New Journal of Chemistry

Supporting Information

Transition metal doping: a new and effective approach for remarkably high nonlinear optical response in aluminum nitride nanocages

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Table 1. Zero point corrected Energies (in au) of doped M@x-$Al_{12}N_{12}$ (x = b_{64}, b_{66}, r_6 and r_4, M=Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn) in four different spin states

Metals	Spin State	ZP ENERGIES			
		M@b_{64}-$Al_{12}N_{12}$	M@b_{66}-$Al_{12}N_{12}$	M@r_6-$Al_{12}N_{12}$	M@r_4-$Al_{12}N_{12}$
Sc	Doublet	-4327.828166	-4327.825633	-4327.87308	-4327.825465
	Quartet	-4327.790376	-4327.790378	-4327.817943	-4327.786508
	Sextet	-4327.694309	-4327.693848	-4327.720338	-4327.694319
	Octet	-4327.610298	-4327.610298	-4327.586442	-4327.596639
Ti	Singlet	-4416.530288	-4416.517895	-4416.55362	-4416.530219
	Triplet	-4416.5445	-4416.53942	-4416.580876	-4416.544503
	Quintet	-4416.505486	-4416.503232	-4416.495367	-4416.504887
	Septet	-4416.411204	-4416.4069	-4416.392571	-4416.411201
V	Doublet	-4511.043127	-4511.039426	-4511.019301	-4511.043128
	Quartet	-4511.066585	-4511.064296	-4511.066585	-4511.066585
	Sextet	-4511.026211	-4511.026314	-4511.02386	-4511.03786
	Octet	-4510.940626	-4510.937692	-4510.923025	-4510.940627
Cr	Singlet	-4611.441639	-4611.434413	-4611.435414	-4611.441399
	Triplet	-4611.500525	-4611.500615	-4611.514901	-4611.500528
	Quintet	-4611.547616	-4611.548152	-4611.547614	-4611.547615
	Septet	-4611.515073	-4611.514274	-4611.506221	-4611.515089
Mn	Doublet	-4717.985329	-4717.98805	-4717.988189	-4717.960025
	Quartet	-4718.035339	-4718.015734	-4718.035356	-4718.03638
	Sextet	-4718.072525	-4718.071932	-4718.038666	-4718.072521
	Octet	-4718.029509	-4718.028365	-4718.003022	-4718.029509
Fe	Singlet	-4830.647535	-4830.64858	-4830.647539	-4830.653482
	Triplet	-4830.717943	-4830.716837	-4830.685732	-4830.714816
	Quintet	-4830.747612	-4830.743752	-4830.746582	-4830.74761
	Septet	-4830.688123	-4830.686591	-4830.659588	-4830.688121
Co	Doublet	-4949.759109	-4949.757997	-4949.759107	-4949.759117
	Quartet	-4949.775685	-4949.77508	-4949.725524	-4949.775683
	Sextet	-4949.714472	-4949.713319	-4949.68523	-4949.714462
	Octet	-4949.622049	-4949.622773	-4949.669097	-4949.622771
Ni	Singlet	-5075.280392	-5075.280243	-5075.238876	-5075.274877
	Triplet	-5075.28653	-5075.286006	-5075.286524	-5075.286533
	Quintet	-5075.21506	-5075.213318	-5075.190153	-5075.204346
	Septet	-5075.122499	-5075.122845	-5075.121742	-5075.122495
Cu	Doublet	-5207.439957	-5207.438586	-5207.409821	-5207.439961
	Quartet	-5207.340936	-5207.336151	-5207.361787	-5207.338199
	Sextet	-5207.247895	-5207.242825	-5207.279274	-5207.242535
	Octet	-5207.158908	-5207.148345	-5207.16246	-5207.145215
Zn	Singlet	-5346.283532	-5346.280842	-5346.269478	-5346.283537
	Triplet	-5346.236287	-5346.236209	-5346.1999	-5346.236286
	Quintet	-5346.14431	-5346.143788	-5346.117674	-5346.144314
	Septet	-5346.055417	-5346.047454	-5346.032952	-5346.047711

Table 2. Total electronic energies (in au) of doped M@x-$Al_{12}N_{12}$ (x = b_{64}, b_{66}, r_6 and r_4, M=Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn) in four different spin states

Metals	Spin State	SCFENERGIES			
		M@b_{64}-$Al_{12}N_{12}$	M@b_{66}-$Al_{12}N_{12}$	M@r_6-$Al_{12}N_{12}$	M@r_4-$Al_{12}N_{12}$
Sc	Doublet	-4327.906305	-4327.903912	-4327.95064	-4327.903476
	Quartet	-4327.8686	-4327.8686	-4327.894479	-4327.864743
	Sextet	-4327.770091	-4327.768887	-4327.794566	-4327.770099
	Octet	-4327.685196	-4327.685196	-4327.65906	-4327.670548
Ti	Singlet	-4416.60826	-4416.596038	-4416.631239	-4416.608114
	Triplet	-4416.622788	-4416.61777	-4416.658496	-4416.622788
	Quintet	-4416.583643	-4416.581543	-4416.572304	-4416.583328
	Septet	-4416.487211	-4416.480903	-4416.467135	-4416.487212
V	Doublet	-4511.121493	-4511.117846	-4511.095903	-4511.121493
	Quartet	-4511.144948	-4511.142781	-4511.144947	-4511.144948
	Sextet	-4511.104901	-4511.105004	-4511.101391	-4511.116506
	Octet	-4511.016988	-4511.013817	-4510.998161	-4511.01699
Cr	Singlet	-4611.519923	-4611.512727	-4611.512923	-4611.519305
	Triplet	-4611.579145	-4611.579397	-4611.592517	-4611.579145
	Quintet	-4611.626232	-4611.626877	-4611.626229	-4611.626232
	Septet	-4611.593747	-4611.59305	-4611.583553	-4611.593763
Mn	Doublet	-4718.06418	-4718.066965	-4718.067023	-4718.037953
	Quartet	-4718.113716	-4718.094366	-4718.113718	-4718.114804
	Sextet	-4718.151217	-4718.150634	-4718.117234	-4718.151217
	Octet	-4718.107701	-4718.106666	-4718.078187	-4718.107704
Fe	Singlet	-4830.72645	-4830.727666	-4830.72645	-4830.731748
	Triplet	-4830.796704	-4830.79572	-4830.762145	-4830.793547
	Quintet	-4830.826507	-4830.822672	-4830.825494	-4830.826507
	Septet	-4830.766262	-4830.764709	-4830.734362	-4830.766263
Co	Doublet	-4949.838119	-4949.837338	-4949.838115	-4949.838119
	Quartet	-4949.854727	-4949.854075	-4949.804168	-4949.854726
	Sextet	-4949.792575	-4949.791626	-4949.760292	-4949.792574
	Octet	-4949.698034	-4949.698542	-4949.745374	-4949.698541
Ni	Singlet	-5075.359593	-5075.359728	-5075.316657	-5075.354146
	Triplet	-5075.365631	-5075.365169	-5075.365628	-5075.365633
	Quintet	-5075.293352	-5075.291592	-5075.265354	-5075.282438
	Septet	-5075.198552	-5075.198868	-5075.196268	-5075.19855
Cu	Doublet	-5207.519273	-5207.517842	-5207.486793	-5207.519273
	Quartet	-5207.418929	-5207.414223	-5207.439032	-5207.415683
	Sextet	-5207.323813	-5207.316806	-5207.354316	-5207.317456
	Octet	-5207.232893	-5207.222289	-5207.236701	-5207.217425
Zn	Singlet	-5346.362432	-5346.359599	-5346.348328	-5346.362443
	Triplet	-5346.314559	-5346.314667	-5346.274943	-5346.31456
	Quintet	-5346.220507	-5346.218033	-5346.193206	-5346.220518
	Septet	-5346.129814	-5346.121812	-5346.106803	-5346.121984

Table 3. Gibbs Energies (in au) of doped M@x-$Al_{12}N_{12}$ (x = b_{64}, b_{66}, r_6 and r_4, M=Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn) in four different spin states

Metals	Spin State	GIBBS ENERGIES			
		M@b_{64}-$Al_{12}N_{12}$	M@b_{66}-$Al_{12}N_{12}$	M@r_6-$Al_{12}N_{12}$	M@r_4-$Al_{12}N_{12}$
Sc	Doublet	-4327.877504	-4327.874569	-4327.922426	-4327.873262
	Quartet	-4327.839782	-4327.839783	-4327.867766	-4327.835895
	Sextet	-4327.746005	-4327.745453	-4327.77149	-4327.746075
	Octet	-4327.662167	-4327.662166	-4327.638936	-4327.648356
Ti	Singlet	-4416.579272	-4416.565075	-4416.602117	-4416.579136
	Triplet	-4416.593981	-4416.589074	-4416.630419	-4416.593984
	Quintet	-4416.555288	-4416.5539	-4416.545374	-4416.554524
	Septet	-4416.463048	-4416.458608	-4416.444122	-4416.463048
V	Doublet	-4511.092176	-4511.08831	-4511.068816	-4511.092178
	Quartet	-4511.116302	-4511.113711	-4511.1163	-4511.116302
	Sextet	-4511.076352	-4511.076539	-4511.073021	-4511.08763
	Octet	-4510.99233	-4510.989187	-4510.973617	-4510.99233
Cr	Singlet	-4611.490663	-4611.48312	-4611.483172	-4611.488624
	Triplet	-4611.549869	-4611.549562	-4611.56382	-4611.549877
	Quintet	-4611.597326	-4611.597648	-4611.597329	-4611.597325
	Septet	-4611.565442	-4611.564443	-4611.557125	-4611.565448
Mn	Doublet	-4718.033969	-4718.03656	-4718.036863	-4718.008421
	Quartet	-4718.085753	-4718.065074	-4718.085804	-4718.085674
	Sextet	-4718.122328	-4718.121797	-4718.090694	-4718.122321
	Octet	-4718.08027	-4718.079003	-4718.056122	-4718.080267
Fe	Singlet	-4830.695615	-4830.696255	-4830.695621	-4830.701023
	Triplet	-4830.767419	-4830.765851	-4830.733592	-4830.762711
	Quintet	-4830.79712	-4830.793162	-4830.796062	-4830.797113
	Septet	-4830.739084	-4830.737454	-4830.71033	-4830.739075
Co	Doublet	-4949.807796	-4949.806242	-4949.807784	-4949.807816
	Quartet	-4949.824828	-4949.82434	-4949.776355	-4949.824815
	Sextet	-4949.765282	-4949.763822	-4949.737328	-4949.765255
	Octet	-4949.673941	-4949.674518	-4949.720242	-4949.674517
Ni	Singlet	-5075.328587	-5075.32772	-5075.287271	-5075.323375
	Triplet	-5075.335361	-5075.334766	-5075.335354	-5075.335359
	Quintet	-5075.26539	-5075.263557	-5075.241264	-5075.255211
	Septet	-5075.17402	-5075.17407	-5075.172647	-5075.174013
Cu	Doublet	-5207.488292	-5207.486975	-5207.459145	-5207.488295
	Quartet	-5207.391885	-5207.386443	-5207.411702	-5207.388003
	Sextet	-5207.299508	-5207.295849	-5207.331439	-5207.293959
	Octet	-5207.21233	-5207.201107	-5207.213749	-5207.197947
Zn	Singlet	-5346.331807	-5346.329445	-5346.32	-5346.331808
	Triplet	-5346.286305	-5346.285897	-5346.250979	-5346.286303
	Quintet	-5346.195587	-5346.195033	-5346.169639	-5346.195585
	Septet	-5346.107528	-5346.099564	-5346.085014	-5346.099993

Table 4. Zero point corrected Binding Energies (in au) of doped M@x-$Al_{12}N_{12}$ (x = b_{64}, b_{66}, r_6 and r_4, M=Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn) in four different spin states

Metals	Spin State	ZP BINDING ENERGY			
		M@b_{64}-$Al_{12}N_{12}$	M@b_{66}-$Al_{12}N_{12}$	M@r_6-$Al_{12}N_{12}$	M@r_4-$Al_{12}N_{12}$
Sc	**Doublet**	-53.23	-51.64	-81.41	-51.5
	Quartet	-29.51	-29.51	-46.81	-27.1
	Sextet	30.77	31.06	14.44	30.76
	Octet	83.49	83.489	98.46	92.06
Ti	**Singlet**	-41.53	-33.75	-56.17	-41.5
	Triplet	-50.44	-47.26	-73.27	-50.4
	Quintet	-25.96	-24.55	-19.61	-25.6
	Septet	33.2	35.9	44.89	33.2
V	**Doublet**	-41.32	-39	-26.37	-41.3
	Quartet	-56.04	-54.6	-56.04	-56
	Sextet	-30.7	-30.77	-29.23	-38
	Octet	23	24.844	34.05	23
Cr	**Singlet**	8.06	12.594	11.97	8.21
	Triplet	-28.89	-28.95	-37.91	-28.9
	Quintet	-58.44	-58.78	-58.44	-58.4
	Septet	-38.02	-37.52	-32.47	-38
Mn	**Doublet**	28.9	27.195	27.11	44.78
	Quartet	-2.479	9.823	-2.49	-3.13
	Sextet	-25.81	-25.44	-4.567	-25.8
	Octet	1.179	1.897	17.8	1.179
Fe	**Singlet**	23.2	22.546	23.2	19.47
	Triplet	-20.98	-20.29	-0.767	-19
	Quintet	-39.6	-37.18	-38.95	-39.6
	Septet	-2.268	-1.306	15.64	-2.27
Co	**Doublet**	-83.91	-83.22	-37.37	-83.9
	Quartet	-94.32	-93.94	-16.3	-94.3
	Sextet	-55.9	-55.18	8.986	-55.9
	Octet	2.092	1.6378	19.11	1.639
Ni	**Singlet**	-49.09	-48.99	-23.04	-45.6
	Triplet	-52.94	-52.61	-52.93	-52.9
	Quintet	-8.09	-6.997	7.539	-1.37
	Septet	49.99	49.775	50.47	49.99
Cu	**Doublet**	-63.9	-63.04	-44.99	-63.9
	Quartet	-1.76	1.2425	-14.84	-0.04
	Sextet	56.62	59.805	36.93	59.99
	Octet	112.5	119.09	110.2	121.1
Zn	**Singlet**	-17.91	-16.22	-9.091	-17.9
	Triplet	11.74	11.786	34.57	11.74
	Quintet	69.45	69.781	86.17	69.45
	Septet	125.2	130.23	139.3	130.1

Table 5. SCF Binding Energies (in au) of doped M@x-$Al_{12}N_{12}$ (x = b_{64}, b_{66}, r_6 and r_4, M=Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn) in four different spin states

Metals	Spin State	SCF BINDING ENERGY			
		M@b_{64}-$Al_{12}N_{12}$	M@b_{66}-$Al_{12}N_{12}$	M@r_6-$Al_{12}N_{12}$	M@r_4-$Al_{12}N_{12}$
Sc	Doublet	-52.84	-52.84	-52.84	-52.84
	Quartet	-29.18	-29.18	-29.18	-29.18
	Sextet	32.63	32.63	32.63	32.63
	Octet	85.91	85.91	85.91	85.91
Ti	Singlet	-41.04	-41.04	-41.04	-41.04
	Triplet	-50.16	-50.16	-50.16	-50.16
	Quintet	-25.59	-25.59	-25.59	-25.59
	Septet	34.92	34.92	34.92	34.92
V	Doublet	-41.08	-41.08	-41.08	-41.08
	Quartet	-55.8	-55.8	-55.8	-55.8
	Sextet	-30.67	-30.67	-30.67	-30.67
	Octet	24.5	24.5	24.5	24.5
Cr	Singlet	8.351	8.351	8.351	8.351
	Triplet	-28.81	-28.81	-28.81	-28.81
	Quintet	-58.36	-58.36	-58.36	-58.36
	Septet	-37.97	-37.97	-37.97	-37.97
Mn	Doublet	28.84	28.84	28.84	28.84
	Quartet	-2.246	-2.246	-2.246	-2.246
	Sextet	-25.78	-25.78	-25.78	-25.78
	Octet	1.528	1.528	1.528	1.528
Fe	Singlet	23.1	23.1	23.1	23.1
	Triplet	-20.99	-20.99	-20.99	-20.99
	Quintet	-39.69	-39.69	-39.69	-39.69
	Septet	-1.886	-1.886	-1.886	-1.886
Co	Doublet	-84.08	-84.08	-37.54	-84.08
	Quartet	-94.5	-94.5	-16.23	-94.5
	Sextet	-55.5	-55.5	11.3	-55.5
	Octet	3.826	3.826	3.826	3.826
Ni	Singlet	-49.37	-49.37	-49.37	-49.37
	Triplet	-53.16	-53.16	-53.16	-53.16
	Quintet	-7.804	-7.804	-7.804	-7.804
	Septet	51.68	51.68	51.68	51.68
Cu	Doublet	-64.25	-64.25	-64.25	-64.25
	Quartet	-1.286	-1.286	-1.286	-1.286
	Sextet	58.4	58.4	58.4	58.4
	Octet	115.5	115.5	115.5	115.5
Zn	Singlet	-18	-18	-18	-18
	Triplet	12.04	12.04	12.04	12.04
	Quintet	71.05	71.05	71.05	71.05
	Septet	128	128	128	128

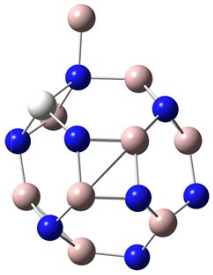
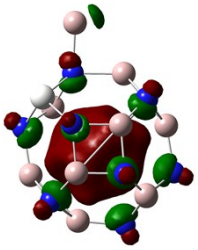
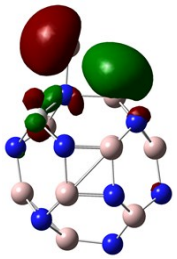
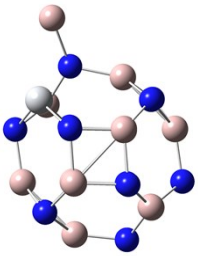
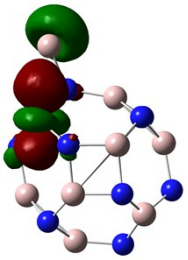
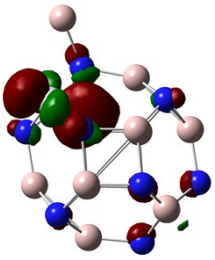
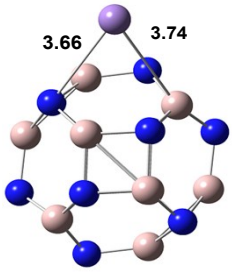
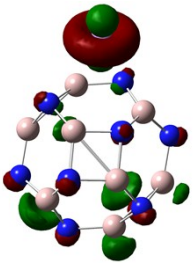
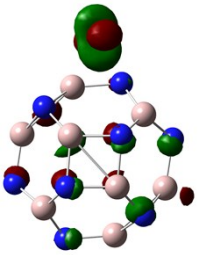
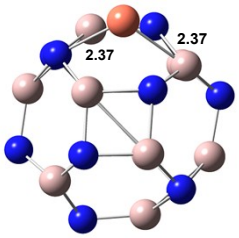
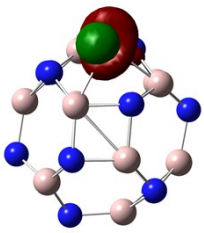
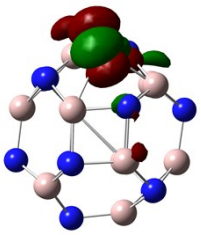
Table 6. Gibbs Binding Energies (in au) of doped M@x-$Al_{12}N_{12}$ (x = b_{64}, b_{66}, r_6 and r_4, M=Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn) in four different spin states

Metals	Spin State	GIBBS BINDING ENERGY			
		M@b_{64}-$Al_{12}N_{12}$	M@b_{66}-$Al_{12}N_{12}$	M@r_6-$Al_{12}N_{12}$	M@r_4-$Al_{12}N_{12}$
Sc	Doublet	-46.13	-44.29	-74.32	-43.47
	Quartet	-22.46	-22.46	-40.02	-20.02
	Sextet	36.385	36.731	20.39	36.34
	Octet	88.994	88.995	103.6	97.66
Ti	Singlet	-33.91	-25	-48.25	-33.83
	Triplet	-43.14	-40.06	-66.01	-43.15
	Quintet	-18.86	-17.99	-12.64	-18.38
	Septet	39.018	41.804	50.89	39.02
V	Doublet	-33.52	-31.09	-18.86	-33.52
	Quartet	-48.66	-47.03	-48.66	-48.66
	Sextet	-23.59	-23.71	-21.5	-30.67
	Octet	29.133	31.106	40.88	29.13
Cr	Singlet	16.021	20.754	20.72	17.3
	Triplet	-21.13	-20.94	-29.89	-21.14
	Quintet	-50.91	-51.11	-50.91	-50.91
	Septet	-30.9	-30.28	-25.68	-30.91
Mn	Doublet	37.263	35.637	35.45	53.29
	Quartet	4.7678	17.744	4.736	4.817
	Sextet	-18.18	-17.85	1.667	-18.18
	Octet	8.2085	9.0035	23.36	8.21
Fe	Singlet	31.822	31.42	31.82	28.43
	Triplet	-13.24	-12.25	7.991	-10.28
	Quintet	-31.87	-29.39	-31.21	-31.87
	Septet	4.5444	5.5673	22.59	4.55
Co	Doublet	-76.17	-75.2	-29.21	-76.18
	Quartet	-86.86	-86.55	-9.491	-86.85
	Sextet	-49.49	-48.58	15	-49.48
	Octet	7.8232	7.4611	25.72	7.462
Ni	Singlet	-40.81	-40.27	-25.41	-37.54
	Triplet	-45.06	-44.69	-45.06	-45.06
	Quintet	-1.154	-0.004	13.99	5.233
	Septet	56.182	56.15	57.04	56.19
Cu	Doublet	-55.88	-55.05	-37.59	-55.88
	Quartet	4.621	8.0359	-7.814	7.057
	Sextet	62.588	64.884	42.55	66.07
	Octet	117.29	124.34	116.4	126.3
Zn	Singlet	-10.25	-8.765	-2.838	-10.25
	Triplet	18.306	18.562	40.47	18.31
	Quintet	75.232	75.58	91.51	75.23
	Septet	130.49	135.49	144.6	135.2

Table 7. Binding energy (Eb, in kcal mol-1), enthalpies of reaction (ΔH, in kcal mol-1), the bond order (B.O). the bond length (dM-Al & dM-N, in Å), the NBO Charge (qM,qAl& qN, in lel), the dipole moment (μ, in Debye), first hyperpolarizability (βo,in au), HOMO (E_{HOME}, in eV), LUMO (E_{LUMO}, in eV) and HOMO LUMO gap (E_{H-L}, in eV) of transition metals doped M@x-$Al_{12}N_{12}$ (x = r_6 and r_4, M = Sc, Ti, Mn, Cu, Zn)

Properties		**Sc@$_{b66}$ (dist)-$Al_{12}N_{12}$**	**Ti@$_{b64}$ (dist)-$Al_{12}N_{12}$**	**Mn@r_6-$Al_{12}N_{12}$**	**Cu@r_6-$Al_{12}N_{12}$**	**Zn@r_6-$Al_{12}N_{12}$**	**Sc@r_4-$Al_{12}N_{12}$**
E_b(kcal/mol^{-1})		-81.41	-73.27	-4.567	-44.99	-9.091	-51.5
ΔH (kcal/mol^{-1})		-81.14	-72.97	-4.874	-44.58	-8.92	-51.93
Bond Order(B.O)		2.57	2.8	0.34	1.56	0.39	1.89
Bond Length (d)(Å)	**d_{M-Al}**	-----	-----	3.74	2.37	3.47	-----
	d_{M-N}	-----	-----	3.66	2.37	3.4	-----
q	**q_M**	1.55	1.04	0.14	0.5	0.13	0.75
	q_{Al}	1.28	1.42	1.81	1.7	1.81	1.54
	q_N	-1.83	-1.82	-1.86	-1.83	-1.87	-1.89
***μ* (D)**		3.65	2.56	0.02	0.20	0.34	4.09
***β*$_o$(au)**		5029	1084	1691	18516	96	10924
LUMO (eV)		-2.53	-2.58	-2.53	-2.1	-2.52	-2.28
HOMO (eV)		-4.23	-3.9	-5.56	-3.98	-5.87	-4.31
E_{H-L} Gap (eV)		1.71	1.32	3.02	1.88	3.35	2.03

Figure S1. Side view of optimized structures, HOMO and LUMO of optimized structures of transition metals doped M@x-$Al_{12}N_{12}$ (x = r_6 and r_4, M = Sc, Ti, Mn, Cu, Zn) (all the given bond lengths are in angstrom Å)

Optimized Structures M@x-$Al_{12}N_{12}$	**HOMO M@x-$Al_{12}N_{12}$**	**LUMO M@x-$Al_{12}N_{12}$**
 **Sc@r_6-$Al_{12}N_{12}$**	 **Sc@r_6-$Al_{12}N_{12}$**	 **Sc@r_6-$Al_{12}N_{12}$**
 **Ti@r_6-$Al_{12}N_{12}$**	 **Ti@r_6-$Al_{12}N_{12}$**	 **Ti@r_6-$Al_{12}N_{12}$**
 **Mn@r_6-$Al_{12}N_{12}$**	 **Mn@r_6-$Al_{12}N_{12}$**	 **Mn@r_6-$Al_{12}N_{12}$**
 **Cu@r_6-$Al_{12}N_{12}$**	 **Cu@r_6-$Al_{12}N_{12}$**	 **Cu@r_6-$Al_{12}N_{12}$**

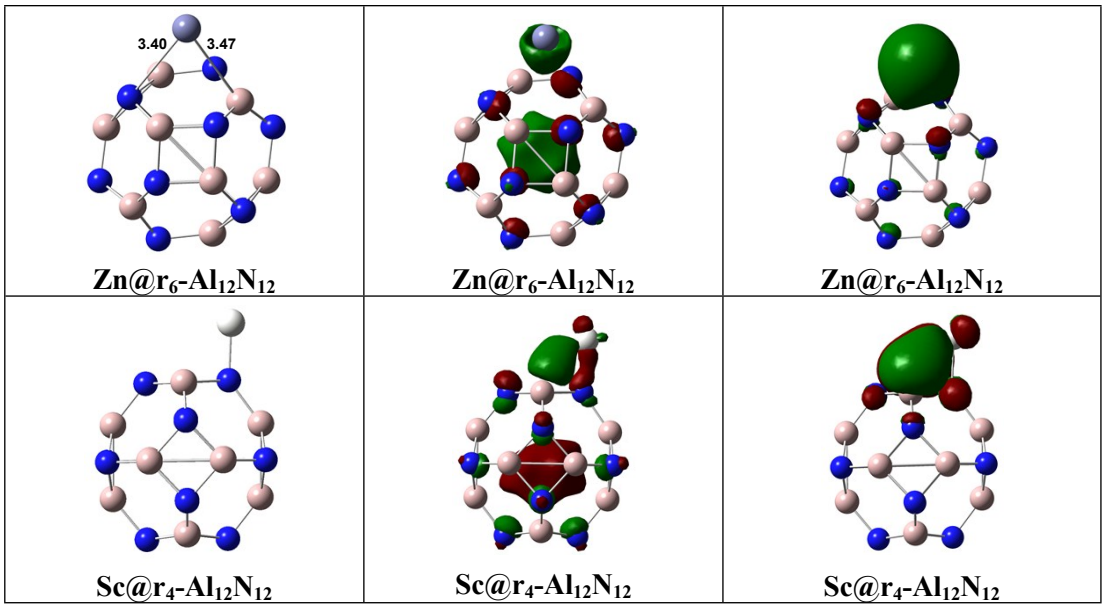
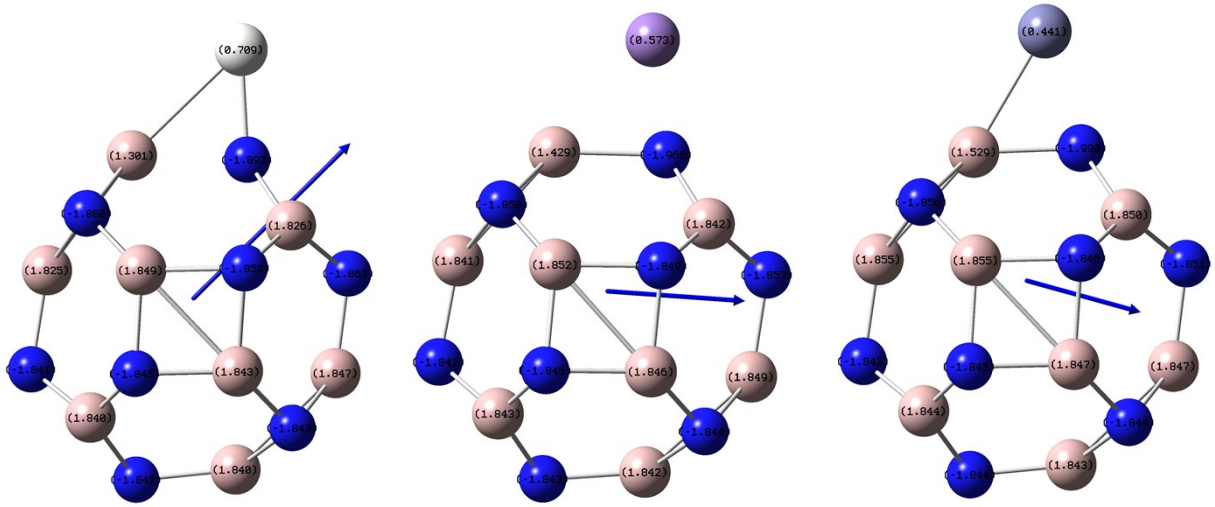


Figure S2. Illustration of changes in dipole moment vector with changes in the charge of transition metal



Sc@b66-Al12N12 **Mn@b66-Al12N12** **Zn@b66-Al12N12**

Cartesian Coordinates

UNDOPED $Al_{12}N_{12}$

Al	2.69554500	0.57149400	-0.35069000
Al	1.36331800	2.21052700	0.98191800
Al	0.48699100	1.95106500	-1.91417100
Al	1.55666900	-0.55053100	2.23287600
Al	1.59231700	-2.25892800	-0.27893700
Al	1.05322800	-0.99867400	-2.36684800
Al	-1.05320800	0.99875000	2.36689300
Al	-1.59223600	2.25909900	0.27895500
N	-0.15582100	-0.44214700	2.94721400
N	2.46584700	0.79989400	1.47931700
N	1.30005300	-2.23487400	1.49067200
N	1.87746200	2.17754800	-0.80343700
N	2.53239500	-0.97696100	-1.24187500
N	0.15564200	0.44207600	-2.94719700
N	-1.30014100	2.23491500	-1.49073000
N	-0.29798500	2.50857700	1.58923800
Al	-2.69577900	-0.57145500	0.35069000
Al	-1.36332000	-2.21078300	-0.98197000
N	-1.87729300	-2.17757100	0.80358500
N	-2.46574300	-0.79990100	-1.47938100
N	-2.53201600	0.97703000	1.24179100
N	0.29812200	-2.50827500	-1.58909800
Al	-0.48708200	-1.95113400	1.91392200

Al	-1.55672500	0.55040400	-2.23269300

Sc@b_{64}-$Al_{12}N_{12}$

Al	-2.36768500	1.75468900	-0.13062300
Al	-1.67329400	-0.52924500	-1.68603500
N	-2.76294200	-0.96689600	-0.22629500
N	-1.49640000	1.29076800	-1.74259800
Al	-0.50786500	0.98590700	2.35167200
Al	0.51708500	2.67614300	0.85972900
N	-1.24097900	2.24122400	1.21750700
N	1.21530300	1.69933500	2.27701300
Al	2.89375900	-1.28202100	0.11100100
Al	2.47197000	0.53169800	1.77491000
N	2.32133300	-1.31635800	1.88056500
N	3.36654000	0.51468300	0.14311900
Al	0.36884400	-2.66506100	-0.85131700
Al	1.28711500	-0.95658300	-2.42081900
N	2.10846100	-2.14744900	-1.25196700
N	-0.40361100	-1.68481500	-2.22185800
Al	0.20813900	1.82248500	-1.98657000
Al	2.51503900	1.49049000	-1.10311800
N	1.23473400	2.79619400	-0.78117100
N	1.63518900	0.79080100	-2.58298900
Al	-1.69428100	-1.63900400	1.08336600
Al	0.61514100	-1.83800100	2.02741900

N	-0.85203700	-0.77760700	2.48397800
N	-0.32930500	-2.85377200	0.79190900
Sc	-4.46740700	-0.07962800	-0.01407100

Ti@b_{64}-$Al_{12}N_{12}$

Al	-2.36366800	1.74917600	-0.14094500
Al	-1.67707600	-0.57651100	-1.66506800
N	-2.75999500	-1.04716100	-0.21018500
N	-1.50057900	1.24529000	-1.74245900
Al	-0.50511300	1.02600500	2.32787600
Al	0.51665800	2.70177000	0.81651400
N	-1.24092000	2.27944200	1.18966000
N	1.21729000	1.74159800	2.24305900
Al	2.90975200	-1.26527100	0.12520900
Al	2.48044400	0.57468500	1.75761300
N	2.34028500	-1.27074000	1.89645200
N	3.37317500	0.53446000	0.12530100
Al	0.39144000	-2.68331900	-0.80472900
Al	1.29127600	-0.99226900	-2.40373300
N	2.12582500	-2.15884900	-1.22007500
N	-0.39358300	-1.72554500	-2.18406200
Al	0.19922500	1.78449900	-2.01083300
Al	2.51213700	1.48399900	-1.13447900
N	1.22592200	2.78843000	-0.83027900
N	1.62946800	0.75362100	-2.59777200

Al	-1.67968500	-1.66093900	1.11689600
Al	0.63735000	-1.79858700	2.05220900
N	-0.84072800	-0.73867500	2.48042000
N	-0.29616800	-2.85673700	0.84533400
Ti	-4.33752400	-0.05809000	-0.02012100

V@b_{64}-$Al_{12}N_{12}$

Al	-2.38478400	1.69327800	-0.15598900
Al	-1.60526300	-0.54844200	-1.71205900
N	-2.71584300	-1.08091600	-0.30251400
N	-1.47939000	1.27875800	-1.75140300
Al	-0.57529000	0.90442700	2.33825400
Al	0.43889500	2.66705400	0.92164100
N	-1.31663800	2.18572200	1.23244500
N	1.12862900	1.66667300	2.32484000
Al	2.94826100	-1.21031700	0.13259000
Al	2.43281700	0.55157400	1.82525300
N	2.33883500	-1.30072300	1.88831400
N	3.36422700	0.59954100	0.21534200
Al	0.48660100	-2.64855100	-0.90787700
Al	1.37732300	-0.87262600	-2.41830100
N	2.21562100	-2.06702700	-1.26490200
N	-0.29451500	-1.65149200	-2.26122400
Al	0.21425200	1.86514300	-1.95095600
Al	2.51020700	1.57918900	-1.02586300

N	1.18572600	2.84059800	-0.70177300
N	1.68049300	0.88696800	-2.53797100
Al	-1.65017500	-1.75380600	0.99889300
Al	0.64660500	-1.87661900	1.98585500
N	-0.86647100	-0.87269600	2.42338700
N	-0.23263900	-2.90777500	0.71609900
V	-4.25952600	-0.06945000	-0.01187900

Cr@b_{64}-$Al_{12}N_{12}$

Al	-2.29352300	1.43449000	0.06915400
Al	-1.59981100	-0.32397500	-1.80427700
N	-2.57604500	-0.69228200	-0.23759000
N	-1.49602500	1.49306700	-1.64255500
Al	-0.45168200	0.62935700	2.51496300
Al	0.47207700	2.50730600	1.18251200
N	-1.25379800	1.92212700	1.47950500
N	1.23438200	1.41973300	2.48719500
Al	2.95243700	-1.22524700	-0.05835400
Al	2.51054100	0.35033000	1.83057000
N	2.40100000	-1.50270800	1.69516900
N	3.38519900	0.56131000	0.20186200
Al	0.44697000	-2.51501100	-1.19041100
Al	1.33703800	-0.61529500	-2.54383100
N	2.17523200	-1.92187800	-1.51957300
N	-0.33916000	-1.41700600	-2.45904400
Al	0.19596000	2.08303300	-1.76695100

Al	2.50248900	1.66466000	-0.90834800
N	1.19050800	2.88267000	-0.41845400
N	1.64266600	1.14692100	-2.47320800
Al	-1.59360000	-1.71124700	0.91345900
Al	0.71039500	-2.08457500	1.79783200
N	-0.75519100	-1.14360300	2.45686100
N	-0.25157800	-2.88444500	0.41903300
Cr	-4.37337800	-0.06529500	-0.01652400

Mn@b_{64}-$Al_{12}N_{12}$

Al	-2.24925100	1.34588100	0.01856300
Al	-1.55640700	-0.43275800	-1.78402800
N	-2.54515900	-0.70180300	-0.19565700
N	-1.50030600	1.39442700	-1.70095400
Al	-0.43269300	0.69723400	2.50634700
Al	0.44532600	2.54631200	1.09891400
N	-1.26864300	1.93117800	1.42269000
N	1.23235600	1.52293700	2.43964400
Al	2.99767400	-1.17893400	-0.01700400
Al	2.52522200	0.45151900	1.81719600
N	2.44963100	-1.40636900	1.74461700
N	3.39281800	0.62443600	0.18118200
Al	0.52120800	-2.55545100	-1.10574100
Al	1.37376800	-0.68764700	-2.52737200
N	2.23599600	-1.93835500	-1.45501900

N	-0.28564800	-1.52292600	-2.41722000
Al	0.17858400	2.02048500	-1.84664100
Al	2.48863800	1.66960300	-0.96612500
N	1.15045400	2.87659800	-0.51737200
N	1.64104600	1.08308300	-2.51367900
Al	-1.52443500	-1.68583100	0.95933400
Al	0.77235400	-2.02264400	1.87277300
N	-0.70684000	-1.07983000	2.49904900
N	-0.17714400	-2.87341200	0.51459300
Mn	-4.45399100	-0.06202900	-0.01415600

Fe@b_{64}-$Al_{12}N_{12}$

Al	-2.26904400	1.32571100	0.03848500
Al	-1.56001900	-0.44438200	-1.78819100
N	-2.52416600	-0.77658800	-0.20224500
N	-1.52071000	1.38202500	-1.67765900
Al	-0.43757700	0.66048000	2.51023100
Al	0.41546000	2.53829400	1.12447600
N	-1.29101900	1.90097900	1.44605100
N	1.21694400	1.50797400	2.44974800
Al	3.01895200	-1.14137500	-0.03579100
Al	2.52630200	0.46411800	1.81519900
N	2.48049100	-1.39374500	1.72547100
N	3.38827800	0.66579500	0.17936100
Al	0.55716000	-2.54368400	-1.12952500

Al	1.37809000	-0.64887000	-2.53418700
N	2.26178200	-1.89776900	-1.47785100
N	-0.26868700	-1.50721400	-2.42645600
Al	0.14830200	2.03353600	-1.82405400
Al	2.46539900	1.70881300	-0.95462200
N	1.11156300	2.89237900	-0.49072100
N	1.62133500	1.12490000	-2.50509500
Al	-1.49607300	-1.74042000	0.95392000
Al	0.81255600	-2.03443800	1.85091800
N	-0.68033900	-1.12091900	2.48769400
N	-0.12672000	-2.89362100	0.49098300
Fe	-4.30595600	-0.05771400	-0.01323500

Co@b_{64}-$Al_{12}N_{12}$

Al	-2.25763900	1.29028100	0.01176200
Al	-1.51844200	-0.44591700	-1.81614600
N	-2.49461100	-0.78389000	-0.24311500
N	-1.50001900	1.38126400	-1.69972800
Al	-0.46182400	0.64014400	2.50256500
Al	0.39518700	2.53176700	1.13826900
N	-1.30964900	1.88043100	1.43395100
N	1.18771900	1.49972700	2.46872600
Al	3.03635000	-1.12407800	-0.00961300
Al	2.51102500	0.46755500	1.84435300
N	2.47681600	-1.38994800	1.74278000

N	3.39097400	0.68386600	0.21969900
Al	0.60023600	-2.53745500	-1.14340300
Al	1.42577400	-0.62832600	-2.52619100
N	2.30427800	-1.87761400	-1.46611400
N	-0.21598500	-1.49968700	-2.44573500
Al	0.16679300	2.04388200	-1.81746300
Al	2.47528500	1.72724900	-0.91990100
N	1.10875200	2.89948600	-0.46637700
N	1.65444300	1.14698600	-2.48393400
Al	-1.48634400	-1.75732800	0.91724400
Al	0.81188700	-2.04300600	1.84343200
N	-0.69467200	-1.14305000	2.46697000
N	-0.10335700	-2.89920700	0.46586200
Co	-4.24853900	-0.05298300	-0.01017400

Ni@b_{64}-$Al_{12}N_{12}$

Al	-2.26294300	1.23894400	-0.00083300
Al	-1.49680500	-0.50018800	-1.80825400
N	-2.46743700	-0.82724400	-0.23382200
N	-1.51250000	1.32904400	-1.71634600
Al	-0.45969800	0.65421200	2.49848400
Al	0.36395000	2.54161800	1.10923400
N	-1.32882200	1.86537600	1.41456500
N	1.17547500	1.54004600	2.45221400
Al	3.06386700	-1.08358700	0.00299600

Al	2.51334700	0.52111900	1.83795000
N	2.50752100	-1.33770800	1.75814500
N	3.38949100	0.73247800	0.21076000
Al	0.65127700	-2.54747700	-1.11414100
Al	1.44699600	-0.64310600	-2.52023600
N	2.34513700	-1.86564600	-1.44504600
N	-0.18001600	-1.54018800	-2.43041400
Al	0.14275800	2.01679500	-1.84253300
Al	2.45590100	1.74707200	-0.94023300
N	1.07076800	2.90193700	-0.50016400
N	1.64557400	1.13624000	-2.49787300
Al	-1.45004200	-1.77046900	0.93866000
Al	0.85246300	-2.01467900	1.86794200
N	-0.66689600	-1.13241600	2.48451800
N	-0.05008500	-2.89686900	0.49860800
Ni	-4.18469300	-0.05066500	-0.01226700

Cu@b_{64}-$Al_{12}N_{12}$

Al	-2.25206500	1.25343500	-0.00928700
Al	-1.49071900	-0.49365800	-1.82249500
N	-2.45434600	-0.84819800	-0.25915800
N	-1.49773900	1.33714600	-1.71905600
Al	-0.46372000	0.64391400	2.49583100
Al	0.36878200	2.53812400	1.11965100
N	-1.32711000	1.86445800	1.41653700

N	1.17216900	1.52916800	2.46101500
Al	3.06892100	-1.08474200	0.00885400
Al	2.51298300	0.51265100	1.84837900
N	2.50699000	-1.34535700	1.76131500
N	3.39509100	0.73042200	0.22531300
Al	0.65897500	-2.54240200	-1.12396100
Al	1.46219800	-0.63268100	-2.51837800
N	2.35510400	-1.86017600	-1.44494200
N	-0.16557700	-1.52766300	-2.43933800
Al	0.15856900	2.02328600	-1.83587100
Al	2.46758700	1.75024900	-0.92568200
N	1.08066300	2.90358300	-0.48605000
N	1.66342300	1.14647000	-2.48920200
Al	-1.44855500	-1.78032600	0.92523400
Al	0.85149600	-2.02272300	1.86042100
N	-0.67084700	-1.14215300	2.47366900
N	-0.04460300	-2.90209700	0.48591800
Cu	-4.09380700	-0.04641000	-0.00679900

Zn@b_{64}-$Al_{12}N_{12}$

Al	-2.18195900	1.12964100	-0.02853400
Al	-1.44665700	-0.64290500	-1.75705100
N	-2.39152900	-0.85290700	-0.14748800
N	-1.50865000	1.19464500	-1.76452400
Al	-0.38887400	0.74720400	2.49092100

Al	0.36341800	2.58544600	0.99145600
N	-1.30869600	1.87832500	1.35714800
N	1.21712500	1.67516500	2.37113800
Al	3.13981700	-1.02128100	0.02504500
Al	2.56966100	0.65524700	1.78772900
N	2.60746000	-1.20406100	1.79686100
N	3.42236100	0.81092700	0.14296600
Al	0.75073800	-2.58988000	-0.99476800
Al	1.48786700	-0.74326200	-2.50620300
N	2.42487900	-1.88545400	-1.37717600
N	-0.11470300	-1.67633800	-2.35905600
Al	0.12637700	1.92000900	-1.94192500
Al	2.44998000	1.74217400	-1.04398000
N	1.03985900	2.88237200	-0.64320800
N	1.64235800	1.04153100	-2.56504000
Al	-1.33817900	-1.74173800	1.03580800
Al	0.97209800	-1.91994400	1.96056400
N	-0.55597600	-1.04022000	2.55709100
N	0.07306200	-2.87613400	0.64071200
Zn	-4.34628500	-0.04013900	-0.01045900

Sc@b_{66}-$Al_{12}N_{12}$

Al	-0.34819800	-1.01144900	2.45578700
Al	1.16468800	0.99041500	2.47920100
N	1.49906200	-0.82093200	2.64711000

N	-0.68133300	0.81403100	2.64699000
Al	-0.07395700	-2.67573500	-0.00007100
Al	-2.34815400	-1.50383300	0.00035700
N	-1.19341900	-2.13745800	1.36318500
N	-1.19388100	-2.13735900	-1.36288700
Al	1.16368400	0.99077000	-2.47931500
Al	-0.34916800	-1.01112100	-2.45564100
N	1.49801400	-0.82055300	-2.64771400
N	-0.68241100	0.81436500	-2.64627400
Al	2.90802800	1.23375900	-0.00041400
Al	0.91510000	2.72680500	0.00006000
N	2.00813400	2.12196200	-1.36772800
N	2.00862100	2.12174100	1.36736200
Al	-1.57000300	1.51121800	1.26911300
Al	-1.57077700	1.51145500	-1.26813800
N	-2.60539000	0.54942600	0.00080400
N	-0.88312100	2.66658900	0.00041400
Al	2.40587200	-1.48505400	1.24747000
Al	2.40531900	-1.48486500	-1.24848100
N	1.72357900	-2.67151100	-0.00044200
N	3.37169000	-0.49541700	-0.00064300
Sc	-4.53421200	0.12690800	-0.00001300

Ti@b_{66}-$Al_{12}N_{12}$

Al	-0.33566900	-1.00846200	2.46018400

Al	1.18864400	0.98411200	2.48005500
N	1.51240900	-0.83024000	2.64516400
N	-0.65794600	0.81917500	2.65389700
Al	-0.07993400	-2.68119200	-0.00192500
Al	-2.30522900	-1.43023900	0.00448800
N	-1.18960700	-2.12552100	1.36356900
N	-1.19566100	-2.12231700	-1.36109600
Al	1.17692500	0.99003900	-2.48107800
Al	-0.34701400	-1.00274000	-2.45926200
N	1.50016400	-0.82395100	-2.65242700
N	-0.67043800	0.82521100	-2.64611000
Al	2.92678600	1.21702500	-0.00445000
Al	0.94481800	2.72512600	0.00173800
N	2.03100500	2.11333200	-1.36894000
N	2.03703300	2.11000600	1.36618100
Al	-1.54296000	1.51687900	1.27288700
Al	-1.55034900	1.51923200	-1.25981200
N	-2.57021800	0.54899500	0.00947000
N	-0.85372100	2.67332900	0.00582700
Al	2.40960100	-1.50025000	1.24176600
Al	2.40351700	-1.49721400	-1.25457200
N	1.71782800	-2.68209100	-0.00613600
N	3.37831800	-0.51548700	-0.00755900
Ti	-4.49240700	0.10212700	-0.00059700

V@b_{66}-$Al_{12}N_{12}$

Al	-0.34758000	-0.99140500	2.45787200
Al	1.21576700	0.96963000	2.47924400
N	1.50300800	-0.85039900	2.64751900
N	-0.63405800	0.84211300	2.64857500
Al	-0.12173600	-2.66991200	-0.00121200
Al	-2.32482500	-1.38093100	0.00016000
N	-1.22270200	-2.09139800	1.36185900
N	-1.22351500	-2.08992900	-1.36297000
Al	1.21382600	0.97248000	-2.47866000
Al	-0.34935600	-0.98871900	-2.45847400
N	1.50110200	-0.84734100	-2.64935500
N	-0.63610300	0.84501000	-2.64670100
Al	2.96436200	1.16507700	-0.00029600
Al	1.01453100	2.71413200	0.00127200
N	2.09010600	2.07902500	-1.36715000
N	2.09105400	2.07743800	1.36824500
Al	-1.50324300	1.55808400	1.26639200
Al	-1.50454100	1.55944200	-1.26321700
N	-2.55836000	0.62138600	0.00176800
N	-0.78406300	2.69770700	0.00186700
Al	2.38870600	-1.53937900	1.24631600
Al	2.38769500	-1.53791000	-1.24950000
N	1.67579800	-2.70779800	-0.00199700
N	3.38109500	-0.57609000	-0.00143900

V	-4.42262600	0.09583800	-0.00000800

$Cr@b_{66}$-$Al_{12}N_{12}$

Al	-0.33170100	-0.98946200	2.46050900
Al	1.22852800	0.97405300	2.47807000
N	1.51885200	-0.84571100	2.64829200
N	-0.62042100	0.84391000	2.64990000
Al	-0.10477100	-2.66936100	0.00229000
Al	-2.30514100	-1.37892100	0.00270200
N	-1.20610900	-2.09101700	1.36490500
N	-1.20775500	-2.09294200	-1.35982200
Al	1.22469600	0.97089100	-2.48045000
Al	-0.33519000	-0.99279900	-2.45820800
N	1.51506100	-0.84912200	-2.64886400
N	-0.62445500	0.84026600	-2.64932500
Al	2.97582900	1.16815700	-0.00256300
Al	1.02411600	2.71481800	-0.00227400
N	2.10051000	2.07930800	-1.37037400
N	2.10244400	2.08116800	1.36526700
Al	-1.49217000	1.55434100	1.26607200
Al	-1.49441100	1.55242800	-1.26518000
N	-2.53908200	0.61651500	0.00230700
N	-0.77399300	2.69315600	-0.00100500
Al	2.40473000	-1.53502400	1.24750300
Al	2.40277700	-1.53658600	-1.24835300

N	1.69263800	-2.70580500	0.00086900
N	3.39555000	-0.57232000	-0.00180700
Cr	-4.37656200	0.09146800	-0.00016400

Mn@b_{66}-$Al_{12}N_{12}$

Al	-0.31326300	-0.98512100	2.46784700
Al	1.26218900	0.96414000	2.48307700
N	1.53641300	-0.86002700	2.64910200
N	-0.58859700	0.84857900	2.65654900
Al	-0.10825300	-2.67123500	-0.00215000
Al	-2.24900400	-1.30855200	0.00061300
N	-1.20099700	-2.06833500	1.36172600
N	-1.20283900	-2.06580500	-1.36332700
Al	1.25804100	0.96933400	-2.48232800
Al	-0.31707200	-0.98020400	-2.46864300
N	1.53225400	-0.85444800	-2.65257400
N	-0.59303400	0.85385700	-2.65309800
Al	3.00592800	1.14591900	-0.00088400
Al	1.06977200	2.71529000	0.00234200
N	2.13871200	2.06703900	-1.36656700
N	2.14092500	2.06425700	1.36813400
Al	-1.44437600	1.55587300	1.26167400
Al	-1.44657400	1.55838000	-1.25542100
N	-2.51643700	0.62813000	0.00330300
N	-0.72939700	2.70472600	0.00363900

Al	2.41261400	-1.55513900	1.24512100
Al	2.41054700	-1.55253900	-1.25138100
N	1.68747800	-2.71736800	-0.00375900
N	3.40899300	-0.59900600	-0.00296000
Mn	-4.45285900	0.07435700	0.00002200

Fe@b_{66}-$Al_{12}N_{12}$

Al	-0.33617100	0.93645500	-2.47464200
Al	1.28884700	-0.97281600	-2.46857500
N	1.51632000	0.85473900	-2.65817500
N	-0.56395400	-0.90652100	-2.64127700
Al	-0.16980900	2.66074300	-0.03027800
Al	-2.28312500	1.25659300	-0.01561500
N	-1.24802900	2.01570500	-1.38630000
N	-1.25001700	2.04742800	1.33845900
Al	1.28341500	-0.91785500	2.49098700
Al	-0.34076000	0.99177500	2.45222900
N	1.51127700	0.91338600	2.64029300
N	-0.56976900	-0.84722900	2.65895500
Al	3.03760500	-1.08200000	0.01451100
Al	1.14363200	-2.70278900	0.03049300
N	2.19338700	-2.00796400	1.39156700
N	2.19632700	-2.03882400	-1.34332800
Al	-1.40186600	-1.62938200	-1.24456100
Al	-1.40459600	-1.60124500	1.27677400

N	-2.48892800	-0.71529600	0.00476500
N	-0.65565500	-2.73957700	0.02951000
Al	2.37582500	1.58866900	-1.26387400
Al	2.37357200	1.61654600	1.23183300
N	1.62458000	2.74917400	-0.02954400
N	3.39559400	0.67238800	-0.00472700
Fe	-4.30743600	-0.07165000	0.00030700

Co@b_{66}-$Al_{12}N_{12}$

Al	-0.32947800	0.94832200	-2.46954600
Al	1.30185300	-0.95542200	-2.47552200
N	1.52291600	0.87445000	-2.65305700
N	-0.55114000	-0.89462200	-2.64761000
Al	-0.16721600	2.66335100	-0.01320100
Al	-2.26031100	1.23419300	-0.00690000
N	-1.24255100	2.02010300	-1.37322800
N	-1.24355100	2.03375300	1.35227300
Al	1.29937000	-0.93145400	2.48533100
Al	-0.33162600	0.97240600	2.45970400
N	1.52056400	0.90003200	2.64528700
N	-0.55377900	-0.86876000	2.65523700
Al	3.05288400	-1.07392600	0.00639500
Al	1.16370100	-2.70061100	0.01332600
N	2.21235200	-2.01098100	1.37796000
N	2.21369700	-2.02434800	-1.35686800

Al	-1.38585800	-1.62577400	-1.25274800
Al	-1.38711000	-1.61343000	1.26666400
N	-2.46136300	-0.71915000	0.00193200
N	-0.63519800	-2.74417000	0.01283800
Al	2.38068300	1.60287100	-1.25486800
Al	2.37963800	1.61503500	1.24096800
N	1.62701900	2.75414500	-0.01286100
N	3.40392400	0.68222800	-0.00200400
Co	-4.25944900	-0.06596500	0.00021700

Ni@b_{66}-$Al_{12}N_{12}$

Al	-0.32686900	0.75095700	-2.53220400
Al	1.32727400	-1.12647000	-2.39831100
N	1.52602800	0.68803900	-2.71201100
N	-0.52627500	-1.10137700	-2.57500600
Al	-0.19308200	2.64744900	-0.20998300
Al	-2.25814300	1.18524700	-0.09449800
N	-1.25727200	1.88487900	-1.51742300
N	-1.25866700	2.10428800	1.20013100
Al	1.31895700	-0.73574300	2.54672900
Al	-0.33244900	1.14140300	2.38270300
N	1.51987800	1.10489200	2.57181700
N	-0.53456400	-0.68234200	2.71371300
Al	3.07778000	-1.03705500	0.08539600
Al	1.20825500	-2.68183800	0.21217000

N	2.24774500	-1.88074900	1.52220000
N	2.25268100	-2.09742800	-1.20359300
Al	-1.35679000	-1.73553400	-1.12963200
Al	-1.35962400	-1.53591600	1.38243700
N	-2.44036500	-0.75665100	0.05569500
N	-0.58923600	-2.74500000	0.21545200
Al	2.37007100	1.52969100	-1.37027400
Al	2.36840000	1.72715700	1.11756600
N	1.60004900	2.75977300	-0.21698800
N	3.40510700	0.71835500	-0.05332900
Ni	-4.19946000	-0.05922400	0.00350400

Cu@b_{66}-$Al_{12}N_{12}$

Al	-0.32525200	0.87623100	-2.48968500
Al	1.33397800	-1.00117200	-2.45212200
N	1.52758400	0.82745400	-2.67364400
N	-0.51927400	-0.97269200	-2.62580600
Al	-0.19014900	2.65507600	-0.07548400
Al	-2.25181200	1.19005000	-0.03376000
N	-1.25498700	1.96050500	-1.41989700
N	-1.25561800	2.04011000	1.30604100
Al	1.33030300	-0.86061700	2.50528900
Al	-0.32760900	1.01692900	2.43623200
N	1.52506100	0.97740400	2.62281600
N	-0.52293100	-0.82167000	2.67605400

Al	3.08622700	-1.03416200	0.03076800
Al	1.22118000	-2.68851600	0.07623700
N	2.26019300	-1.95152700	1.42407700
N	2.26245900	-2.02962800	-1.30954300
Al	-1.34591300	-1.68539900	-1.21554500
Al	-1.34725500	-1.61338000	1.30697900
N	-2.41842800	-0.77081600	0.02017300
N	-0.57626700	-2.76086200	0.07787200
Al	2.37258100	1.60162300	-1.29275600
Al	2.37211000	1.67298600	1.20176000
N	1.60253600	2.77153700	-0.07818800
N	3.41018500	0.72680200	-0.01921100
Cu	-4.11560800	-0.05730200	0.00075500

Zn@b_{66}-$Al_{12}N_{12}$

Al	-0.29740000	1.58437400	-2.11282500
Al	1.39924000	-0.17917700	-2.64050100
N	1.55471700	1.63387600	-2.28431200
N	-0.45419100	-0.13526200	-2.80843000
Al	-0.20751200	2.53959200	0.74510200
Al	-2.17953800	1.03473100	0.30236100
N	-1.25086100	2.25687100	-0.75950800
N	-1.25172600	1.48760800	1.85687700
Al	1.39856700	-1.57930500	2.12579300
Al	-0.29830200	0.19039100	2.63245800

N	1.55352100	0.13905200	2.80496500
N	-0.45519600	-1.63240100	2.28867000
Al	3.15104500	-0.93932300	-0.27482400
Al	1.32047700	-2.56658900	-0.75319400
N	2.34732100	-2.25932700	0.76139900
N	2.34746800	-1.48892100	-1.86043900
Al	-1.26057700	-1.25396000	-1.67405100
Al	-1.26105200	-1.95907600	0.72903300
N	-2.36747600	-0.77333700	-0.22827300
N	-0.47414600	-2.67510300	-0.78591800
Al	2.37887800	1.96206300	-0.72432800
Al	2.37831500	1.25886200	1.67078800
N	1.58175300	2.68337300	0.78815400
N	3.43378200	0.75868700	0.22341800
Zn	-4.35808700	-0.03898000	-0.01039300

Sc@r_6-$Al_{12}N_{12}$

Al	-4.48833300	0.79231900	-0.14983900
Al	-1.53652000	-0.10131300	-1.90632700
N	-1.28090800	-1.90353300	-1.64661400
N	-2.68343300	0.23621400	-0.46065600
Al	0.57798300	-2.32522800	1.45803000
Al	-0.64835300	-0.43233700	2.51114900
N	-1.24274600	-1.96914900	1.62637600
N	1.11338500	-1.02176300	2.65533600

Al	2.69266500	1.54641200	-0.04319500
Al	2.30171400	0.13019300	1.97101900
N	3.31322000	-0.14374900	0.43426200
N	1.97568400	1.92068700	1.62531000
Al	1.35178400	0.49500900	-2.53439700
Al	0.13294900	2.38822900	-1.43604300
N	1.94550500	1.98862800	-1.61384600
N	-0.41033300	1.07249300	-2.63385600
Al	-2.10130000	1.69904100	0.67293900
Al	0.21423200	2.27222300	1.54813800
N	-1.16405900	1.25458600	2.24276300
N	-0.73055900	2.82916600	0.05970800
Al	0.48510400	-2.25107000	-1.56383200
Al	2.64022500	-1.45016300	-0.59262200
N	1.43464000	-2.76672000	-0.05780400
N	1.85175600	-1.20468400	-2.25783800
Sc	-2.37823800	-1.80801600	0.04917900

Ti@r_6-$Al_{12}N_{12}$

Al	-0.06110600	1.71653900	-2.10361600
Al	-2.34520600	1.57575700	-1.10462500
N	-0.94445000	2.77202100	-0.85798100
N	-1.58101700	0.76401100	-2.58925400
Al	4.55396000	-0.73870700	0.11360700
Al	1.60621300	-0.75692500	-1.77326000

N	1.60752400	1.05724700	-1.96510600
N	2.67395800	-0.91496100	-0.22321900
Al	-0.65166900	-1.76149100	2.12087400
Al	1.61472700	-1.64845900	1.08677700
N	0.88092000	-0.78591100	2.54151300
N	0.21564700	-2.82926000	0.86653900
Al	-2.33623300	0.73020100	1.80040000
Al	-2.92415400	-1.10571800	0.21274000
N	-2.31655800	-1.11995900	1.97081900
N	-3.25433300	0.72194700	0.18609700
Al	-1.36872900	-1.00139500	-2.38216100
Al	-0.53264100	-2.70256300	-0.75720700
N	0.26864400	-1.86626100	-2.20099900
N	-2.23619600	-2.07328600	-1.13441100
Al	-0.21083800	2.67345600	0.77747700
Al	0.65756400	0.99178600	2.38295000
N	1.51827800	2.11776800	1.18383900
N	-0.99379500	1.82880500	2.23763800
Ti	2.50477700	1.30239200	-0.22589800

Mn@r$_6$-Al$_{12}$N$_{12}$

Al	1.64325300	1.30388600	1.16791300
Al	0.18758800	-0.04559600	2.68763200
N	1.80193300	-0.42351300	1.83940000
N	0.23377100	1.76815700	2.28459100

Al	1.64317400	0.34076500	-1.71331900
Al	0.20721100	2.34505300	-1.30445100
N	1.81685300	1.78487100	-0.55350300
N	0.24098100	1.08877700	-2.67350700
Al	-2.67239700	-1.30388800	-1.16723500
Al	-1.21905000	0.04568000	-2.68555100
N	-1.26298000	-1.76904600	-2.28627600
N	-2.82881100	0.42259300	-1.83663800
Al	-1.23882400	-2.34336300	1.30381400
Al	-2.67275100	-0.34046600	1.71352800
N	-2.84376500	-1.78234900	0.55371500
N	-1.27035100	-1.08981400	2.67555600
Al	-1.21774900	2.30805100	1.37800900
Al	-2.66020100	1.67402300	-0.56164100
N	-1.24631800	2.86875200	-0.39300600
N	-2.83004900	1.38927800	1.26726200
Al	1.63048300	-1.67405200	0.56205800
Al	0.18637900	-2.30965200	-1.37867700
N	1.80301800	-1.39053300	-1.26876200
N	0.21686100	-2.86647800	0.39344700
Mn	4.94237900	-0.00042400	-0.00171900

Cu@r_6-$Al_{12}N_{12}$

Al	1.74543100	-1.01663400	1.55745900
Al	0.32776800	-2.67568900	0.31929000

N	1.94851500	-1.84158900	-0.14530100
N	0.33499900	-2.06774700	2.08228700
Al	1.75430000	1.85633800	0.10037900
Al	0.33242900	1.61343000	2.15581900
N	1.95005400	0.78861400	1.66491200
N	0.34333400	2.83626600	0.74875100
Al	-2.53602600	0.98191200	-1.45542900
Al	-1.10898100	2.68286900	-0.30445200
N	-1.11102600	2.02917100	-2.04369700
N	-2.71057900	1.87533300	0.16655100
Al	-1.11322800	-1.60287200	-2.17039600
Al	-2.54146800	-1.74775200	-0.12209600
N	-2.71211000	-0.78674500	-1.70525500
N	-1.11831600	-2.78369100	-0.73613800
Al	-1.11625700	-1.07645800	2.47306400
Al	-2.53989900	0.77341600	1.57340000
N	-1.11600800	0.75596900	2.77571500
N	-2.71514200	-1.07819600	1.53401800
Al	1.75169200	-0.84422400	-1.65612600
Al	0.33511900	1.05994100	-2.47483400
N	1.95315800	1.04437100	-1.51689600
N	0.34140400	-0.77049300	-2.82889500
Cu	3.22415700	-0.00222200	0.00271100

Zn@r_6-$Al_{12}N_{12}$

Al	1.58104000	-0.24895700	-1.72911200
Al	0.13943200	1.77247600	-2.01892600
N	1.74971300	1.50070800	-1.12623400
N	0.17700700	0.12938400	-2.88536400
Al	1.57682100	-1.38011400	1.08039900
Al	0.12996900	-2.63577100	-0.52548000
N	1.74360400	-1.73324700	-0.73586500
N	0.16893800	-2.56570400	1.33098300
Al	-2.72573800	0.25064500	1.73468100
Al	-1.28616800	-1.77173000	2.01835500
N	-1.31997500	-0.13101700	2.88966600
N	-2.89226500	-1.49692300	1.12483000
Al	-1.27638300	2.63538000	0.52553000
Al	-2.72125800	1.38466700	-1.08393300
N	-2.88605800	1.73067800	0.73399300
N	-1.31162800	2.57083900	-1.33124900
Al	-1.28072500	-0.86020000	-2.54461200
Al	-2.72783300	-1.62504700	-0.65688900
N	-1.32023100	-2.43593200	-1.56124900
N	-2.88808000	-0.22156800	-1.86444200
Al	1.58337200	1.61987600	0.65554500
Al	0.13399400	0.86074700	2.54532100
N	1.74583300	0.22176000	1.86874100
N	0.17755800	2.43360100	1.55760800
Zn	4.57814300	-0.00145700	-0.00071300

Sn@r_4-$Al_{12}N_{12}$

Al	-2.11770800	-1.04218100	1.20206800
Al	-2.08001000	-0.68600700	-1.44683100
N	-1.66847100	-2.06776700	-0.28218000
N	-2.61669300	0.55383700	0.04372800
Al	0.77071300	-1.49483300	2.28840300
Al	-0.01195300	0.84565500	2.59297200
N	-0.91726000	-0.76135600	2.52692300
N	1.67867700	0.08051200	2.68696100
Al	2.77892200	0.92167200	-1.12194000
Al	2.76259400	0.59930100	1.35634100
N	3.36727300	-0.46934200	-0.03909100
N	2.51977200	2.10540900	0.28982100
Al	0.80611500	-0.85700100	-2.58969400
Al	0.02592100	1.48711400	-2.29800200
N	1.71768100	0.76524900	-2.55857500
N	-0.87982700	-0.08157400	-2.65612800
Al	-1.53653800	2.00836400	0.24474700
Al	0.84186800	2.72245400	0.35749100
N	-0.42153900	2.33495800	1.67356800
N	-0.39960300	2.69167100	-1.03383300
Al	0.00719500	-2.69535900	-0.35305700
Al	2.38528900	-1.95940300	-0.24062500
N	1.24349600	-2.68402100	1.03342700

N	1.26229000	-2.32840800	-1.67390800
Sc	-4.49627900	0.04660700	0.00146100