Molecular crystals vs. superatomic lattice: A case study with superalkali-superhalogen compounds

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1. Computational methods

The plane-wave DFT computations were performed using the GW projector augmented wave (PAW) potentials within the VASP 5.4.4 software. [1-4] All calculations have been performed spin-polarized and without symmetry constraints. Electronic wave functions were expanded to an energy cutoff of 650 eV.

All the calculations have been performed with the VASP 5.4.4 commercial software (https://www.vasp.at). Initial structures have been carried out with GaussView 5.0 commercial software (http://www.gaussian.com). Visualization of the structures and electron localization function (ELF) maps have been carried out with the VESTA ver. 3.4.6 open-source software (http://www.geocities.jp/kmo_mma). The chemical bonding analysing have been performed with CHARGEMOL open-source software (ver. 09_26_2017, http://www.ddec.sourceforge.net.).

2. Results

2.1. Lattice parameters

Table S 1 Lattice parameters (a, b, c, in Å; α, β, γ, in degrees), and unit-cell volume (in $Å^3$) for dNaCl, dCsI, dZnS phases of N_4Mg_6**M**-Al$\mathbf{X}_4$ supersalts (M=Li, Na, K; X=F, Cl) as obtained by a full structure relaxation with the PBEsol functional.

species	a	b	c	α	β	γ	Unit-cell volume
Li/Cl dNaCl	12.14	18.80	17.49	43.14	55.82	47.48	1994.49
Li/Cl dCsI	9.45	9.44	9.51	88.48	88.64	88.70	847.10

Li/Cl dZnS	7.25	7.43	7.81	62.18	61.34	64.16	314.00
Na/Cl dNaCl	11.62	17.39	17.94	44.79	55.49	61.83	2089.55
Na/Cl dCsI	7.87	7.87	7.88	75.01	74.92	75.07	445.50
Na/Cl dZnS	7.32	9.12	7.54	65.28	60.30	68.60	389.13
K/Cl dNaCl	16.02	15.97	16.32	74.82	50.76	56.42	2669.87
K/Cl dCsI	8.51	8.56	8.53	63.40	80.82	80.61	545.66
K/Cl dZnS	8.13	8.12	8.13	60.04	59.97	60.07	379.63
Li/F dNaCl	8.30	7.04	8.33	66.44	66.03	69.39	396.50
Li/F dCsI	9.24	9.23	9.24	91.92	91.91	92.14	786.33
Li/F dZnS	8.08	6.96	6.95	61.14	63.58	64.58	294.87
Na/F dNaCl	10.00	9.84	9.74	64.23	64.61	61.40	726.93
Na/F dCsI	7.36	7.35	7.36	79.15	79.13	79.15	378.77
Na/F dZnS	6.20	6.93	7.18	70.78	75.77	76.66	278.50
K/F dNaCl	11.06	11.36	10.54	63.33	63.19	59.75	977.82
K/F dCsI	7.39	7.36	7.47	70.89	71.23	71.42	353.17
K/F dZnS	5.94	7.71	7.55	71.42	69.85	79.55	306.64

2.2. Intermolecular distances in superalkali-superhalogen systems.

Table S 2 Cohesive energies (E_{coh}, in eV), the shortest interatomic distance (r_1, in Å), the second shortest interatomic distance (r_2, in Å), and the r_1/r_2 ratio for dNaCl, dCsI, dZnS phases of N_4Mg_6**M**-Al**X**$_4$ supersalts (M=Li, Na, K; X=F, Cl) as obtained by a full structure relaxation with the PBEsol functional.

	E_{coh}	E_{coh}	E_{coh}	r_1	r_2	r_1/r_2	r_1	r_2	r_1/r_2	r_1	r_2	r_1/r_2
	dNaCl	dCsI	dZnS	dNaCl	dNaCl	dNaCl	dCsI	dCsI	dCsI	dZnS	dZnS	dZnS
Li/Cl	-3.02	-4.14	-8.42	3.170	4.828	0.66	2.204	3.758	0.6	2.422	2.671	0.91
Na/Cl	-3.14	-4.43	-8.38	3.674	5.048	0.73	2.545	3.238	0.8	2.318	2.433	0.95
K/Cl	-4.58	-4.41	-8.69	3.142	5.868	0.54	2.866	2.866	1.0	2.774	2.774	1.00
Li/F	-11.57	-6.05	-11.05	1.892	1.921	0.98	1.716	4.250	0.4	2.024	2.035	0.99
Na/F	-10.28	-6.19	-12.84	1.969	2.303	0.86	2.120	3.068	0.7	2.000	2.020	0.99
K/F	-6.19	-6.02	-12.30	2.454	4.597	0.53	2.438	3.474	0.7	1.972	2.013	0.98

2.3. Chemical bond analysis

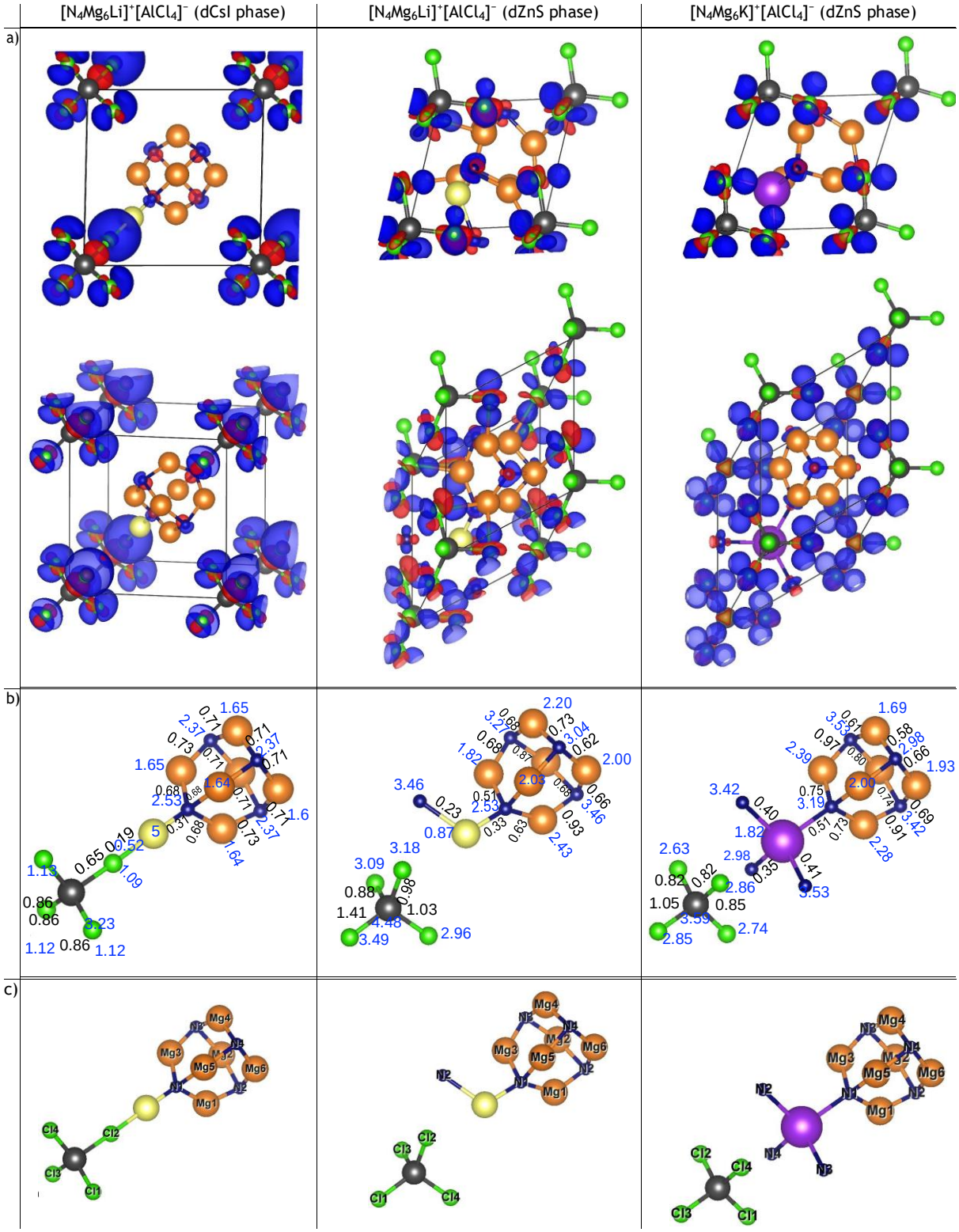

Figure S 1. (a) The electron density difference between superalkali-superhalogen and its superalkali superhalogen subunits and (b) DDEC6 bonding analysis for ground state structures. The bond orders (BOs) and sum of bond orders (SBOs) are provided in black and blue, respectively. Atoms are coloured yellow (Li), pink (Na), orange (Mg), blue (N), and grey (Al).

2.4. Electronic localization function (ELF)

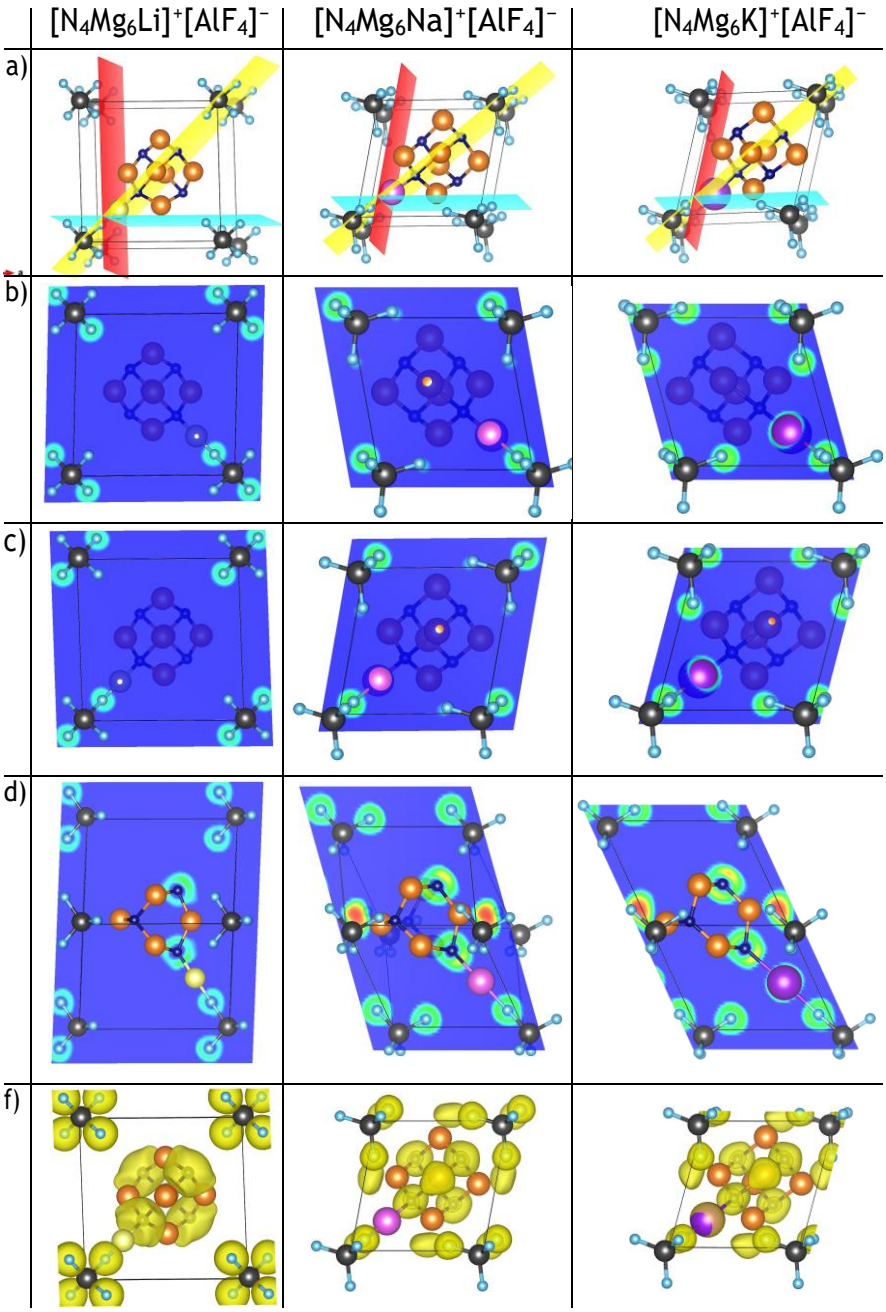

Figure S 2. (a) The vertical (red), horizontal (cyan), and slant (yellow) planes of the bulk-body-centred cubic of $[N_4Mg_6M]^+[AlF_4]^-$ salts. (b) The 2D ELF of the vertical plane, (c) horizontal plane, (d) slant plane and (f) the 3D ELF.

2.5. Band structure and band gap

The band structure and bandgaps were calculated at the PBEsol and PBE-D3 level of theory and are presented in Figure S 3 and Table S 3, respectively. Based on our and other experience, [5-6] we consider the band structure and bandgap obtained at PBE-D3 level of theory as the most

reliable results. The only issue we want to raise is the observation that the bandgap values are underestimated at the PBEsol level of theory (with respect to PBE-D3) values.

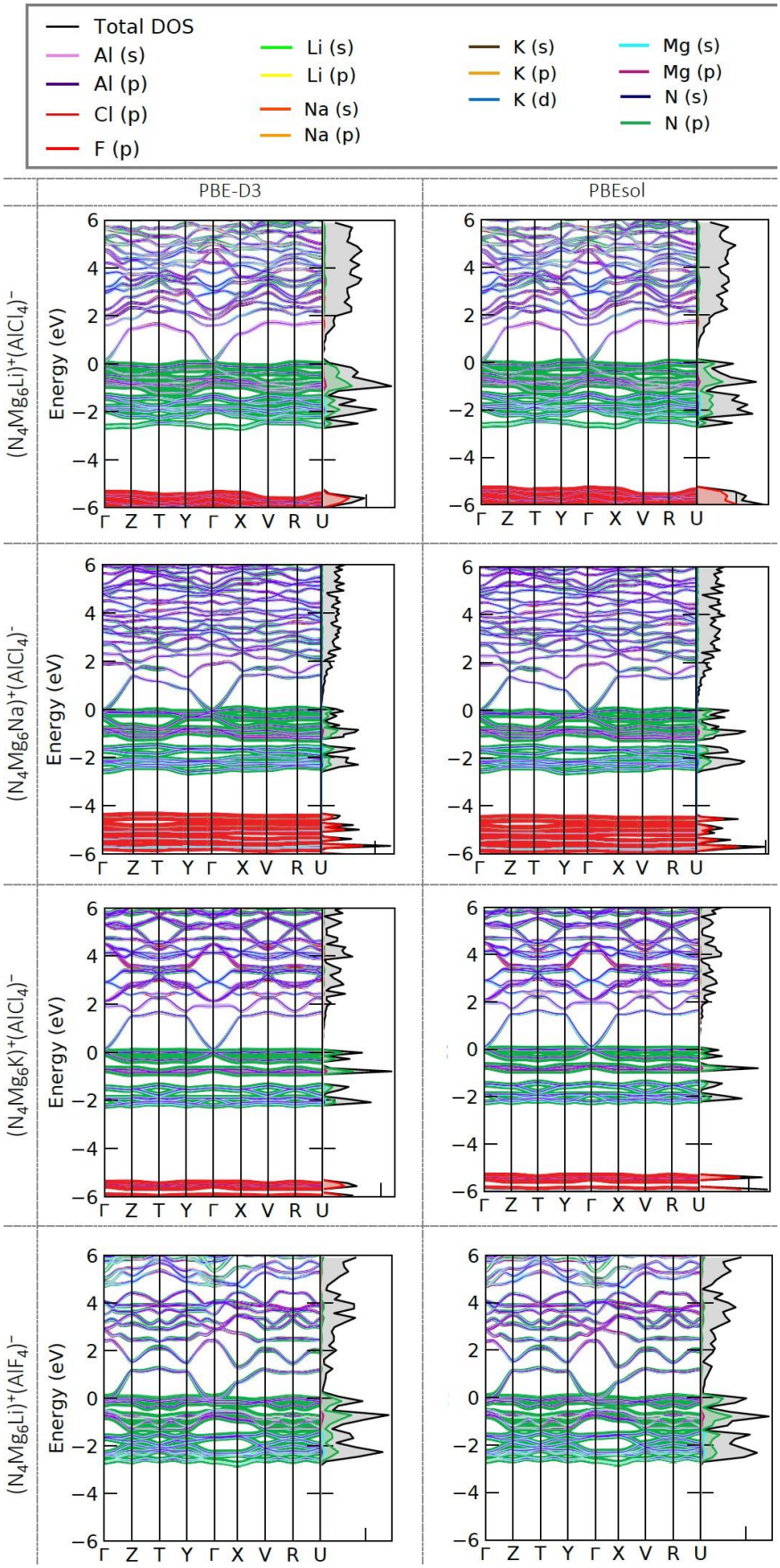

Figure S 3 Electronic band structure for dZnS phase of $[N_4Mg_6\mathbf{M}]^+[Al\mathbf{X}_4]^-$ as obtained from PBEsol and PBE-D3.

Table S 3 Bandgap (in eV), valence band maximum (VBM, in eV), and conduction band minimum (CBM, in eV) for $N_4Mg_6\mathbf{M}$-Al$\mathbf{X}_4$ supersalts (M=Li, Na, K; X=F, Cl) as obtained from PBEsol and PBE-D3.

	Theory level	GAP Direct	GAP Indirect	VBM	CBM
Li/Cl	PBEsol	0.087	0.097	2.553	2.640
	PBE-D3	0.117	0.122	2.678	2.795
Na/Cl	PBE-D3	metallic			
K/Cl	PBEsol	0.108	0.119	1.571	1.679
	PBE-D3	0.141	0.151	1.692	1.833
Li/F	PBE-D3	metallic			
Na/F	PBE-D3	metallic			
K/F	PBE-D3	0.037	0.103	1.676	1.714

2.6. Total (TDOS) and partial (PDOS) density of states

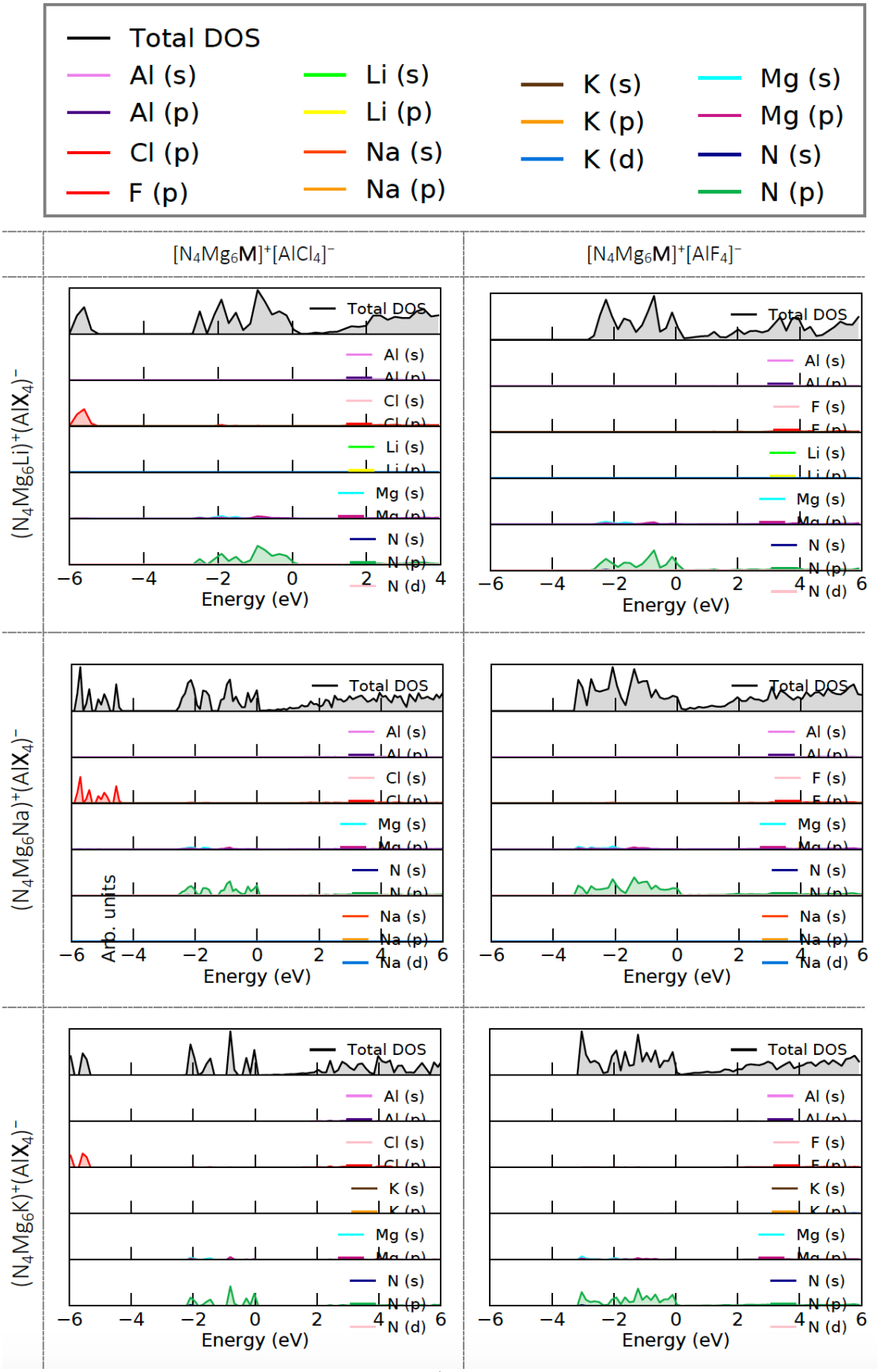

Figure S 4. DOS for dZnS phase of $[N_4Mg_6\mathbf{M}]^+[Al\mathbf{X}_4]^-$ as obtained from PBE-D3.

2.7. The positions of ions and the lattice geometry

Below, we provide the positions of the ions and the lattice geometry as have been written in POSCAR files.

dNaCl phase of N_4Mg_6**Li**-Al**Cl**$_4$
1.0
12.1437397003 0.0000000000 0.0000000000
12.7077213525 13.8574381977 0.0000000000
9.8289620328 8.3059612024 11.8521487704
Li N Mg Al Cl
1 4 6 1 4
Cartesian
16.123947144 8.130017281 4.385201931
16.952489853 9.541401863 5.144154072
16.375167847 12.913895607 6.477078915
19.388542175 12.205095291 4.700802803
18.857549667 10.824999809 7.920364857
15.923585892 11.203112602 5.674460888
17.442058563 12.179022789 7.959528446
17.960391998 9.454777718 6.896099567
19.946853638 11.612910271 6.491164684
18.390552521 10.620136261 4.217730999
17.877708435 13.325238228 5.268257141
23.949098587 13.844906807 0.018128403
1.230318189 0.256681144 0.212793976
23.039657593 13.825656891 1.965898275
20.257383347 9.878129005 10.679673195
21.239336014 20.266952515 10.879776955

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dNaCl phase of N_4Mg_6**Na**-Al**Cl**$_4$
1.0
11.6188058853 0.0000000000 0.0000000000
8.2108258663 15.3338895496 0.0000000000
10.1633747223 9.0009499276 11.7284071351
Na N Mg Al Cl
1 4 6 1 4
Cartesian
14.109049797 8.605779648 4.327173710
14.776293755 10.563177109 5.021842957
13.620538712 13.821369171 6.238298416
16.664253235 13.558148384 4.435431957
16.462059021 12.254500389 7.740195274
13.474553108 12.024142265 5.503787994
14.820756912 13.334778786 7.721824646
15.795716286 10.725337029 6.749980927
17.349567413 13.151018143 6.231971741

15.969140053	11.808060646	3.985558510
14.992930412	14.444652557	4.967744827
19.219068527	15.257740021	0.319221050
9.730149269	15.532999039	0.465001225
18.384120941	15.088608742	2.280879259
20.274343491	10.572014809	11.008125305
17.345462799	22.436750412	10.966012001

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dNaCl phase of N_4Mg_6**K**-Al**Cl**$_4$

1.0

16.0211429596	0.0000000000	0.0000000000
8.8343197179	13.3062615915	0.0000000000
10.3239831084	-1.7227752454	12.5239377546

K N Mg Al Cl

1 4 6 1 4

Cartesian

16.808580399	2.567688704	2.840664864
17.269563675	4.380910873	4.693862438
15.652656555	6.799100876	6.887006283
18.917886734	7.500524521	5.576979160
18.496932983	4.951328278	8.067481995
15.773736000	5.425181389	5.500241280
16.754302979	5.860033512	8.225835800
18.076000214	3.923085690	6.459573269
19.422023773	6.438875675	7.160861492
18.420352936	5.990332603	4.439532757
17.098352432	7.945898056	6.191030979
16.159187317	0.317667127	0.500896811
2.184621096	1.026124120	0.494792998
24.637928009	12.925080299	2.519968510
14.948822975	2.099929333	0.309980005
18.922054291	10.447169304	11.536885262

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dNaCl phase of N_4Mg_6**Li**-Al**F**$_4$

1.0

8.2963647842	0.0000000000	0.0000000000
2.4762573158	6.5856810352	0.0000000000
3.3830958086	2.2836438114	7.2570322922

N Mg Al F Li

4 6 1 4 1

Cartesian

7.484244823	3.233193636	2.604689121
4.820322037	5.236618519	3.749040127
7.979525089	6.827735424	3.396810293
7.360050678	4.329019070	5.981033325
5.552226067	3.676822901	2.811433792
5.469958782	4.668256760	5.526824474
7.809274673	3.094253063	4.561948776
8.012446404	6.052554607	5.284998417
8.113057137	5.085024834	2.426369667
5.981769562	6.716495037	3.300990105
6.205443859	8.603759766	6.991270065
4.245002747	3.245478868	5.935839653
11.185162544	6.961010456	1.263439059

12.932163239 8.172604561 6.662016869
7.281083107 7.321647167 6.665443897
7.378832817 1.413878322 2.118439198

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dNaCl phase of N_4Mg_6**Na**-Al**F**$_4$
1.0
7.3119087219 0.0000000000 0.0000000000
1.9615717968 7.1254282223 0.0000000000
1.7922046997 2.5140953145 6.6598512587
N Mg Al F Na
4 6 1 4 1
Cartesian
6.054072857 3.620164871 2.418287516
3.278635502 5.646234989 3.329203129
6.410636425 7.157509327 3.015608072
5.670924664 4.784308910 5.717621326
4.162408352 4.194770813 2.342290163
3.798196554 5.016440392 5.118526459
6.217169285 3.454859734 4.380907536
6.320736408 6.462417126 4.887226582
6.873811722 5.403318405 2.196261644
4.439660549 7.128968716 2.793731451
4.122291088 9.376958847 6.474014282
2.654790401 3.430787563 5.354003429
0.509424686 0.578200400 1.264842868
9.788086891 9.045392036 6.246946335
5.071404934 7.987343311 6.213206291
5.755572796 1.472442269 1.749379277

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dNaCl phase of N_4Mg_6**K**-Al**F**$_4$
1.0
11.0553932190 0.0000000000 0.0000000000
5.7240308843 9.8151548573 0.0000000000
4.7547705557 2.7040884911 9.0113067026
K N Mg Al F
1 4 6 1 4
Cartesian
10.856709480 2.830663204 1.760033607
10.825547218 4.857167244 3.411291599
8.691488266 7.499320030 4.764267445
12.149277687 8.150138855 4.128197670
11.190888405 5.987413406 6.835669041
9.166031837 5.942535877 3.679757833
9.452496529 6.821570396 6.444209576
11.195993423 4.697113037 5.368284702
12.264095306 7.366554737 5.929408073
11.977679253 6.463913918 3.165623188
10.234634399 8.593727112 4.225868225
10.560482979 12.402822495 8.948824883
5.434547901 3.733328581 7.860495567
11.575264931 0.501950681 1.474137902
19.938716888 12.409403801 8.879892349
11.226198196 10.860038757 8.731470108

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dCsI phase of N_4Mg_6**Li**-Al**Cl**$_4$
1.0
9.4457559586 0.0000000000 0.0000000000
0.2141019716 9.4403834752 0.0000000000
0.2258592647 0.2472323884 9.4997140269
Al Cl Mg N Li
1 4 6 4 1
Cartesian
0.063173369 0.057237815 0.058026247
1.817457914 8.568310738 8.370824814
1.400620818 1.356582642 1.312218189
8.553030968 1.651941657 8.414124489
8.587502480 8.351528168 1.442525268
5.079112053 4.989421368 2.839485407
5.117799759 7.088163376 4.893286705
3.038353682 5.016568661 4.943675518
5.144662857 5.037695408 6.989163876
5.105335236 2.939084768 4.934395313
7.185856342 5.011533737 4.884946823
3.777954817 3.691186905 3.636431217
6.347605228 6.250053406 3.607465982
3.859458923 6.282979488 6.172354221
6.379994392 3.750312567 6.160872936
2.684964895 2.614515781 2.587848186

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dCsI phase of N_4Mg_6**Na**-Al**Cl**$_4$
1.0
7.8741445541 0.0000000000 0.0000000000
2.0260886728 7.5996888941 0.0000000000
2.0490147299 1.5619844042 7.4446545197
Al Cl Mg N Na
1 4 6 4 1
Cartesian
11.737206459 8.989701271 7.314239025
2.163720608 1.643716693 5.203054428
1.338383675 1.034349203 0.835141778
5.799132824 0.663259864 0.547540486
2.164209127 5.418537617 0.562345088
6.023328781 4.626518726 1.835034132
6.662752628 7.074128151 3.736974001
4.215128899 5.112431049 4.150872707
6.662119389 5.101395607 6.142919064
6.020379543 2.736028194 4.145362854
8.542865753 4.597017765 3.737047672
4.701719284 3.611695766 2.930754423
7.478223801 5.740835190 2.547524452
5.488619804 6.276237011 5.094282627
7.476668835 3.657243490 5.091464043
3.144856453 2.429426670 1.960179806

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dCsI phase of N_4Mg_6**K**-Al**Cl**$_4$
1.0
8.5114679337 0.0000000000 0.0000000000
1.3969826356 8.4463458683 0.0000000000

1.3606499738 3.6469088046 7.5901695196
Al Cl Mg N K
1 4 6 4 1
Cartesian
11.029224396 12.040990829 7.562627792
1.821749926 6.533607006 0.883377016
0.925564051 1.486765027 0.953903198
1.797515988 3.612660646 5.496608734
6.206965446 0.396408856 0.252578437
5.840446472 4.263812542 4.396738052
8.284817696 6.096166611 3.831740618
5.850462914 5.820864677 1.934614420
6.199152946 8.350624084 3.526664019
3.916461229 6.508100510 4.073831081
6.192945480 6.802459240 5.970874310
4.520728111 4.885595322 3.061828613
7.258094311 5.292999744 5.282682896
7.268982410 7.067572594 2.477831125
4.934378147 7.934121132 4.971994400
2.470744371 3.606487989 2.248376846

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dCsI phase of N_4Mg_6**Li**-Al**F**$_4$
1.0
9.2360410690 0.0000000000 0.0000000000
-0.3451986950 9.2283777783 0.0000000000
-0.3078546046 -0.3212621665 9.2256319180
Al F Mg N Li
1 4 6 4 1
Cartesian
0.174845070 0.181675807 0.197690666
0.618011713 8.207673073 8.508811951
1.146282315 1.188854337 1.239661336
8.181824684 0.923302770 8.509241104
8.148335457 8.457267761 1.229395032
4.439478397 4.607137203 2.659343958
4.372745514 6.648082733 4.773436069
2.334768534 4.531859398 4.692855835
4.376210213 4.541669369 6.806839943
4.443064213 2.501260042 4.692838192
6.481439114 4.617084026 4.773418903
3.146096468 3.264388561 3.378358364
5.656588554 5.870849609 3.502103329
3.087998867 5.779316902 5.983458996
5.661274910 3.300826788 5.983417034
2.103459358 2.182125092 2.261163235

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dCsI phase of N_4Mg_6**Na**-Al**F**$_4$
1.0
7.3566818237 0.0000000000 0.0000000000
1.3840652699 7.2185476170 0.0000000000
1.3868314783 1.1436523532 7.1325790922
Al F Mg N Na
1 4 6 4 1
Cartesian

9.840214729	8.121125221	6.931663036
1.354372859	1.110992670	5.269407749
0.883962631	0.738322794	0.626846015
5.534467697	0.304611444	0.266013503
1.360354662	5.372713089	0.276196480
5.242788792	4.332562447	1.761869788
5.695048809	6.753268719	3.682531357
3.370624065	4.690836430	3.997735262
5.695576191	4.704405308	6.086281776
5.244650841	2.429326057	3.998753786
7.709528446	4.316776276	3.680544615
3.875850201	3.201448202	2.728950262
6.631165981	5.477019310	2.533815384
4.558102608	5.874188900	5.008652687
6.633847713	3.367951393	5.009970665
2.326257706	1.920953870	1.634949088

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dCsI phase of N_4Mg_6**K**-Al**F**$_4$

1.0

7.3873500824	0.0000000000	0.0000000000
2.3469223523	6.9798631655	0.0000000000
2.4046039229	1.7723641967	6.8494042717

Al F Mg N K

1 4 6 4 1

Cartesian

0.337242544	0.220159292	0.194508240
9.917944908	3.593489408	6.505883694
11.231784821	8.050787926	6.289340973
6.553511143	8.282495499	6.511379242
9.799353600	7.026969910	1.869028807
5.982636929	6.101014137	2.933170319
5.115692139	3.697825670	0.914974332
7.671012402	3.746288061	2.932596922
5.109682083	1.815503001	3.370446444
5.997145176	4.336261749	5.255395412
3.308610439	4.309136391	3.369541883
7.403659344	5.337589264	4.175339222
4.500424385	5.163464069	2.066276789
6.314188480	2.639417648	2.056919098
4.513151646	3.281917572	4.531613827
9.424457550	6.791789055	5.243528366

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dZnS phase of N_4Mg_6**Li**-Al**Cl**$_4$

1.0

7.2482247353	0.0000000000	0.0000000000
3.2379803073	6.6851815083	0.0000000000
3.7466937615	2.2356286051	6.4800873326

Mg N Li Al Cl

6 4 1 1 4

Cartesian

7.839487076	3.283279896	1.924229503
8.610732079	6.035164356	2.343698502
5.754899025	5.412484646	2.504255533
7.317896843	6.229508400	4.925728321

6.501388073	3.444824934	4.536676884
9.370955467	4.052566051	4.343323708
5.972781181	3.441632986	2.615888119
9.559966087	4.246171951	2.347852230
6.986596584	6.872258186	3.068068504
7.864672661	4.442196846	5.565157413
4.141841888	2.708681583	1.953759193
0.345491529	0.134072766	0.302678406
12.820941925	8.224664688	5.915380478
10.993103981	7.279005051	2.400094748
11.526214600	4.373383522	5.888461590
9.081541061	7.971695423	6.132845402

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dZnS phase of N_4Mg_6**Na**-Al**Cl**$_4$

1.0

7.3212351799	0.0000000000	0.0000000000
3.3265867355	8.4874634624	0.0000000000
3.7368250481	1.9226174603	6.2622304114

Mg N Na Al Cl

6 4 1 1 4

Cartesian

6.376979828	6.534925461	3.685040951
5.000317097	5.576819897	1.284865618
7.925308228	5.223011494	1.489133358
6.152397156	2.857104778	1.806935310
7.620537281	3.888435125	4.156392574
4.625113487	4.200571537	3.937671661
8.118970871	5.656304359	3.404198647
4.557468414	6.009737492	3.162827253
6.411186695	4.364986897	0.517191350
6.012744904	2.815677166	3.783733606
9.996762276	6.614188671	4.373641968
6.841628551	10.062458038	6.064869881
9.062775612	8.861804962	1.311035514
9.976684570	2.400302172	4.233105183
5.109666824	8.185284615	0.488817155
6.395115376	7.866002083	6.007057190

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dZnS phase of N_4Mg_6**K**-Al**Cl**$_4$

1.0

8.1269683838	0.0000000000	0.0000000000
4.0517796518	7.0376690942	0.0000000000
4.0680375518	2.3431939721	6.6374182445

Mg N K Al Cl

6 4 1 1 4

Cartesian

8.994054794	3.514097691	2.381412745
10.384674072	6.116188526	2.475119829
7.432787895	6.018470287	2.497328520
8.902346611	6.819983482	4.929218769
7.512624264	4.216522694	4.836334705
10.463834763	4.315455437	4.814637184
7.175408840	4.097953320	2.891544819

10.777832031	4.218170643	2.864371300
8.872252464	7.275255203	3.005529165
8.968651772	5.076581478	5.860681057
4.885251045	2.820189714	1.995845079
0.824140131	0.475513160	0.337539285
10.689627647	8.804863930	6.282488823
13.050709724	4.834177494	6.219838142
15.301654816	8.856229782	6.270521641
13.000431061	7.554299831	2.489091635

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dZnS phase of N_4Mg_6**Li**-AlF_4

1.0

8.0763034821	0.0000000000	0.0000000000
2.9893531589	6.2901490393	0.0000000000
3.0922405516	2.2433421719	5.8043202744

Mg	N	Li	Al	F
6	4	1	1	4

Cartesian

8.741708755	3.595942497	3.642537355
7.419517040	2.521132469	1.156412721
5.768519402	3.170653820	3.477313519
5.737245560	4.947399616	0.972735822
6.857778549	5.878010750	3.497908115
8.694988251	5.247183323	1.212360859
7.073143482	4.213146210	4.525355816
9.094182968	3.385069609	1.718186378
5.545615196	3.068682194	1.522782564
7.043117523	6.297810555	1.581662297
4.133636475	1.857108116	0.736300290
3.003481865	2.289968252	5.277630329
10.616876602	3.851391315	4.744555473
10.571693420	6.512235641	1.130484343
7.595794201	8.073440552	4.916934013
12.911085129	7.509762764	4.686314106

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dZnS phase of N_4Mg_6**Na**-AlF_4

1.0

8.0763034821	0.0000000000	0.0000000000
2.9893529542	6.2901486086	0.0000000000
3.0922409659	2.2433424236	5.8043199564

Mg	N	Li	Al	F
6	4	1	1	4

Cartesian

8.741705894	3.595939398	3.642535925
7.419518948	2.521130800	1.156412005
5.768524647	3.170656919	3.477315664
5.737241268	4.947398663	0.972734332
6.857775688	5.878008842	3.497909546
8.694991112	5.247184753	1.212359905
7.073146343	4.213143826	4.525355339
9.094186783	3.385070801	1.718188882
5.545617104	3.068684101	1.522780776
7.043119907	6.297812939	1.581659794

4.133637428	1.857107878	0.736301184
3.003486633	2.289969921	5.277630329
10.616874695	3.851389170	4.744555473
10.571690559	6.512235641	1.130484104
7.595793247	8.073441505	4.916932106
12.911083221	7.509761333	4.686315060

dZnS phase of N_4Mg_6**K**-Al**F**$_4$

1.0

5.8556785583	0.0000000000	0.0000000000
1.3830068056	7.5825313263	0.0000000000
2.7063251467	1.7307183508	6.5674443695

Mg	N	K	Al	F
6	4	1	1	4

Cartesian

6.761940002	4.392823219	2.268697739
6.918702602	7.261553288	3.122364759
4.033015728	5.700304508	2.726112127
5.025623798	6.543181896	5.272932529
4.817797661	3.591478825	4.578132629
7.424364567	4.910500050	5.123794556
4.940977573	3.845946312	2.623966932
7.970463753	5.566680431	3.323017120
4.984113693	7.363774300	3.473431110
5.620276928	4.775535107	5.959651947
3.234620333	1.952047467	1.850046992
8.226595879	1.810582638	6.404568195
4.786188602	8.040641785	6.533564091
2.886077166	3.086188316	5.352822781
8.024843216	8.975398064	6.072780609
5.794246197	0.732757270	1.398939252

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