333680	
8	1.184212	-3.068529	1.537517	8	1.567316	-2.90016	1.5377130	
8	-1.408808	-0.838709	3.080561	8	-1.31071	-1.04707	3.0716870	
20	0.594082	-1.760141	3.159507	20	0.804908	-1.68533	3.1602960	
20	2.769655	0.956080	1.602291	20	2.560576	1.305925	1.5927600	
20	-0.548109	1.182058	3.100589	20	-0.73463	1.072039	3.1206410	

20	-2.618102	2.024565	0.000000
20	2.769655	0.956080	-1.602291
20	-0.548109	1.182058	-3.100589
20	-2.861081	-1.419248	-1.576155
20	0.594082	-1.760141	-3.159507
20	-0.257764	-3.715860	0.000000
20	-2.861081	-1.419248	1.576155
20	2.638862	-2.465407	0.000000
25	0.251173	2.976680	0.000000
7	0.177610	4.586794	0.000000
8	-0.231059	5.714172	0.000000

NO/CoCa₁₁O₁₂

8	2.426429	1.922224	0.000000
8	-0.336492	2.449974	1.390509
8	-3.264727	0.746544	0.000000
8	1.529671	-0.052903	3.175294
8	3.216814	-1.053519	0.000000
8	0.583332	-3.261336	-1.536363
8	-2.696652	-2.293033	0.000000
8	1.529671	-0.052903	-3.175294
8	-1.492100	-0.566663	-3.110698
8	-0.336492	2.449974	-1.390509
8	0.583332	-3.261336	1.536363
8	-1.492100	-0.566663	3.110698
20	0.291737	-1.876351	3.171173
20	2.907340	0.428437	1.584568
20	-0.232856	1.220602	3.162414
20	-2.041768	2.535637	0.000000
20	2.907340	0.428437	-1.584568
20	-0.232856	1.220602	-3.162414
20	-3.012428	-0.789182	-1.573934
20	0.291737	-1.876351	-3.171173
20	-0.960207	-3.592724	0.000000
20	-3.012428	-0.789182	1.573934
20	2.129832	-2.939865	0.000000
27	0.818879	2.883055	0.000000
7	0.291024	4.546953	0.000000
8	-0.857660	4.905591	0.000000

NO/CuCa₁₁O₁₂

8	2.117994	0.000000	-2.107650
8	2.515330	-1.444436	0.936767
8	0.203231	0.000000	3.421776
8	0.189143	-3.125898	-1.465596
8	-0.649417	0.000000	-3.387725
8	-3.149026	1.538519	-1.019091
8	-2.699527	0.000000	2.379252
8	0.189143	3.125898	-1.465596
8	-0.772143	3.082444	1.445389
8	2.515330	1.444436	0.936767
8	-3.149026	-1.538519	-1.019091
8	-0.772143	-3.082444	1.445389
20	-1.792914	-3.150458	-0.511491
20	0.775996	-1.587605	-2.854006
20	1.201764	-3.106996	0.478895

20	-2.87322	1.599183	0.0000000
20	2.560576	1.305925	-1.5927600
20	-0.73463	1.072039	-3.1206410
20	-2.66428	-1.84517	-1.5788180
20	0.804908	-1.68533	-3.1602960
20	0.235434	-3.74519	0.0000000
20	-2.66428	-1.84517	1.5788180
20	2.930227	-2.10204	0.0000000
26	-0.27126	3.028814	0.0000000
7	-0.24381	4.871881	0.0000000
8	0.408322	5.877289	0.0000000

NO/NiCa₁₁O₁₂

8	2.117994	0.000000	-2.107650
8	2.515330	-1.444436	0.936767
8	0.203231	0.000000	3.421776
8	0.189143	-3.125898	-1.465596
8	-0.649417	0.000000	-3.387725
8	-3.149026	1.538519	-1.019091
8	-2.699527	0.000000	2.379252
8	0.189143	3.125898	-1.465596
8	-0.772143	3.082444	1.445389
8	2.515330	1.444436	0.936767
8	-3.149026	-1.538519	-1.019091
8	-0.772143	-3.082444	1.445389
20	-1.792914	-3.150458	-0.511491
20	0.775996	-1.587605	-2.854006
20	1.201764	-3.106996	0.478895
20	2.178143	0.000000	2.530746
20	0.775996	1.587605	-2.854006
20	1.201764	3.106996	0.478895
20	-1.261637	1.575578	2.927280
20	-1.792914	3.150458	-0.511491
20	-3.703626	0.000000	0.457476
20	-1.261637	-1.575578	2.927280
20	-2.643521	0.000000	-2.515022
28	2.797540	0.000000	-0.349634
7	4.651231	0.000000	-0.611244
8	5.406359	0.000000	0.271575

NO/ZnCa₁₁O₁₂

8	3.072804	0.572398	0.000000
8	0.640271	2.523438	1.489428
8	-2.657700	1.932427	0.000000
8	1.461888	-0.711280	3.131422
8	2.641701	-2.442952	0.000000
8	-0.690960	-3.297348	-1.536845
8	-3.305546	-1.082869	0.000000
8	1.461888	-0.711280	-3.131422
8	-1.519506	0.016212	-3.106783
8	0.640271	2.523438	-1.489428
8	-0.690960	-3.297348	1.536845
8	-1.519506	0.016212	3.106783
20	-0.401064	-1.884692	3.153433
20	2.954852	-0.956126	1.593868
20	0.346474	1.180149	3.157965

20	2.178143	0.000000	2.530746
20	0.775996	1.587605	-2.854006
20	1.201764	3.106996	0.478895
20	-1.261637	1.575578	2.927280
20	-1.792914	3.150458	-0.511491
20	-3.703626	0.000000	0.457476
20	-1.261637	-1.575578	2.927280
20	-2.643521	0.000000	-2.515022
29	2.797540	0.000000	-0.349634
7	4.651231	0.000000	-0.611244
8	5.406359	0.000000	0.271575

20	-0.854983	3.136792	0.000000
20	2.954852	-0.956126	-1.593868
20	0.346474	1.180149	-3.157965
20	-3.006733	0.424069	-1.577268
20	-0.401064	-1.884692	-3.153433
20	-2.234907	-2.967304	0.000000
20	-3.006733	0.424069	1.577268
20	0.843926	-3.670884	0.000000
30	1.746514	1.900949	0.000000
7	0.393376	6.772617	0.000000
8	-0.281019	5.840846	0.000000

HCN/ScCa₁₁O₁₂

8	2.388101	-0.007894	-1.754796
8	2.424872	-1.499219	1.185958
8	-0.243758	-0.072674	3.415767
8	0.350377	-3.097834	-1.452924
8	-0.194908	0.068605	-3.397762
8	-2.955150	1.607513	-1.349097
8	-2.991040	0.002931	2.039960
8	0.447454	3.134228	-1.330536
8	-0.870802	3.044893	1.426548
8	2.444274	1.352892	1.234858
8	-3.403174	0.005410	-1.731936
8	-3.002119	-1.465749	-1.409700
8	-0.469361	1.386967	1.968729
8	0.175082	-9.002629	-3.740149
20	-0.140407	3.151540	-1.733054
20	0.185886	0.005457	0.372229
20	2.865164	-0.698730	2.732304
20	2.963545	10.004800	22.064957
20	-0.207395	3.079612	0.738267
20	0.914134	13.048813	1.798508
20	-1.462619	3.137439	-0.641017
20	2.966854	0.855598	0.097818
20	0.917389	3.664452	1.740883
20	1.704701	0.988976	-0.802138
20	3.195892	-0.056969	0.030492
20	-1.122960	1.615478	-2.684488
20	5.326935	-0.070038	-0.034900
20	-1.145418	3.137887	0.681462
20	6.516236	0.183146	0.010214
20	-1.873015	-0.002394	2.825677
20	7.345920	-0.559758	-0.139701
20	-1.125101	-1.604733	-2.687890
20	-1.148838	-3.137358	0.673073
20	1.607987	-1.588347	2.781922
20	1.700937	-3.155830	-0.701120

HCN/TiCa₁₁O₁₂

8	-2.308077	-0.219097	-1.730104
8	-2.474803	1.182916	1.068034
8	0.130473	0.022255	3.424153
8	-0.594817	3.059941	-1.443886
8	0.234181	-0.034500	-3.394807
8	3.080082	-1.344303	-1.300481
8	2.896544	0.220582	2.097189
8	-0.143686	-3.179634	-1.375343
8	1.074052	-2.997167	1.417249
8	-2.345225	-1.565488	1.128308
8	-2.391089	-0.358193	-1.434090
8	2.867413	1.719489	-1.537278
8	0.246810	3.123158	-1.553368
20	0.447856	9.545238	-3.700687
20	-0.250757	13.351020	0.861556
20	-0.050318	30.550516	0.360226
20	2.799170	10.378053	2.794164
20	30.093215	0.409502	-2.819456
20	-0.062630	28.206079	0.642808
20	0.862829	3.242747	2.812069
20	1.293384	13.042823	-0.675633
20	3.691894	0.265326	0.987823
20	1.037660	12.792768	2.782667
20	1.716225	0.125436	0.751598
20	-1.960854	-0.239794	-0.051851
20	-1.270391	-0.031023	2.312135
20	-4.930575	-0.161696	-0.095511
20	-1.006516	-0.985521	-1.189436
20	-6.113286	0.230011	0.001281
20	-1.636279	0.387720	-2.906561
20	-6.890629	-0.581392	-0.005703
20	-1.397005	1.089749	2.786979
20	-1.249806	3.122759	-0.248941
20	1.733048	2.041221	-2.387228
20	1.506751	3.040468	1.285580

HC
N/V
Ca₁₁
O₁₂
HC
N/C
rCa
11O₁
2

20	3.701571	-0.002616	0.029514
20	1.609799	1.578589	2.786027
20	2.298407	0.002294	-2.799580
23	-2.994686	0.002841	0.001025
7	-4.969310	-0.002829	-0.087845
6	-6.131626	-0.004709	-0.111117
1	-7.197735	-0.009790	-0.094427

20	3.703027	0.104334	0.243601
20	1.857064	-1.076237	-2.869061
20	2.068498	-0.386462	2.901302
24	-2.970432	-0.048521	-0.282537
7	-4.740449	-0.073209	-0.069072
6	-5.867974	-0.116474	0.368735
1	-6.809407	0.187505	-0.094620

HCN/MnCa₁₁O₁₂

8	-2.403298	0.001829	1.777205
8	-2.381620	-1.396696	-1.239024
8	0.235175	0.006373	-3.452533
8	-0.407130	-3.124800	1.393248
8	0.180301	-0.006154	3.409727
8	2.974950	1.531559	1.393157
8	2.970644	-0.001201	-2.035051
8	-0.396471	3.122076	1.404249
8	0.933444	3.078537	-1.358702
8	-2.378584	1.411282	-1.235133
8	2.969899	-1.546280	1.387738
8	0.922959	-3.076538	-1.369550
20	1.682096	-3.149773	0.705165
20	-1.172132	-1.587846	2.695152
20	-1.160301	-3.092484	-0.662871
20	-1.830219	0.008862	-2.809134
20	-1.166225	1.583247	2.701228
20	-1.149699	3.099314	-0.652005
20	1.623718	1.579557	-2.766022
20	1.692862	3.141999	0.716235
20	3.716471	-0.006164	0.000566
20	1.617944	-1.574476	-2.771419
20	2.271332	-0.008744	2.806544
25	-2.919463	0.005834	-0.033221
7	-4.717104	0.001093	0.044086
6	-5.887284	-0.004850	0.103024

HCN/FeCa₁₁O₁₂

8	1.916674	2.315037	0.000000
8	-1.164556	2.418821	1.397869
8	-3.474812	-0.071858	0.000000
8	1.431015	0.336770	3.117031
8	3.420546	-0.339258	0.000000
8	1.266718	-3.032270	-1.539068
8	-2.161555	-2.863856	0.000000
8	1.431015	0.336770	-3.117031
8	-1.393146	-0.868177	-3.075120
8	-1.164556	2.418821	-1.397869
8	1.266718	-3.032270	1.539068
8	-1.393146	-0.868177	3.075120
20	0.641141	-1.717141	3.144652
20	2.773378	1.037287	1.589686
20	-0.596633	1.183656	3.075381
20	-2.753966	1.980595	0.000000
20	2.773378	1.037287	-1.589686
20	-0.596633	1.183656	-3.075381
20	-2.836824	-1.478326	-1.574437
20	0.641141	-1.717141	-3.144652
20	-0.163157	-3.701093	0.000000
20	-2.836824	-1.478326	1.574437
20	2.711589	-2.399428	0.000000
26	0.123779	2.831289	0.000000
7	0.155342	4.612730	0.000000
6	0.107581	5.772986	0.000000

1	-6.949054	0.005913	0.032351
N/CoCa₁₁O₁₂			
8	-2.377870	-1.366807	-1.140733
8	-2.658618	1.474299	0.924145
8	0.426988	1.623197	3.027195
8	-1.175566	1.940151	-2.495019
8	0.043772	-1.620855	-2.998798
8	3.222805	-1.481091	-0.946914
8	3.027489	1.478758	1.382695
8	0.340022	-3.511293	0.231984
8	1.708320	-1.881447	2.442230
8	-1.909896	-1.092820	2.018146
8	2.470134	1.169492	-2.321534
8	0.291984	3.452345	-0.266226
20	0.889250	2.649439	-2.233550
20	-1.588822	-0.155404	-2.810162
20	-1.788825	2.783299	-0.561076
20	-1.617184	0.943391	2.744862
20	-0.857845	-2.917332	-1.461435
20	-0.349952	-2.586601	2.094602
20	2.104730	0.196703	2.920405
20	2.393946	-2.804805	0.556726
20	3.631995	0.641263	-0.524006
20	1.383052	2.937559	1.536651
20	2.100818	-0.956385	-2.773986
27	-2.859606	-0.440219	0.451386
7	-4.791462	-0.324095	0.043402
6	-5.927722	-0.281437	-0.139970
1	-6.983833	-0.250803	-0.289394

HCN/CuCa₁₁O₁₂

8	-3.073906	0.010928	-0.205124
8	-1.272540	1.520095	2.341319
8	2.023617	0.078146	2.958601
8	-0.968246	3.080635	-0.982937
8	-1.510344	-0.078018	-2.860841
8	1.910877	-1.628571	-2.554442
8	3.651288	-0.012016	0.340181
8	-0.999990	-3.127110	-0.791526
8	1.561085	-3.076688	0.889292
8	-1.301391	-1.336587	2.418666
8	1.931042	1.440376	-2.650330
8	1.597783	3.115243	0.692362
20	1.182913	3.094780	-1.475900
20	-2.325475	1.564204	-1.667250
20	-0.541646	3.187961	1.159804
20	-0.069063	0.110614	3.490917
20	-2.336449	-1.635993	-1.565658
20	-0.580264	-3.085514	1.353935
20	2.863622	-1.543042	1.709505
20	1.150882	-3.199098	-1.276740
20	3.278886	-0.077622	-1.793585
20	2.872099	1.610367	1.606376
20	0.589961	-0.111726	-3.447149
29	-2.114888	0.075708	1.422736

1	0.069745	6.836105	0.000000	HC
HCN/NiCa₁₁O₁₂				
8	-3.074464	0.119152	-0.286734	
8	-1.240047	2.055143	1.898829	
8	1.977217	0.665214	2.938219	
8	-0.783000	2.825908	-1.685925	
8	-1.474335	-0.648938	-2.834773	
8	1.851900	-2.263000	-2.054817	
8	3.633765	-0.114172	0.451029	
8	-1.176422	-3.164862	-0.117453	
8	1.336420	-2.848676	1.609883	
8	-1.409682	-0.588757	2.517667	
8	2.043659	0.697175	-2.846141	
8	1.751529	3.101897	0.020815	
20	1.375660	2.613550	-2.100948	
20	-2.204033	1.254607	-2.046531	
20	-0.387212	3.375392	0.389864	
20	-0.118248	0.934943	3.375662	
20	-2.413672	-1.821389	-1.244573	
20	-0.810538	-2.603421	1.957005	
20	2.717651	-1.244683	2.101058	
20	0.976721	-3.461971	-0.483004	
20	3.285949	-0.647430	-1.620654	
20	2.935048	1.794405	1.291119	
20	0.635214	-0.928058	-3.312289	
28	-2.097554	0.551982	1.245423	
7	-6.984389	-0.017678	0.171457	
6	-5.835143	0.084640	0.141796	
1	-4.710008	0.152822	0.058226	

HCN/ZnCa₁₁O₁₂

8	2.353679	-0.019433	-1.845786
8	2.322040	-1.538718	1.252461
8	-0.227556	-0.024763	3.441263
8	0.284514	-3.138450	-1.429243
8	-0.270077	0.025304	-3.405005
8	-3.023971	1.585315	-1.352553
8	-2.985065	0.022343	2.062313
8	0.367183	3.144555	-1.385637
8	-0.950385	3.103321	1.390337
8	2.360775	1.453941	1.273744
8	-3.063623	-1.492684	-1.373736
8	-1.031517	-3.101554	1.347628
20	-1.798805	-3.128629	-0.721374
20	1.064938	-1.585547	-2.710960
20	1.051784	-3.164670	0.630333
20	1.838782	-0.046589	2.775451
20	1.106238	1.590634	-2.689971
20	1.134200	3.122078	0.674244
20	-1.601200	1.575365	2.786143
20	-1.716156	3.177631	-0.677881
20	-3.764039	0.045943	0.039884
20	-1.643422	-1.577636	2.764815
20	-2.354390	0.047220	-2.783630
30	2.679436	-0.038359	0.018779

7	-6.997778	-0.041115	-0.028400
6	-5.845825	-0.016753	0.041108
1	-4.712357	0.002662	0.045959

7	5.372207	-0.040277	-0.039354
6	6.502044	0.015721	-0.235646
1	7.552636	0.068940	-0.421372

Table S3.

The electronic configuration, orbital diagram, spin multiplicity and total electronic energy of free TM in the low-spin state and $\text{TMCa}_{11}\text{O}_{12}$ at B3LYP/6-311+G(D)D3 level of theory

Electronic configuration	Orbital diagram	Spin multiplicity	Energy (E_h)	$\text{TMCa}_{11}\text{O}_{12}$
$^{21}\text{Sc}[\text{Ar}] 3d^1 4s^2$ $3d^3$	$\downarrow\uparrow \uparrow$	doublet	-760.620460	$[\text{core}]4s^{(0.46)}3d^{(1.09)}4p^{(0.25)}4d^{(0.04)}$
$^{22}\text{Ti}[\text{Ar}] 3d^2 4s^2$ $3d^4$	$\downarrow\uparrow \downarrow\uparrow$	singlet	-849.290003	$[\text{core}]4s^{(0.63)}3d^{(2.26)}4p^{(0.26)}4d^{(0.04)}$
$^{23}\text{V}[\text{Ar}] 3d^3 4s^2$ $3d^5$	$\downarrow\uparrow \downarrow\uparrow \uparrow$	doublet	-943.828778	$[\text{core}]4s^{(0.17)}3d^{(2.53)}4p^{(0.15)}4d^{(0.02)}$
$^{24}\text{Cr}[\text{Ar}] 3d^5 4s^1$ $3d^6$	$\downarrow\uparrow \uparrow \uparrow \uparrow \uparrow$	triplet	-1044.223886	$[\text{core}]4s^{(0.50)}3d^{(4.59)}4p^{(0.30)}4d^{(0.02)}$
$^{25}\text{Mn}[\text{Ar}] 3d^5 4s^2$ $3d^7$	$\downarrow\uparrow \downarrow\uparrow \uparrow \uparrow \uparrow$	doublet	-1150.827718	$[\text{core}]4s^{(0.15)}3d^{(4.22)}4p^{(0.16)}4d^{(0.01)}$
$^{26}\text{Fe}[\text{Ar}] 3d^6 4s^2$ $3d^8$	$\downarrow\uparrow \downarrow\uparrow \downarrow\uparrow \uparrow \uparrow$	triplet	-1263.521952	$[\text{core}]4s^{(0.30)}3d^{(6.57)}4p^{(0.29)}$
$^{27}\text{Co}[\text{Ar}] 3d^7 4s^2$ $3d^9$	$\downarrow\uparrow \downarrow\uparrow \downarrow\uparrow \downarrow\uparrow \uparrow$	doublet	-1382.693183	$[\text{core}]4s^{(0.29)}3d^{(7.45)}4p^{(0.30)}4d^{(0.01)}$
$^{28}\text{Ni}[\text{Ar}] 3d^8 4s^2$ $3d^{10}$	$\downarrow\uparrow \downarrow\uparrow \downarrow\uparrow \downarrow\uparrow \downarrow\uparrow$	singlet	-1508.200249	$[\text{core}]4s^{(0.30)}3d^{(8.54)}4p^{(0.30)}$
$^{29}\text{Cu}[\text{Ar}] 3d^{10} 4s^1$ $3d^{10} 4s^1$	$\downarrow\uparrow \downarrow\uparrow \downarrow\uparrow \downarrow\uparrow \downarrow\uparrow \uparrow$	doublet	-1640.472257	$[\text{core}]4s^{(0.28)}3d^{(9.32)}4p^{(0.32)}$
$^{30}\text{Zn}[\text{Ar}] 3d^{10} 4s^2$ $3d^{10} 4s^2$	$\downarrow\uparrow \downarrow\uparrow \downarrow\uparrow \downarrow\uparrow \downarrow\uparrow \downarrow\uparrow$	singlet	-1779.353534	$[\text{core}]4s^{(0.33)}3d^{(9.96)}4p^{(0.37)}$

Table S4.

NBO charges (Q , $|e|$), for (CO, NO, HCN), gas/ $\text{Ca}_{12}\text{O}_{12}$ and gas/TM $\text{Ca}_{11}\text{O}_{12}$ systems at B3LYP/6-311+G(D)D3 level of theory.

System	Q _{site}	Q _C	Q _O	Q _{CO}	
CO	---	0.478	-0.478	0.000	
CO/Ca ₁₂ O ₁₂	0.316	0.217	-0.533	-0.316	
CO/ScCa ₁₁ O ₁₂	0.162	0.372	-0.534	-0.162	
CO/TiCa ₁₁ O ₁₂	-0.139	0.601	-0.462	0.139	
CO/VCa ₁₁ O ₁₂	-0.015	0.605	-0.590	0.015	
CO/CrCa ₁₁ O ₁₂	-0.119	0.680	-0.561	0.119	
CO/MnCa ₁₁ O ₁₂	-0.204	0.736	-0.532	0.204	
CO/FeCa ₁₁ O ₁₂	-0.168	0.644	-0.476	0.168	
CO/CoCa ₁₁ O ₁₂	-0.038	0.664	-0.626	0.038	
CO/NiCa ₁₁ O ₁₂	0.048	0.561	-0.609	-0.048	
CO/CuCa ₁₁ O ₁₂	-0.002	0.510	-0.508	0.002	
CO/ZnCa ₁₁ O ₁₂	0.316	0.217	-0.533	-0.316	
System	Q _{site}	Q _N	Q _O	Q _{NO}	
NO	---	0.186	-0.186	0.000	
NO/Ca ₁₂ O ₁₂	0.461	-0.150	-0.311	-0.461	
NO/ScCa ₁₁ O ₁₂	0.319	-0.055	-0.264	-0.319	
NO/TiCa ₁₁ O ₁₂	0.404	0.102	-0.506	-0.404	
NO/VCa ₁₁ O ₁₂	0.253	0.164	-0.417	-0.253	
NO/CrCa ₁₁ O ₁₂	0.113	0.282	-0.395	-0.113	
NO/MnCa ₁₁ O ₁₂	0.203	0.105	-0.308	-0.203	
NO/FeCa ₁₁ O ₁₂	0.211	0.154	-0.365	-0.211	
NO/CoCa ₁₁ O ₁₂	-0.022	0.202	-0.180	0.022	
NO/NiCa ₁₁ O ₁₂	-0.099	0.253	-0.154	0.099	
NO/CuCa ₁₁ O ₁₂	-0.026	0.250	-0.224	0.026	
NO/ZnCa ₁₁ O ₁₂	0.460	-0.150	-0.310	-0.460	
System	Q _{site}	Q _H	Q _C	Q _N	Q _{HCN}
HCN	----	0.217	0.095	-0.312	0.000
HCN/Ca ₁₂ O ₁₂	0.639	-0.722	-0.020	0.103	-0.639
HCN/ScCa ₁₁ O ₁₂	0.509	-0.612	-0.015	0.118	-0.509
HCN/TiCa ₁₁ O ₁₂	-0.024	-0.343	0.140	0.227	0.024
HCN/VCa ₁₁ O ₁₂	0.361	-0.367	-0.157	0.163	-0.361
HCN/CrCa ₁₁ O ₁₂	0.083	-0.273	-0.022	0.212	-0.083
HCN/MnCa ₁₁ O ₁₂	-0.036	-0.226	0.044	0.217	0.036
HCN/FeCa ₁₁ O ₁₂	-0.064	-0.287	0.133	0.218	0.064
HCN/CoCa ₁₁ O ₁₂	0.085	-0.416	0.061	0.270	-0.085
HCN/NiCa ₁₁ O ₁₂	0.086	-0.416	0.060	0.270	-0.086
HCN/CuCa ₁₁ O ₁₂	-0.038	-0.302	0.125	0.215	0.038
HCN/ZnCa ₁₁ O ₁₂	0.639	-0.722	-0.020	0.103	-0.639

Table S5.

The electronic configuration of TM, TMCa₁₁O₁₂, NO/TMCa₁₁O₁₂, TMCO/Ca₁₁O₁₂ and HCN/TMCa₁₁O₁₂ nanocages obtained from the natural bond orbital analysis (NBO) at B3LYP/6-311+G(D)D3 level of theory.

Electronic Configuration				
TM		NO/TMCa ₁₁ O ₁₂	CO/TMCa ₁₁ O ₁₂	HCN/TMCa ₁₁ O ₁₂
Sc	[Ar]3d ¹ 4s ²	[core]3d ^(1.23) 4p ^(0.37) 5S ^(0.12) 4d ^(0.05)	[core]4S ^(0.15) 3d ^(1.27) 4p ^(0.44) 4d ^(0.05)	[core]4S ^(0.12) 3d ^(1.10) 4p ^(0.32) 4d ^(0.05)
Ti	[Ar]3d ² 4s ²	[core]4S ^(0.16) 3d ^(2.31) 4p ^(0.46) 4d ^(0.05) 5p ^(0.01)	[core]3d ^(1.27) 4p ^(0.26) 5S ^(0.10) 4d ^(0.02)	[core]4S ^(0.17) 3d ^(2.24) 4p ^(0.41) 4d ^(0.05)
V	[Ar]3d ³ 4s ²	[core]4S ^(0.17) 3d ^(3.61) 4p ^(0.49) 4d ^(0.03)	[core]3d ^(2.44) 4p ^(0.29) 5S ^(0.10) 4d ^(0.03)	[core]4S ^(0.16) 3d ^(3.37) 4p ^(0.43) 4d ^(0.06) 5p ^(0.01)
Cr	[Ar]3d ⁵ 4s ¹	[core]3d ^(2.44) 4p ^(0.27) 5S ^(0.10) 4d ^(0.02)	[core]4S ^(0.23) 3d ^(4.84) 4p ^(0.54) 4d ^(0.02)	[core]3d ^(4.55) 4p ^(0.43) 5S ^(0.18) 4d ^(0.02) 5p ^(0.01) 6S ^(0.01)
Mn	[Ar]3d ⁵ 4s ²	[core]4S ^(0.22) 3d ^(5.69) 4p ^(0.54) 4d ^(0.02)	[core]4S ^(0.25) 3d ^(5.78) 4p ^(0.56) 4d ^(0.02)	[core]4S ^(0.19) 3d ^(5.57) 4p ^(0.43) 4d ^(0.01)
Fe	[Ar]3d ⁶ 4s ²	[core]3d ^(3.92) 4p ^(0.26) 5S ^(0.10)	[core]4S ^(0.27) 3d ^(6.78) 4p ^(0.57) 4d ^(0.01)	[core]3d ^(6.58) 4p ^(0.46) 5S ^(0.20) 4d ^(0.01) 5p ^(0.01)
Co	[Ar]3d ⁷ 4s ²	[core]3d ^(7.49) 4p ^(0.50) 5S ^(0.22) 4d ^(0.01)	[core]4S ^(0.26) 3d ^(7.50) 4p ^(0.60) 4d ^(0.01)	[core]4S ^(0.21) 3d ^(7.52) 4p ^(0.43) 4d ^(0.01)
Ni	[Ar]3d ⁸ 4s ²	[core]4S ^(0.25) 3d ^(8.32) 4p ^(0.52) 4d ^(0.01)	[core]4S ^(0.36) 3d ^(8.79) 4p ^(0.36) 4d ^(0.01)	[core]4S ^(0.29) 3d ^(8.54) 4p ^(0.29)
Cu	[Ar]3d ¹⁰ 4s ¹	[core]3d ^(9.36) 4p ^(0.53) 5S ^(0.27) 4d ^(0.01)	[core]4S ^(0.38) 3d ^(9.54) 4p ^(0.36)	[core]4S ^(0.13) 3d ^(4.96) 4p ^(0.15)
Zn	[Ar]3d ¹⁰ 4s ²	[core]4S ^(0.32) 3d ^(9.96) 4p ^(0.37)	[core]4S ^(0.32) 3d ^(9.96) 4p ^(0.38) 6p ^(0.01)	[core]4S ^(0.30) 3d ^(9.97) 4p ^(0.39) 5p ^(0.01)

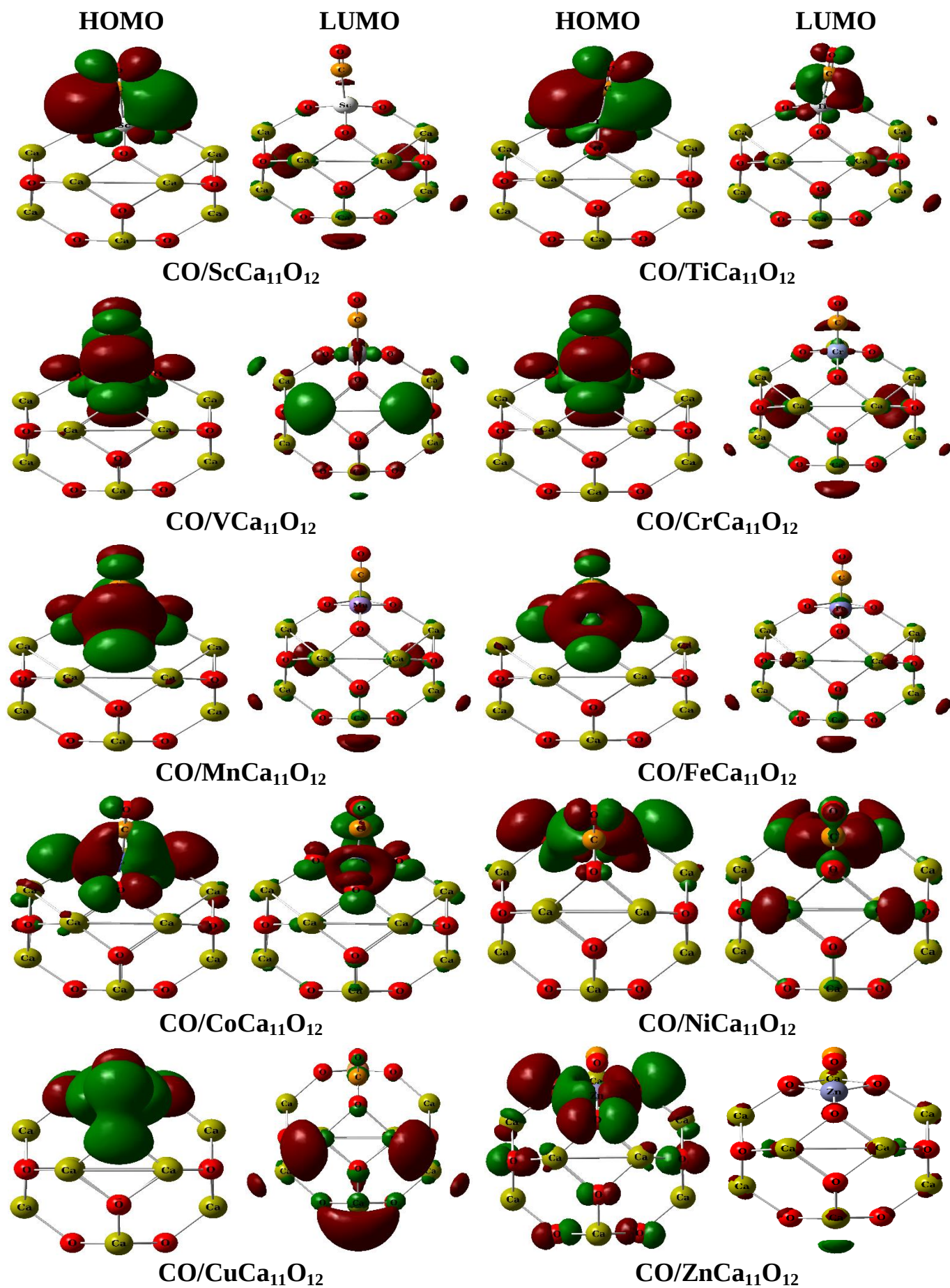


Fig. S1 HOMO-LUMO plot (isodensity contours = 0.2 a.u) of CO/TM_{Ca₁₁O₁₂} (TM = Sc to Zn).

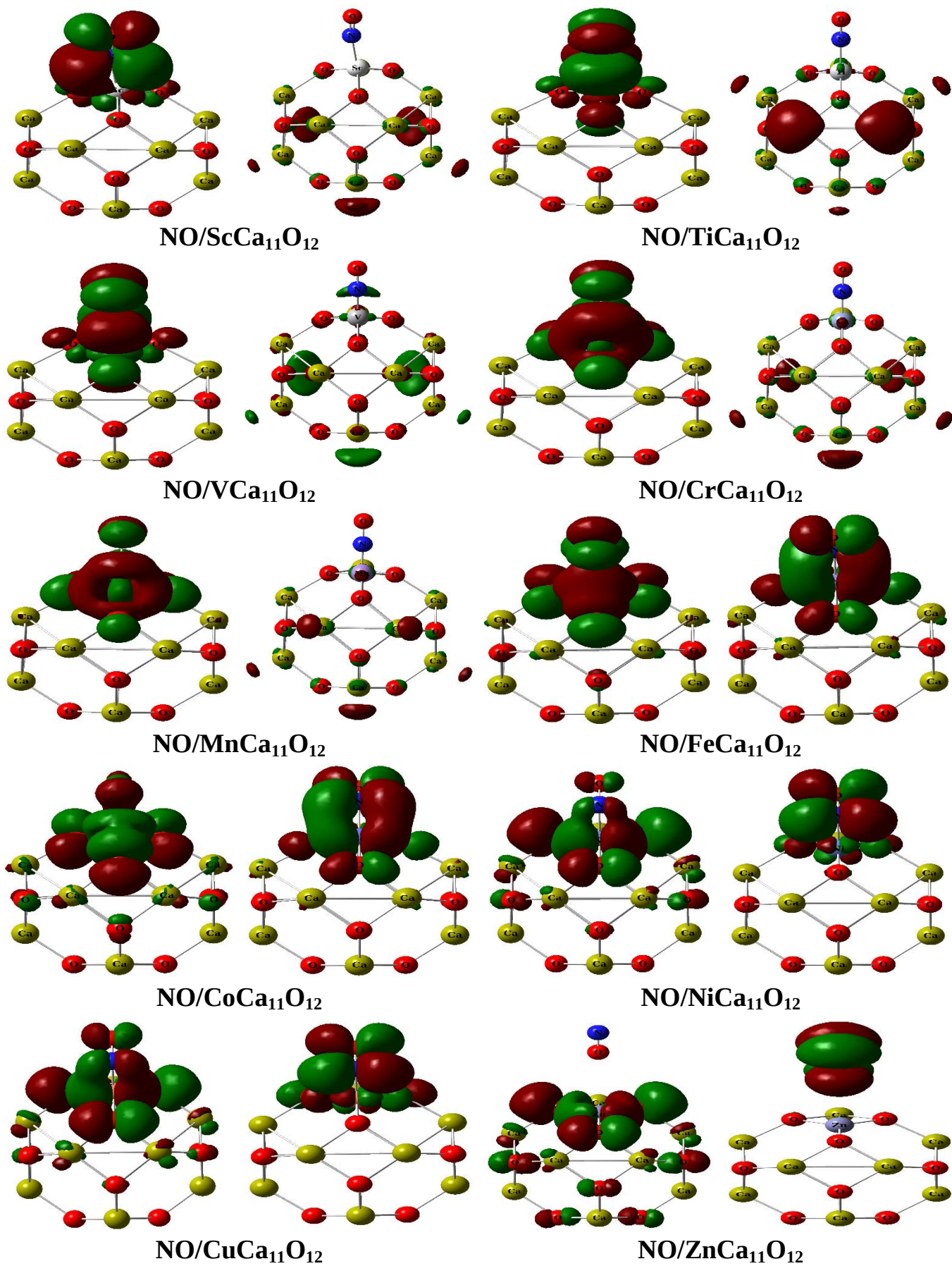
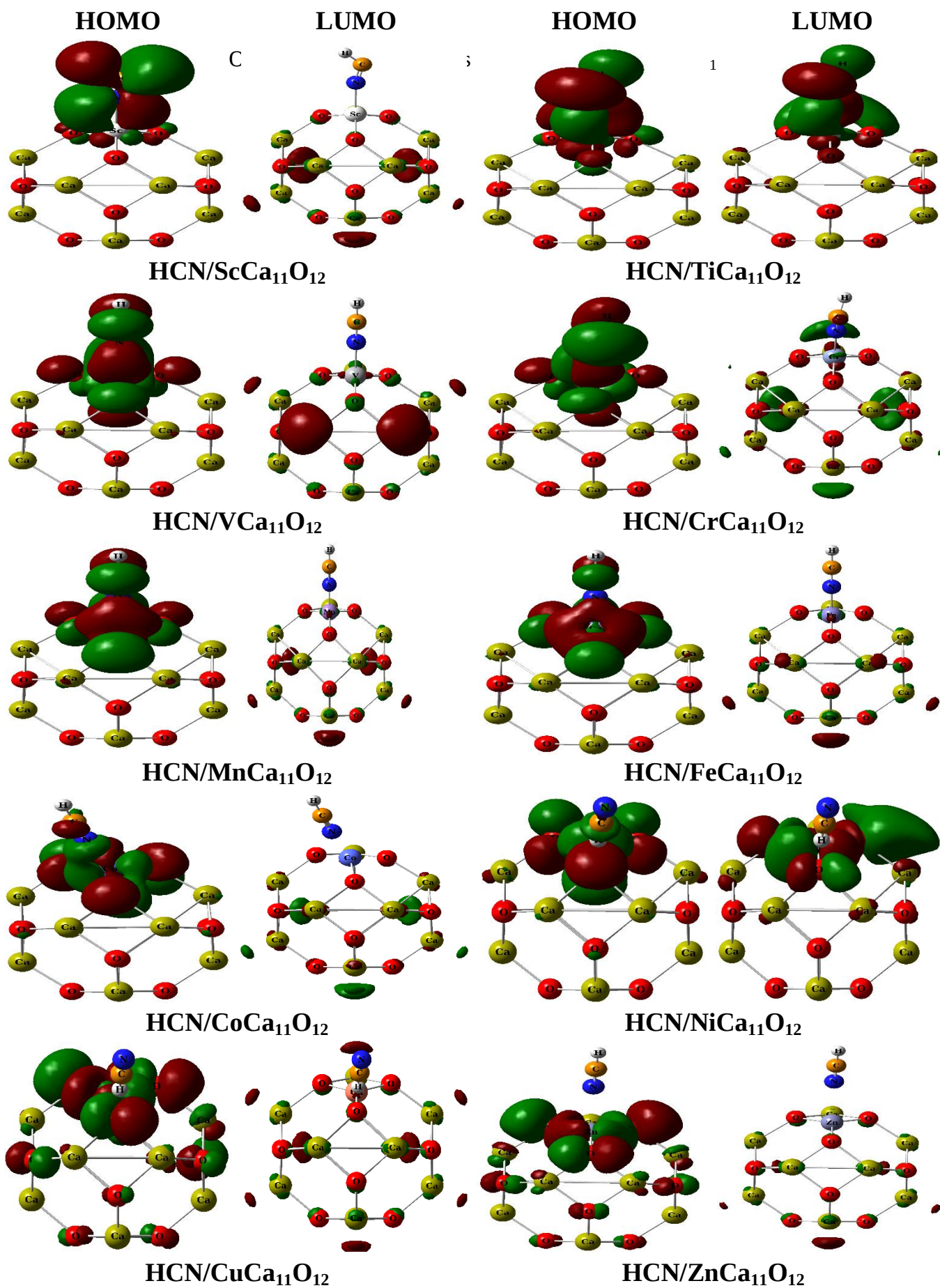


Fig. S2 HOMO-LUMO plot (isodensity contours = 0.2 a.u) of NO-TMCA₁₁O₁₂ (TM = Sc to Zn).



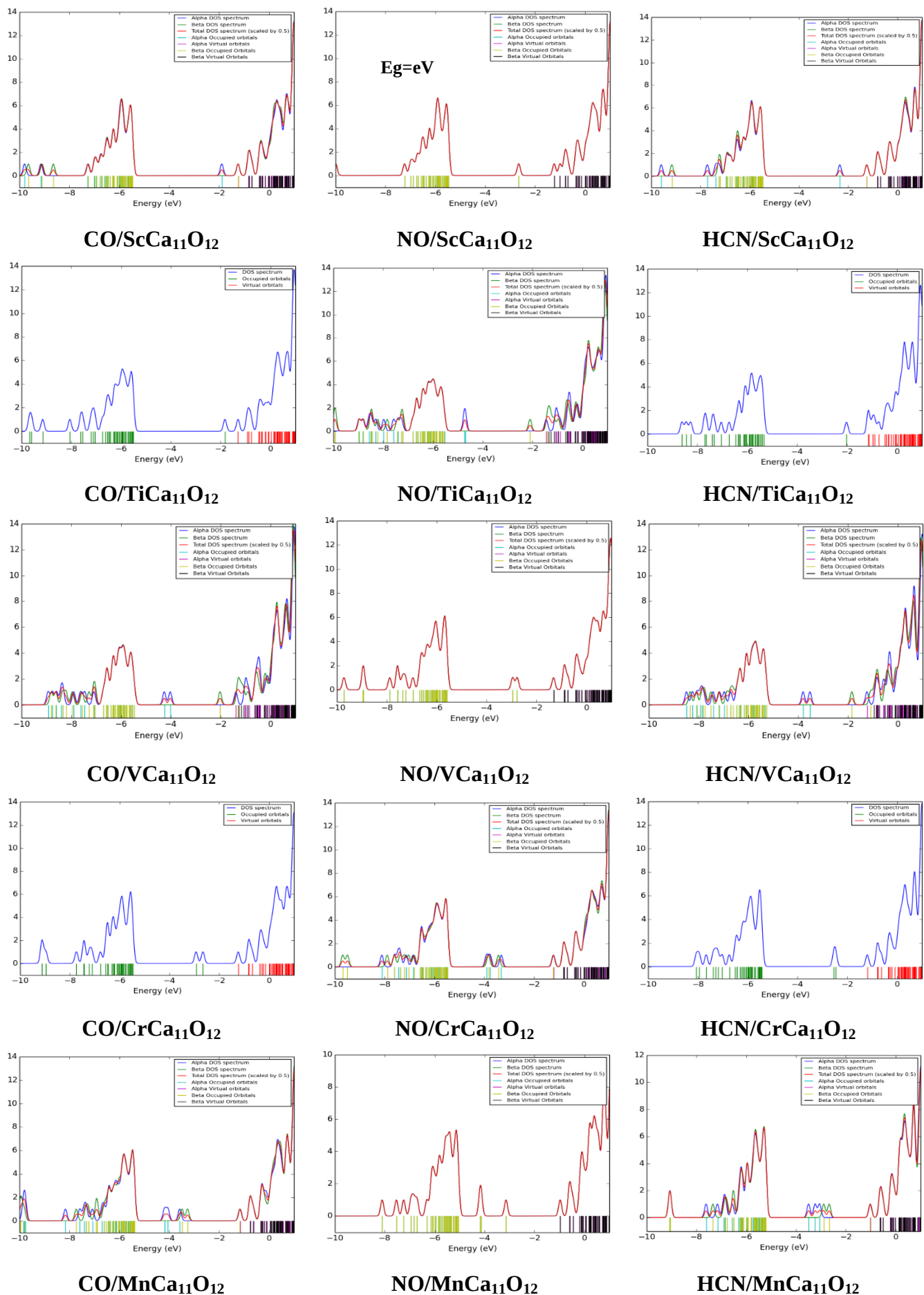


Fig. S4 Density of states (DOS) of NO/TM_{Ca11}O₁₂, CO/TM_{Ca11}O₁₂ and HCN/TM_{Ca11}O₁₂ (TM = Sc, V, Ti, Cr, Mn).

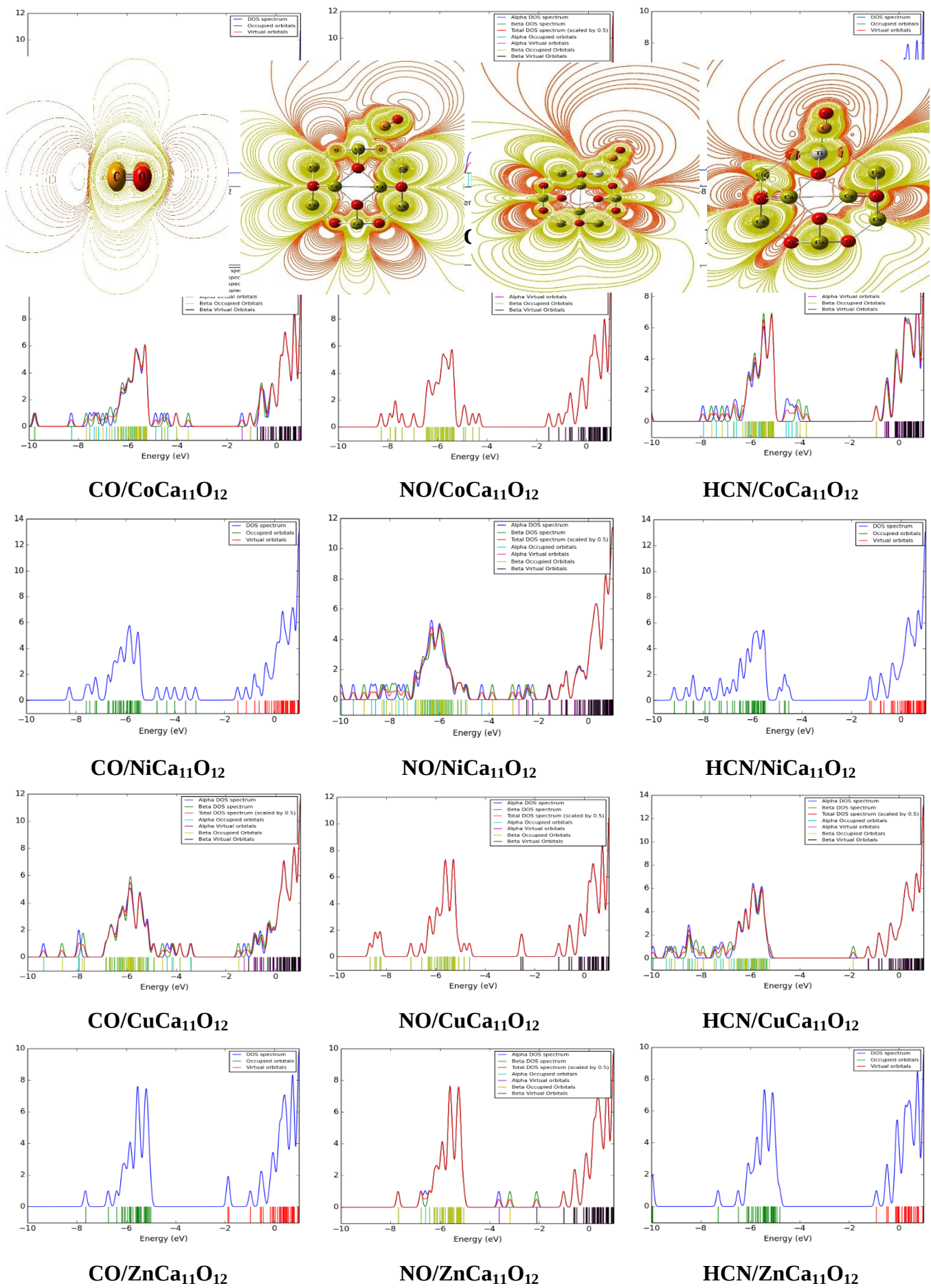


Fig. S5 Density of states (DOS) of NO/TMCo₁₁O₁₂, CO/TMCo₁₁O₁₂ and HCN/TMCo₁₁O₁₂ (TM = Fe, Co, Ni, Cu, Zn).

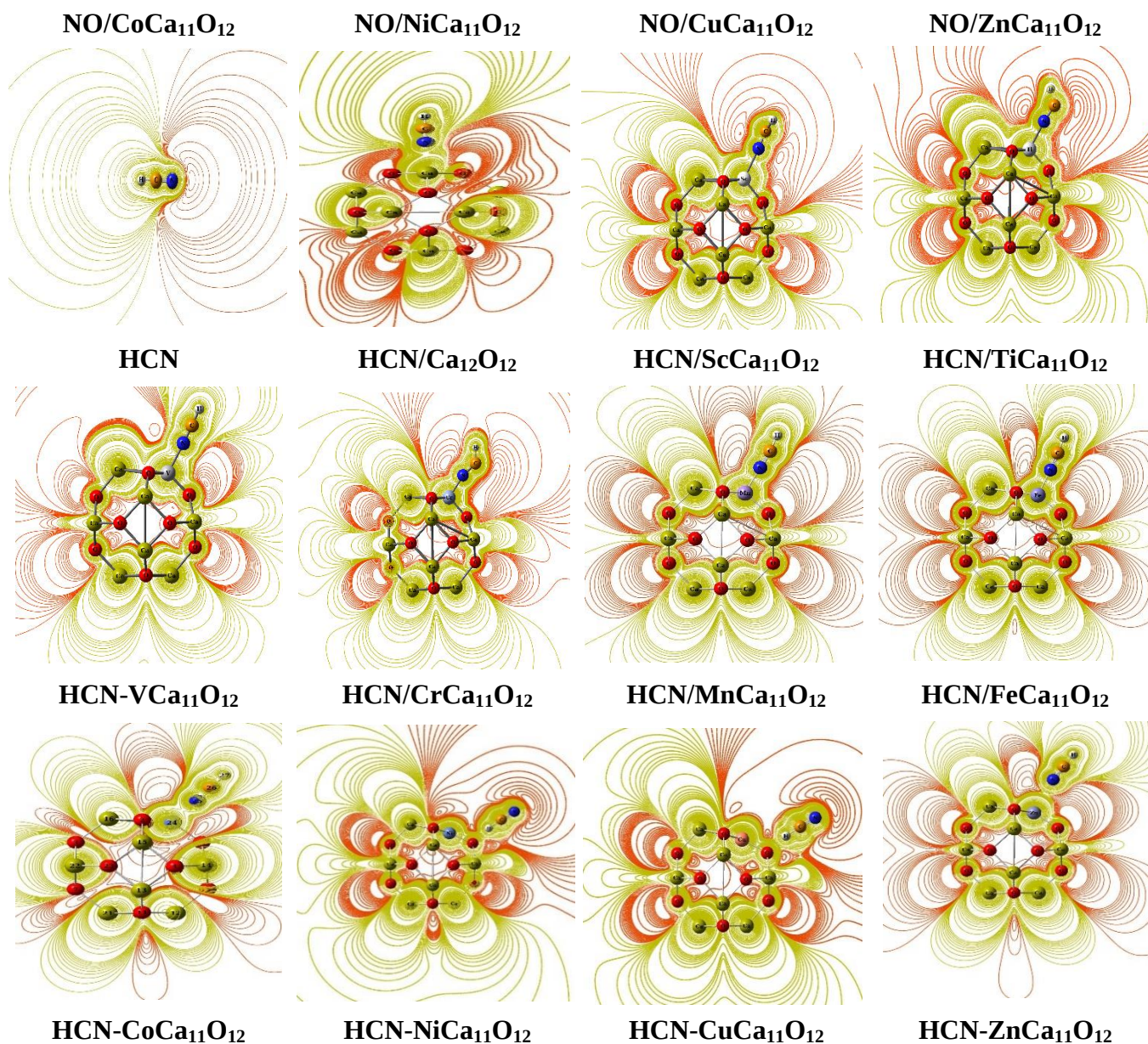
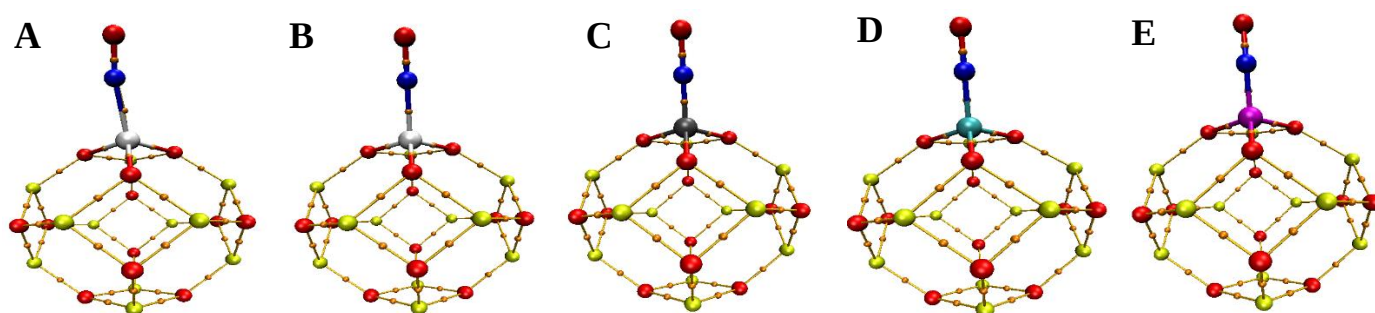


Fig. S7 Molecular electrostatic potential (MEP) contours of NO/TMCa₁₁O₁₂, (TM= Co to Zn), HCN, HCN/Ca₁₂O₁₂, and HCN/TMCa₁₁O₁₂ (TM= Sc to Zn).



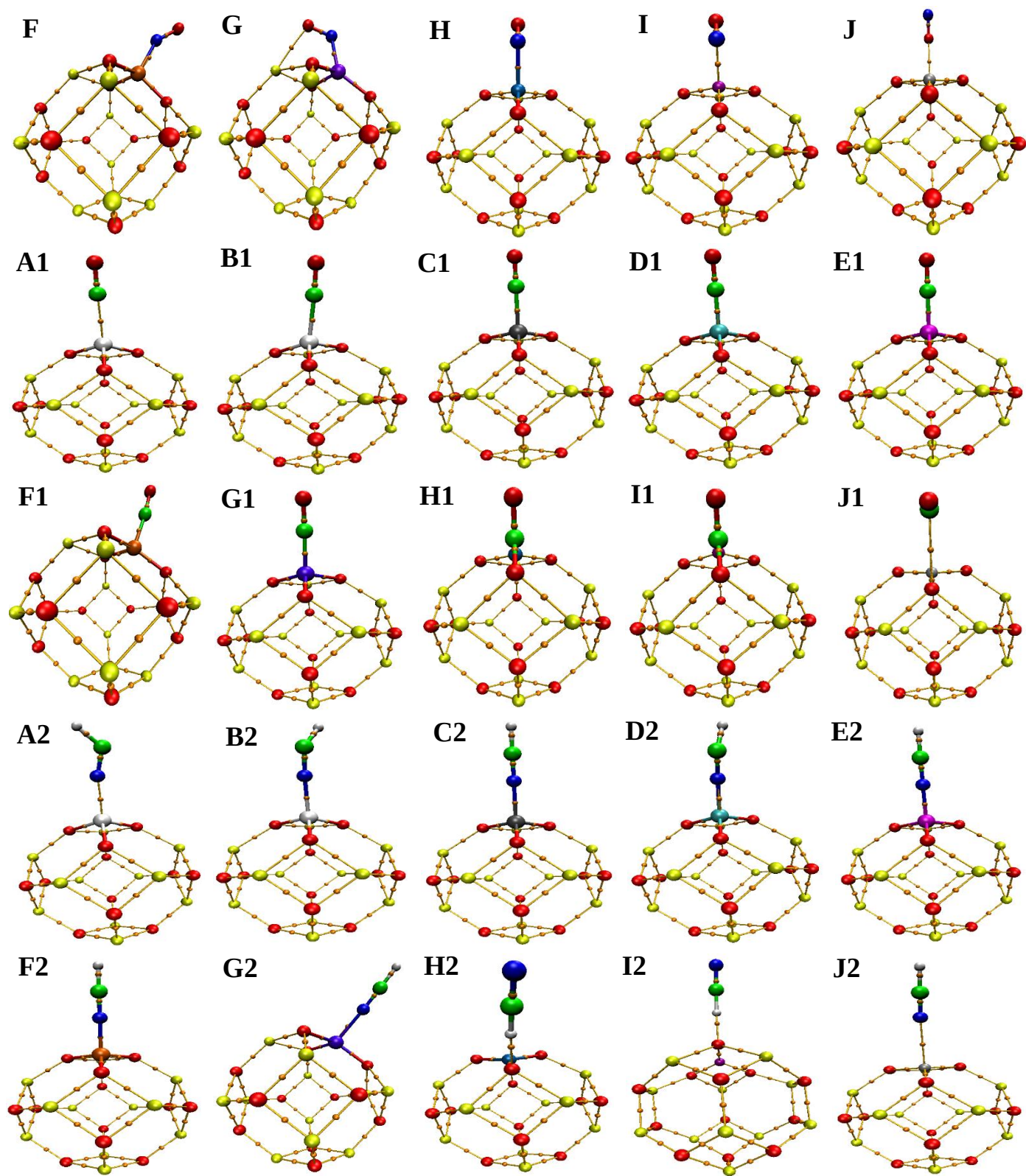
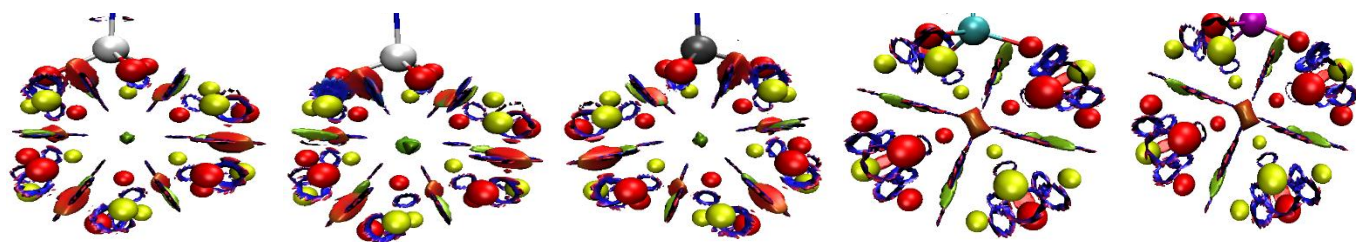


Fig. S8 QTAIM molecular graphs (A-J) for NO/TM $\text{Ca}_{11}\text{O}_{12}$, (A1-J1) for CO/TM $\text{Ca}_{11}\text{O}_{12}$, A and (A₂-J₂) for HCN/TM $\text{Ca}_{11}\text{O}_{12}$ complexes. The orange dots represent the BCPs.



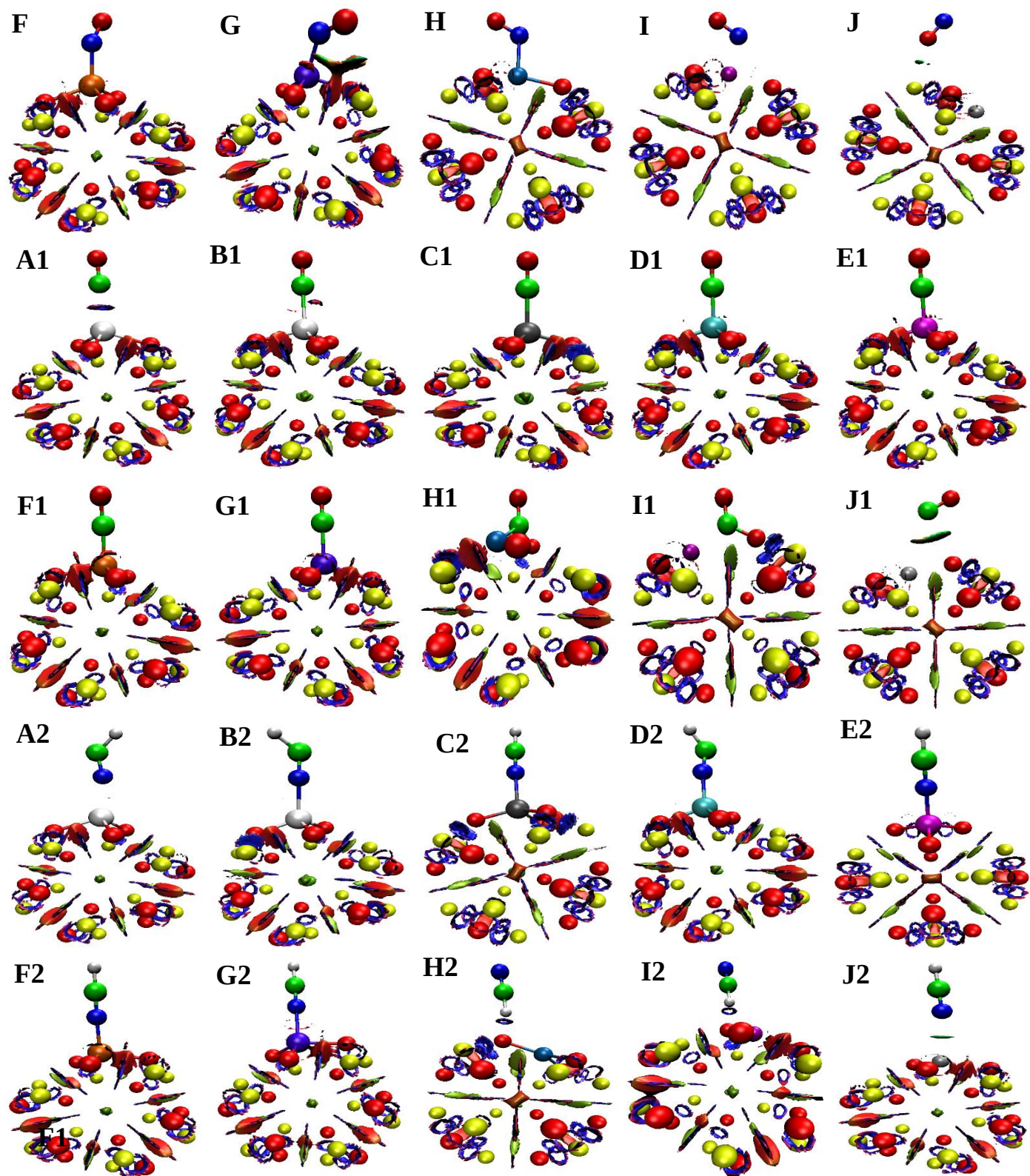
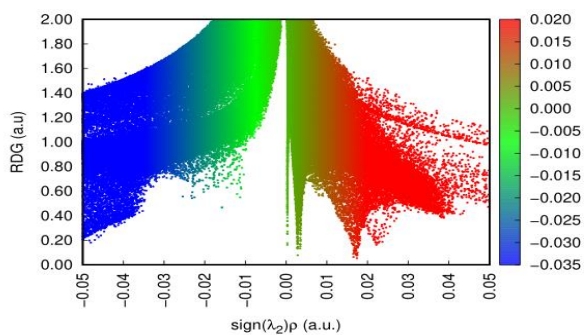
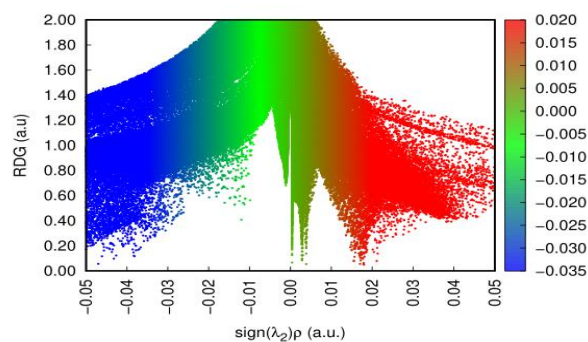


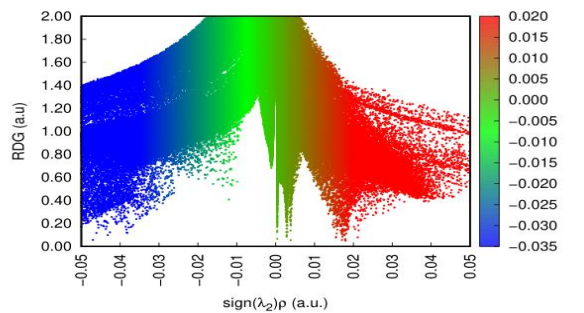
Fig. S9 NCI molecular graphs (A-J) for NO/TMCa₁₁O₁₂, (A1-J1) for CO/TMCa₁₁O₁₂, and (A₂-J₂) for HCN/TMCa₁₁O₁₂ complexes.



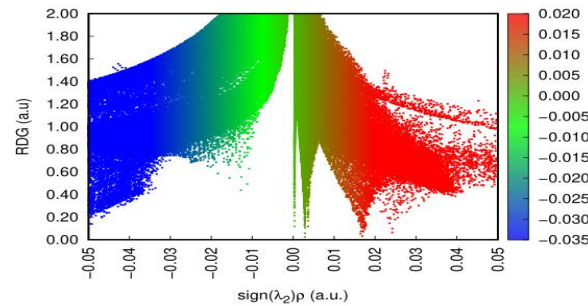
NO-Sc-Ca₁₁O₁₂



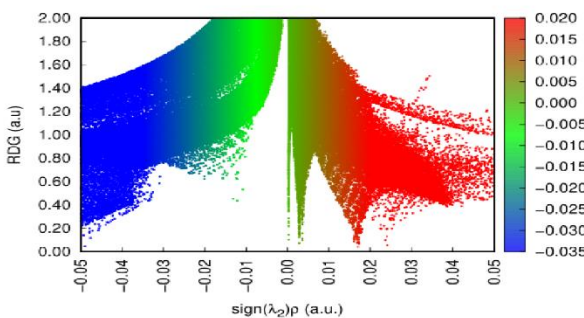
NO-Ti-Ca₁₁O₁₂



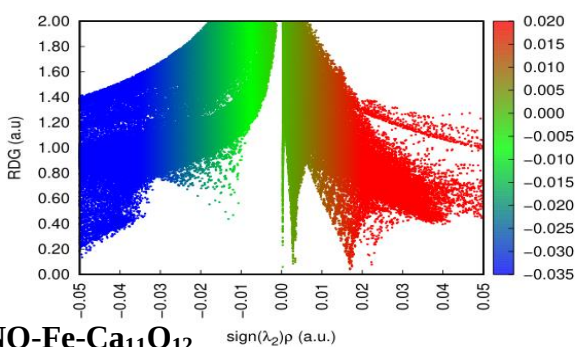
NO-V-Ca₁₁O₁₂



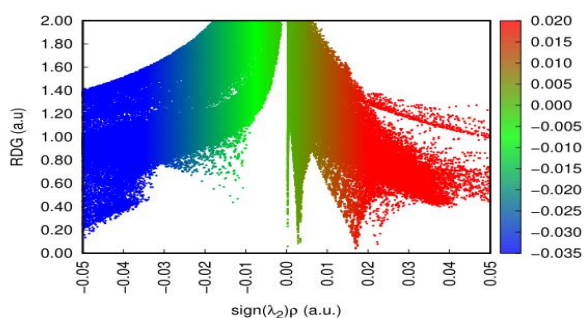
NO-Cr-Ca₁₁O₁₂



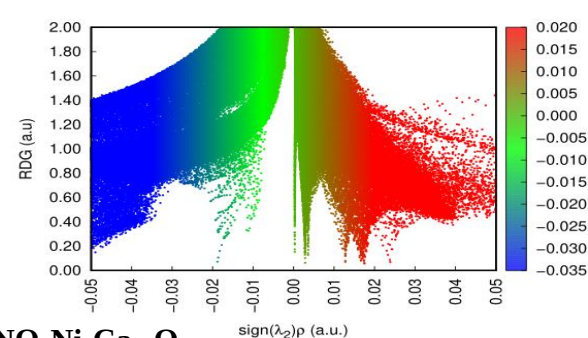
NO-Mn-Ca₁₁O₁₂



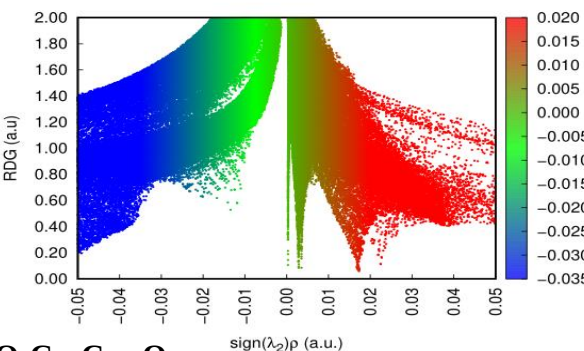
NO-Fe-Ca₁₁O₁₂



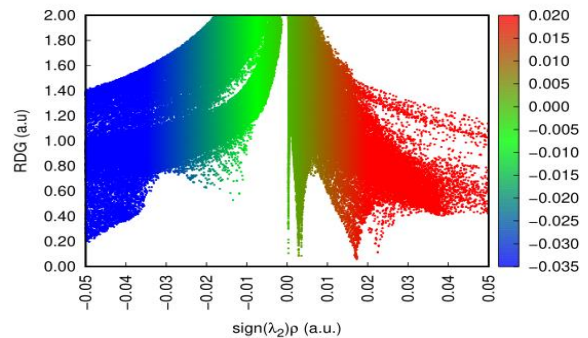
NO-Co-Ca₁₁O₁₂



NO-Ni-Ca₁₁O₁₂

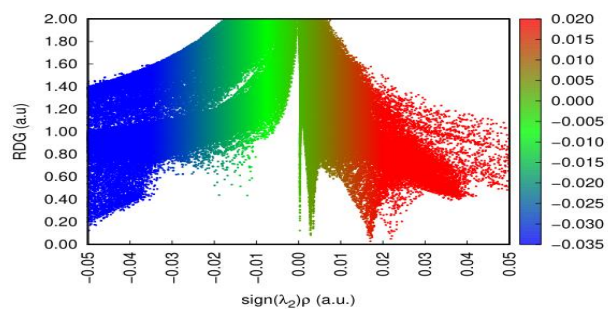


NO-Cu-Ca₁₁O₁₂

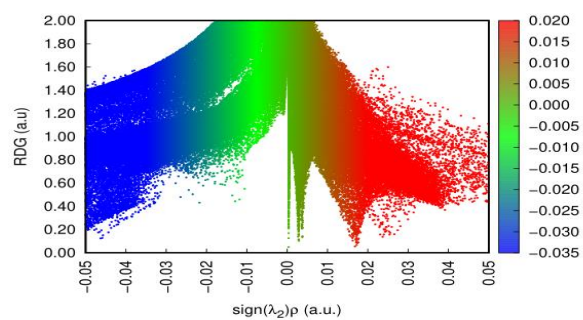


NO-Zn-Ca₁₁O₁₂

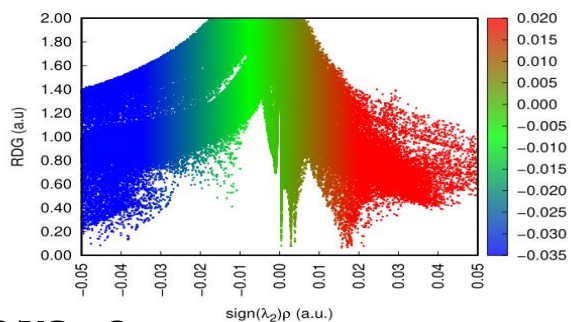
Fig. S10 Reduced density gradient scatter maps for NO/TM₁₁Ca₁₁O₁₂



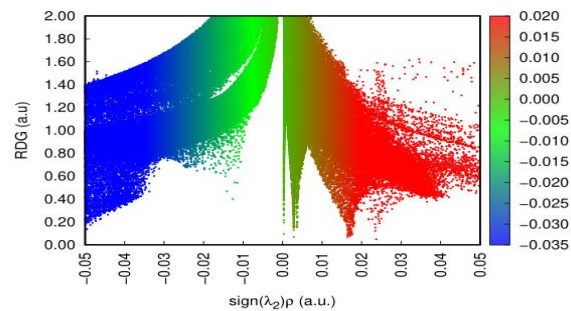
CO/ScCa₁₁O₁₂



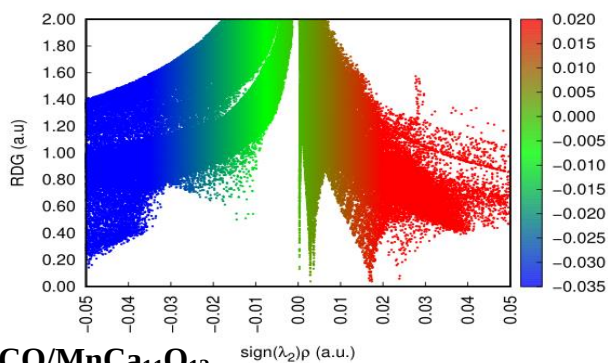
CO/TiCa₁₁O₁₂



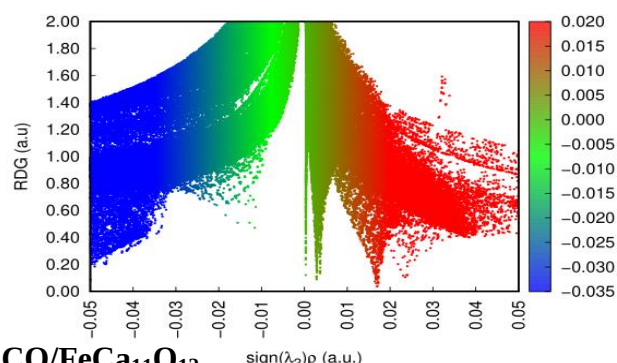
CO/VCa₁₁O₁₂



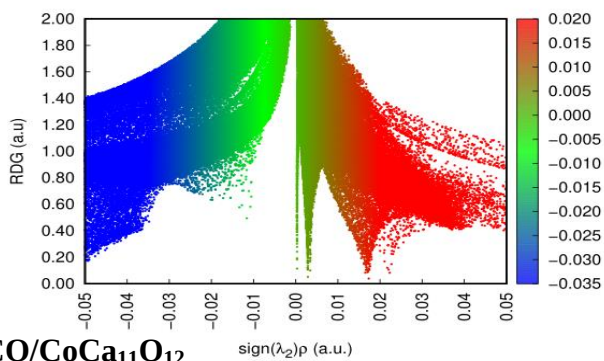
CO/CrCa₁₁O₁₂



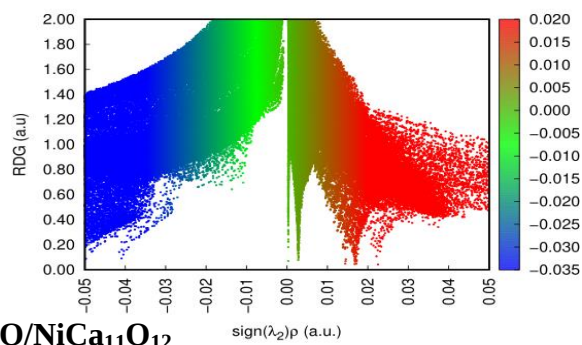
CO/MnCa₁₁O₁₂



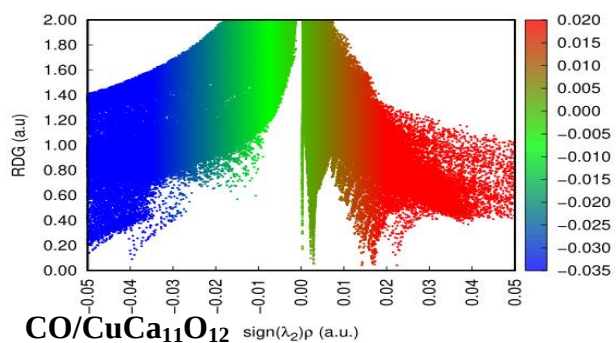
CO/FeCa₁₁O₁₂



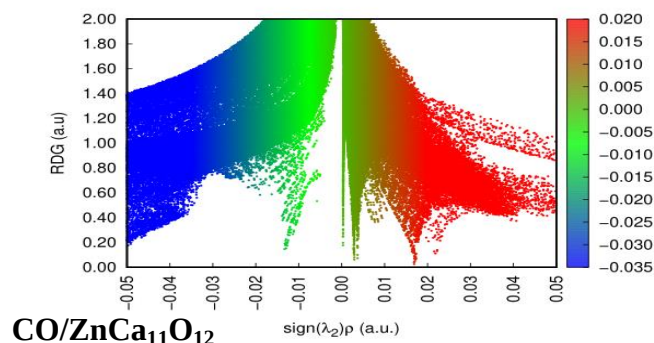
CO/CoCa₁₁O₁₂



CO/NiCa₁₁O₁₂



CO/CuCa₁₁O₁₂



CO/ZnCa₁₁O₁₂

Fig. S11 Reduced density gradient scatter maps for CO/TMCA₁₁O₁₂

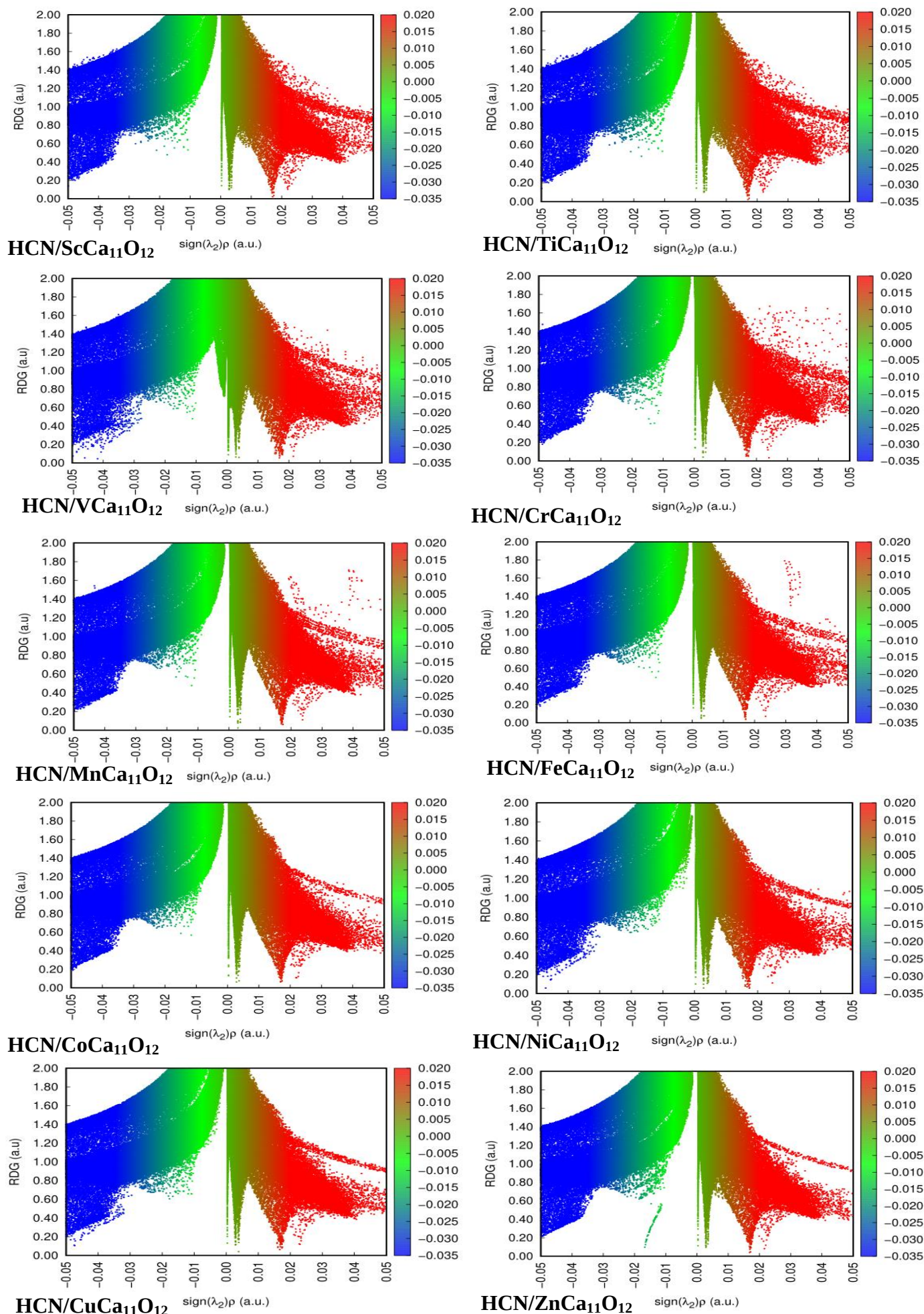


Fig. S12 Reduced density gradient scatter maps for HCN/TMCA₁₁O₁₂