

## Supplementary Information

### **The first-row transition metal doped germanium clusters $\text{Ge}_{16}\text{M}$ : Some remarkable superhalogens**

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**Table S1.** Cartesian coordinates of the most stable isomers of Ge<sub>16</sub>M at both neutral and anionic states

Cluster	Atom number	Element	Cartesian Coordinates		
<b>Ge<sub>16</sub>Sc</b> neutral	1	Ge	0.00000000	1.53274500	-2.63169500
	2	Ge	-1.32739600	-0.76637200	-2.63169500
	3	Ge	0.00000000	-2.68331300	-0.94784200
	4	Ge	-1.29485800	-2.28817900	1.59878100
	5	Ge	0.00000000	0.00000000	2.74986000
	6	Ge	1.33419200	2.26547000	1.59878100
	7	Ge	0.00000000	2.94711500	-0.53685100
	8	Ge	1.32739600	-0.76637200	-2.63169500
	9	Ge	2.32381800	1.34165700	-0.94784200
	10	Ge	2.62905100	0.02271000	1.59878100
	11	Ge	1.29485800	-2.28817900	1.59878100
	12	Ge	-1.33419200	2.26547000	1.59878100
	13	Ge	-2.55227700	-1.47355800	-0.53685100
	14	Ge	-2.62905100	0.02271000	1.59878100
	15	Ge	-2.32381800	1.34165700	-0.94784200
	16	Ge	2.55227700	-1.47355800	-0.53685100
	17	Sc	0.00000000	0.00000000	0.01008700
<b>Ge<sub>16</sub>Sc<sup>-</sup></b> anion	1	Ge	0.90194700	-0.90194700	2.75513800
	2	Ge	-0.90194700	0.90194700	2.75513800
	3	Ge	-0.90194700	2.75513800	0.90194700
	4	Ge	0.90194700	2.75513800	-0.90194700
	5	Ge	-2.75513800	-0.90194700	-0.90194700
	6	Ge	-2.75513800	0.90194700	0.90194700
	7	Ge	2.75513800	-0.90194700	0.90194700
	8	Ge	2.75513800	0.90194700	-0.90194700
	9	Ge	-0.90194700	-0.90194700	-2.75513800
	10	Ge	0.90194700	0.90194700	-2.75513800
	11	Ge	0.90194700	-2.75513800	0.90194700
	12	Ge	-0.90194700	-2.75513800	-0.90194700
	13	Ge	-1.63773500	-1.63773500	1.63773500
	14	Ge	1.63773500	1.63773500	1.63773500
	15	Ge	1.63773500	-1.63773500	-1.63773500
	16	Ge	-1.63773500	1.63773500	-1.63773500
	17	Sc	0.00000000	0.00000000	0.00000000

<b>Ge<sub>16</sub>Ti</b> neutral	1	Ge	0.89497100	-0.89497100	2.73165100
	2	Ge	-0.89497100	0.89497100	2.73165100
	3	Ge	-0.89497100	2.73165100	0.89497100
	4	Ge	0.89497100	2.73165100	-0.89497100
	5	Ge	-2.73165100	-0.89497100	-0.89497100
	6	Ge	-2.73165100	0.89497100	0.89497100
	7	Ge	2.73165100	-0.89497100	0.89497100
	8	Ge	2.73165100	0.89497100	-0.89497100
	9	Ge	-0.89497100	-0.89497100	-2.73165100
	10	Ge	0.89497100	0.89497100	-2.73165100
	11	Ge	0.89497100	-2.73165100	0.89497100
	12	Ge	-0.89497100	-2.73165100	-0.89497100
	13	Ge	-1.58811600	-1.58811600	1.58811600
	14	Ge	1.58811600	1.58811600	1.58811600
	15	Ge	1.58811600	-1.58811600	-1.58811600
	16	Ge	-1.58811600	1.58811600	-1.58811600
	17	Ti	0.00000000	0.00000000	0.00000000
<b>Ge<sub>16</sub>Ti</b> anion	1	Ge	-1.28722700	-0.74318100	-2.63887800
	2	Ge	2.26478500	1.30757400	-0.88949500
	3	Ge	1.28722700	-0.74318100	-2.63887800
	4	Ge	0.00000000	1.48636200	-2.63887800
	5	Ge	0.00000000	2.97932700	-0.56219800
	6	Ge	-2.26478500	1.30757400	-0.88949500
	7	Ge	-1.31072900	2.21986400	1.58439300
	8	Ge	-2.57782300	0.02519300	1.58439300
	9	Ge	1.31072900	2.21986400	1.58439300
	10	Ge	0.00000000	0.00000000	2.75227700
	11	Ge	1.26709400	-2.24505700	1.58439300
	12	Ge	2.57782300	0.02519300	1.58439300
	13	Ge	-2.58017300	-1.48966400	-0.56219800
	14	Ge	0.00000000	-2.61514800	-0.88949500
	15	Ge	-1.26709400	-2.24505700	1.58439300
	16	Ge	2.58017300	-1.48966400	-0.56219800
	17	Ti	0.00000000	0.00000000	0.01902600

<b>Ge<sub>16</sub>V</b> neutral	1	Ge	-0.88887700	2.49087000	-1.60784600
	2	Ge	1.63313100	-1.16921000	-2.20621400
	3	Ge	1.74778700	-1.01253900	2.19552000
	4	Ge	-1.10058700	2.12283600	1.19630400
	5	Ge	1.45882900	1.54856500	2.09265400
	6	Ge	1.26589200	2.69759400	-0.12855200
	7	Ge	2.79069300	0.31080200	-0.08383500
	8	Ge	1.35121400	1.32139600	-2.30779000
	9	Ge	-2.46533800	-1.60641100	-0.61589400
	10	Ge	-0.29914600	-2.74572800	-1.39631300
	11	Ge	-0.61261700	-2.21176800	1.37363800
	12	Ge	-2.55615200	-0.22256300	1.56927000
	13	Ge	-0.48068100	0.06952600	3.05412800
	14	Ge	-2.75576400	0.96376800	-0.72217200
	15	Ge	1.83354000	-2.35177900	0.07685300
	16	Ge	-0.95176400	-0.20857900	-2.48919800
	17	V	0.04151400	0.00448000	-0.00077100
<b>Ge<sub>16</sub>V<sup>-</sup></b> anion	1	Ge	0.01092300	-0.05868700	-2.66016100
	2	Ge	-0.53036600	-2.55424400	0.98395800
	3	Ge	0.81890400	-2.50568500	-1.54713900
	4	Ge	2.17376400	-1.91656100	0.58153700
	5	Ge	1.13051200	-0.95191000	2.65156800
	6	Ge	2.49001600	0.85222300	0.92098000
	7	Ge	0.58022600	2.86007800	0.46953600
	8	Ge	-0.82746400	2.42551100	-1.66145600
	9	Ge	0.29422200	1.55157300	2.59305700
	10	Ge	-1.97109400	1.76339600	0.88300300
	11	Ge	-2.54058700	0.49609400	-1.62715900
	12	Ge	-2.76073600	-0.90864300	0.53953100
	13	Ge	1.74042000	1.90297300	-1.64081500
	14	Ge	-1.70895600	-1.98811800	-1.56740700
	15	Ge	-1.45617200	-0.42470800	2.62925900
	16	Ge	2.55653000	-0.54418100	-1.58242600
	17	V	-0.00019900	0.00123800	0.04749100

<b>Ge<sub>16</sub>Cr</b> neutral	1	Ge	-3.18524400	-0.02453000	0.00000000
	2	Ge	1.79598300	-1.54145700	2.69206200
	3	Ge	2.05213300	-1.54128700	0.00000000
	4	Ge	-0.21248200	-2.50302900	-1.24999600
	5	Ge	-2.18324100	-1.14317000	-1.95206700
	6	Ge	-0.24781400	2.33033000	-1.54108400
	7	Ge	-0.24781400	2.33033000	1.54108400
	8	Ge	2.03694500	0.79556400	1.34923200
	9	Ge	-0.21248200	-2.50302900	1.24999600
	10	Ge	-0.23166700	0.16563900	2.79119700
	11	Ge	-2.20864100	2.23684100	0.00000000
	12	Ge	-2.18324100	-1.14317000	1.95206700
	13	Ge	1.75926500	3.12409500	0.00000000
	14	Ge	1.79598300	-1.54145700	-2.69206200
	15	Ge	-0.23166700	0.16563900	-2.79119700
	16	Ge	2.03694500	0.79556400	-1.34923200
	17	Cr	-0.44394900	-0.00383300	0.00000000
<b>Ge<sub>16</sub>Cr<sup>-</sup></b> anion	1	Ge	-2.09091200	-0.12886300	1.55069000
	2	Ge	-1.81448000	0.27493100	-3.08512300
	3	Ge	-1.77444000	2.55341000	1.79290100
	4	Ge	-1.79065600	-2.81382400	1.32716600
	5	Ge	-2.10071900	1.40252000	-0.63812800
	6	Ge	-2.11213500	-1.25826100	-0.86936200
	7	Ge	0.21048500	-2.76702900	-0.39297900
	8	Ge	0.22924800	2.79384800	0.09113700
	9	Ge	0.19811700	-1.31726900	-2.46772800
	10	Ge	0.23272400	-1.47801800	2.37173200
	11	Ge	0.20991200	1.72183100	-2.20232100
	12	Ge	0.24021600	1.04421400	2.59111000
	13	Ge	2.17038900	-1.89566600	0.86793600
	14	Ge	2.18180000	1.70390500	1.18186600
	15	Ge	2.15404800	0.17397400	-2.09245100
	16	Ge	3.59832900	-0.00911800	-0.02512600
	17	Cr	0.34409800	-0.00077900	-0.00176100

<b>Ge<sub>16</sub>Mn</b> neutral	1	Ge	-1.68530427	-1.96119541	1.27433801
	2	Ge	-2.21129906	0.45566004	-1.68414802
	3	Ge	-1.68530427	-1.96119541	-1.27433801
	4	Ge	-2.21129906	0.45566004	1.68414802
	5	Ge	-0.44163707	2.49520225	0.00000000
	6	Ge	-0.05419419	0.22268686	2.87552292
	7	Ge	1.54170390	1.60460839	1.57038175
	8	Ge	2.30581214	-0.82530186	1.28470289
	9	Ge	1.54170390	1.60460839	-1.57038175
	10	Ge	2.30581214	-0.82530186	-1.28470289
	11	Ge	0.69626404	-2.68828117	0.00000000
	12	Ge	0.58580936	-2.33042790	-2.65527801
	13	Ge	0.58580936	-2.33042790	2.65527801
	14	Ge	-0.05419419	0.22268686	-2.87552292
	15	Ge	-2.90578517	2.23373215	0.00000000
	16	Ge	1.77292335	3.65470744	0.00000000
	17	Mn	-0.11087399	-0.03497387	0.00000000
<b>Ge<sub>16</sub>Mn<sup>-</sup></b> anion	1	Ge	-1.84041300	2.58001800	0.00000000
	2	Ge	-2.63470600	-2.47712700	0.00000000
	3	Ge	-1.38649000	1.61113800	2.28427100
	4	Ge	-1.38649000	1.61113800	-2.28427100
	5	Ge	-1.19256900	-0.89156100	-1.36829200
	6	Ge	0.82079800	2.80648900	-1.50440000
	7	Ge	2.69376400	1.85041800	0.00000000
	8	Ge	1.85163700	-3.28196100	0.00000000
	9	Ge	2.09894200	-0.65168400	0.00000000
	10	Ge	0.82079800	2.80648900	1.50440000
	11	Ge	1.18339400	-1.61741900	2.18211800
	12	Ge	-0.21029000	4.59558100	0.00000000
	13	Ge	-0.44665300	-3.52068100	1.36749800
	14	Ge	-0.44665300	-3.52068100	-1.36749800
	15	Ge	1.18339400	-1.61741900	-2.18211800
	16	Ge	-1.19256900	-0.89156100	1.36829200
	17	Mn	0.10765400	0.77929000	0.00000000

<b>Ge<sub>16</sub>Fe</b> neutral	1	Ge	-1.44171500	-1.27553900	2.07884000
	2	Ge	1.08587500	1.50416300	1.91940700
	3	Ge	-1.43956600	1.27213800	2.08118600
	4	Ge	1.08352000	-1.50801900	1.91625200
	5	Ge	2.40570300	-0.00114800	0.00060400
	6	Ge	0.24522300	-2.82754500	-0.00251300
	7	Ge	1.08537300	-1.50477800	-1.91862300
	8	Ge	-1.44007100	-1.27051800	-2.08192100
	9	Ge	1.08681000	1.50700100	-1.91596600
	10	Ge	-1.43872900	1.27715500	-2.07961500
	11	Ge	-2.82135800	0.00132900	-0.00066400
	12	Ge	-2.37615900	2.63560300	0.00226400
	13	Ge	-2.37920200	-2.63408900	-0.00348900
	14	Ge	0.24853400	2.82746700	0.00256200
	15	Ge	3.10272600	-0.00417500	2.41383400
	16	Ge	3.10469400	0.00064800	-2.41202200
	17	Fe	-0.13742700	0.00037700	-0.00016600
<b>Ge<sub>16</sub>Fe<sup>-</sup></b> anion	1	Ge	2.65183100	-1.68389000	0.75955300
	2	Ge	-1.92022100	-2.33346800	1.08397700
	3	Ge	1.67005400	-2.19246800	-1.57745300
	4	Ge	1.66548800	-0.26132800	2.68451400
	5	Ge	-0.72752200	-0.16156000	1.78263300
	6	Ge	2.66717300	1.50093300	1.07032000
	7	Ge	1.67033100	2.46209500	-1.12013600
	8	Ge	-3.43330000	1.41712200	-0.66265900
	9	Ge	-0.73150700	1.64522000	-0.74671600
	10	Ge	2.69250200	0.18092900	-1.82455600
	11	Ge	-1.89525900	0.22989800	-2.55543100
	12	Ge	4.41767800	-0.01038500	0.02480100
	13	Ge	-3.43278900	-1.27019300	-0.90812700
	14	Ge	-3.44207000	-0.14237100	1.54446000
	15	Ge	-1.92002000	2.09782000	1.48567700
	16	Ge	-0.72764700	-1.48609700	-1.02694100
	17	Fe	0.97880200	0.00952900	-0.01712700

<b>Ge<sub>16</sub>Co</b> neutral	1	Ge	-1.29886700	1.39071300	-2.07456900
	2	Ge	0.90538500	-1.56791700	-1.88681500
	3	Ge	-1.58358300	-1.13693600	-2.03734000
	4	Ge	1.23320400	1.40433400	-1.96587900
	5	Ge	2.39213500	-0.18205900	0.00000200
	6	Ge	0.57532600	2.75905300	-0.00006800
	7	Ge	1.23320500	1.40443200	1.96581200
	8	Ge	-1.29886100	1.39080300	2.07451000
	9	Ge	0.90538800	-1.56782200	1.88689200
	10	Ge	-1.58358300	-1.13684700	2.03738600
	11	Ge	-2.78032200	0.23972300	-0.00000200
	12	Ge	-2.66933200	-2.48085500	0.00005000
	13	Ge	-2.03102800	2.86453800	-0.00006000
	14	Ge	-0.05888200	-2.83043100	0.00006900
	15	Ge	3.07434900	-0.33451500	-2.40090300
	16	Ge	3.07435200	-0.33439300	2.40091200
	17	Co	-0.10534600	0.14006300	0.00000200
<b>Ge<sub>16</sub>Co<sup>-</sup></b> anion	1	Ge	2.62154600	-1.82771000	0.00400100
	2	Ge	-2.00658300	-2.59598400	0.00561900
	3	Ge	1.62428100	-1.35756900	-2.30261300
	4	Ge	1.62464300	-1.34717200	2.30866600
	5	Ge	-0.73147100	-0.86811800	1.43613300
	6	Ge	2.72991500	0.88277400	1.60042700
	7	Ge	1.69604200	2.66357100	-0.00603400
	8	Ge	-3.41367200	1.59945800	-0.00352100
	9	Ge	-0.74447100	1.79512500	-0.00380200
	10	Ge	2.72969700	0.87535900	-1.60442700
	11	Ge	-1.93793100	1.27226100	-2.24289300
	12	Ge	4.46489000	-0.05763400	-0.00001800
	13	Ge	-3.43179900	-0.77319700	-1.36243700
	14	Ge	-3.43185500	-0.76722100	1.36554000
	15	Ge	-1.93812100	1.28205100	2.23748000
	16	Ge	-0.73143000	-0.87445900	-1.43201600
	17	Co	1.03859900	0.11669900	-0.00012400



<b>Ge<sub>16</sub>Ni</b> neutral	1	Ge	2.14227000	1.07358500	1.08730100
	2	Ge	1.79100800	-2.18846100	-2.20826800
	3	Ge	1.79067500	-0.82133900	2.99794900
	4	Ge	1.79899700	3.00268700	-0.78922000
	5	Ge	2.13730800	-1.48284400	0.38922500
	6	Ge	2.14199600	0.39938800	-1.47372100
	7	Ge	-0.21295900	1.84487100	-2.03675800
	8	Ge	-0.22096600	-2.05557100	1.82410500
	9	Ge	-0.21713200	-0.55078100	-2.69097600
	10	Ge	-0.21258900	2.60884100	0.86824700
	11	Ge	-0.22051600	-2.68641000	-0.57846600
	12	Ge	-0.21702300	0.84247600	2.61453700
	13	Ge	-2.13250100	1.65130000	-0.43281000
	14	Ge	-2.13777600	-0.44708300	1.64296900
	15	Ge	-2.13738300	-1.19645100	-1.21216000
	16	Ge	-4.00166900	0.00629400	-0.00249600
	17	Ni	-0.10484500	-0.00057400	0.00061700
<b>Ge<sub>16</sub>Ni<sup>-</sup></b> anion	1	Ge	-2.62662500	-1.53963400	0.89052400
	2	Ge	2.22133500	-2.23598300	1.34607200
	3	Ge	-1.46004300	0.00017200	2.52055300
	4	Ge	-1.71506200	-2.32270700	-1.30595900
	5	Ge	0.69266100	-1.77221500	-0.60962500
	6	Ge	-2.85353800	-0.00017100	-1.57469500
	7	Ge	-1.71508600	2.32246300	-1.30624800
	8	Ge	3.28523300	1.36753800	-1.07502200
	9	Ge	0.69313400	1.77164600	-0.61088400
	10	Ge	-2.62637100	1.53985500	0.89033300
	11	Ge	2.22163700	2.23686800	1.34467200
	12	Ge	-4.59063900	0.00033500	0.31868900
	13	Ge	3.62476300	0.00023700	1.24157800
	14	Ge	3.28485400	-1.36839600	-1.07429700
	15	Ge	1.36794400	-0.00083500	-2.42121700
	16	Ge	0.89102500	0.00076400	1.61375500
	17	Ni	-0.79454200	0.00007500	-0.21511800

<b>Ge<sub>16</sub>Cu</b> neutral	1	Ge	2.70326600	1.50864000	1.09806300
	2	Ge	-1.95653200	2.11248600	1.53555700
	3	Ge	1.63175300	-0.27989500	2.64057900
	4	Ge	1.63133300	2.42694900	-1.07800400
	5	Ge	-0.75682000	1.57753200	-0.70168200
	6	Ge	2.70279400	0.19701500	-1.85460200
	7	Ge	1.63197400	-2.14718100	-1.56277100
	8	Ge	-3.40581000	-1.28930900	-0.93722300
	9	Ge	-0.75645000	-1.39703600	-1.01447300
	10	Ge	2.70356400	-1.70510800	0.75709300
	11	Ge	-1.95613400	-2.38595100	1.06245100
	12	Ge	4.40027300	0.00032300	-0.00019100
	13	Ge	-3.40725100	-0.16650600	1.58366100
	14	Ge	-3.40623100	1.45598100	-0.64925100
	15	Ge	-1.95452300	0.27288900	-2.59714200
	16	Ge	-0.75764700	-0.18068100	1.71765200
	17	Cu	1.05097100	-0.00016500	0.00031200
<b>Ge<sub>16</sub>Cu<sup>-</sup></b> anion	1	Ge	2.75962100	-1.75020800	0.04241100
	2	Ge	-2.02141200	-2.58808200	0.06238300
	3	Ge	1.67309000	-1.37988100	-2.25223700
	4	Ge	1.67299900	-1.26866000	2.31628300
	5	Ge	-0.78927900	-0.83291400	1.50269800
	6	Ge	2.76336500	0.90784900	1.50214300
	7	Ge	1.68653400	2.63658000	-0.06433000
	8	Ge	-3.46635300	1.58905200	-0.03824900
	9	Ge	-0.78552700	1.73453400	-0.04107400
	10	Ge	2.76408800	0.83346000	-1.54412300
	11	Ge	-2.00358800	1.23685600	-2.26834400
	12	Ge	4.62598100	-0.00327400	0.00041900
	13	Ge	-3.47171000	-0.81699800	-1.35245900
	14	Ge	-3.47231500	-0.75094700	1.38838100
	15	Ge	-2.00416100	1.34342000	2.20756500
	16	Ge	-0.78890000	-0.90388300	-1.46094100
	17	Cu	0.94628100	0.01445000	-0.00058100

<b>Ge<sub>16</sub>Zn</b> neutral	1	Ge	2.82325100	-1.76769300	0.18133000
	2	Ge	-2.04498000	-2.59711800	0.26549100
	3	Ge	1.69692100	-1.54840100	-2.13573700
	4	Ge	1.69686000	-1.08220600	2.40510200
	5	Ge	-0.84607700	-0.72479200	1.59216400
	6	Ge	2.82294900	1.03928900	1.44598700
	7	Ge	1.70549100	2.62176900	-0.26922600
	8	Ge	-3.49774600	1.58426500	-0.16225400
	9	Ge	-0.84282700	1.75141900	-0.17746000
	10	Ge	2.82310500	0.72299100	-1.62616400
	11	Ge	-2.02666900	1.06540000	-2.37929400
	12	Ge	4.67044800	-0.00046700	0.00059500
	13	Ge	-3.50261600	-0.92138600	-1.28884700
	14	Ge	-3.50442600	-0.64236500	1.44527600
	15	Ge	-2.02985800	1.52456100	2.11541400
	16	Ge	-0.84490100	-1.03234600	-1.41152600
	17	Zn	0.96114400	0.00755000	-0.00090800
<b>Ge<sub>16</sub>Zn<sup>-</sup></b> anion	1	Ge	2.90746800	0.71336000	-1.60505000
	2	Ge	-2.07794600	1.04216600	-2.34153400
	3	Ge	1.70487800	2.59030300	-0.27291000
	4	Ge	1.70431300	-1.53253500	-2.10626300
	5	Ge	-0.84241100	-1.01700000	-1.39786300
	6	Ge	2.90790100	-1.74609700	0.18456600
	7	Ge	1.70452500	-1.05802900	2.38033000
	8	Ge	-3.60257500	-0.63083700	1.41695100
	9	Ge	-0.84124500	-0.70277600	1.57833500
	10	Ge	2.90811600	1.03275300	1.41983500
	11	Ge	-2.07740600	1.50646200	2.07348200
	12	Ge	4.78943700	-0.00005300	-0.00072700
	13	Ge	-3.60316200	1.54232500	-0.16211800
	14	Ge	-3.60363900	-0.91082600	-1.25455800
	15	Ge	-2.07811200	-2.54895300	0.26873000
	16	Ge	-0.84206600	1.71968200	-0.18096100
	17	Zn	1.00471700	0.00005800	-0.00026200