Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Structural Evolution, Photoelectron Spectra and Vibrational Properties of Anionic $GdGe_n^-$ (n=5-18) Nanoalloy Clusters: A DFT Insight

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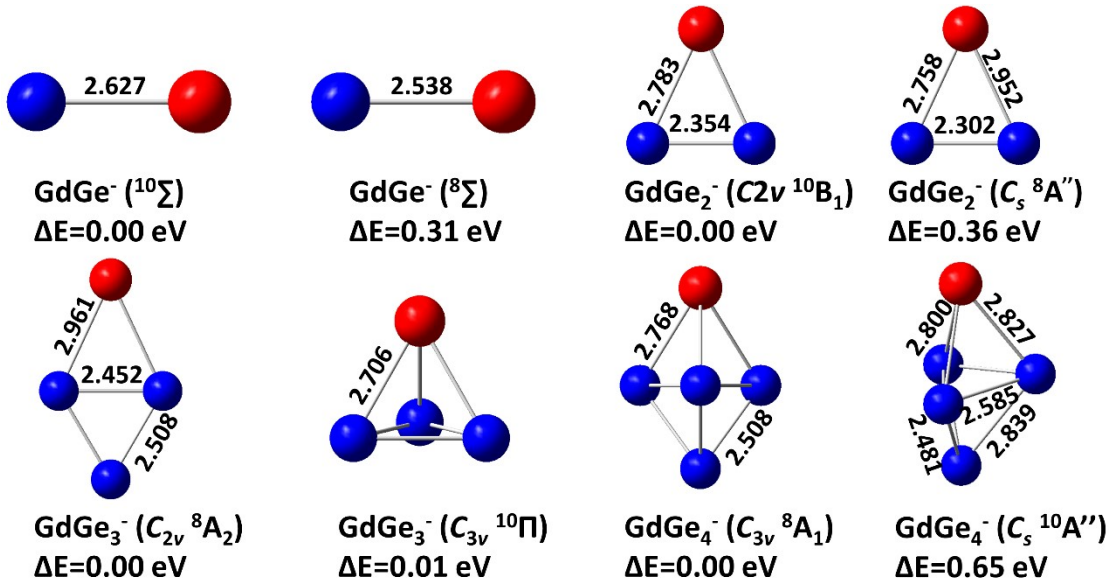

Figure S1. Lowest energy structure and isomers of $GdGe_n^-$ (n=1-4) anionic clusters, point group, electronic state and relative energy (in eV) calculated at mPW2PLYP/aug-cc-pVTZ,def2-TZVP//mPW2PLYP/cc-pVTZ-PP,def2-TZPV level. The blue and red circles stand for germanium and gadolinium atoms, respectively.

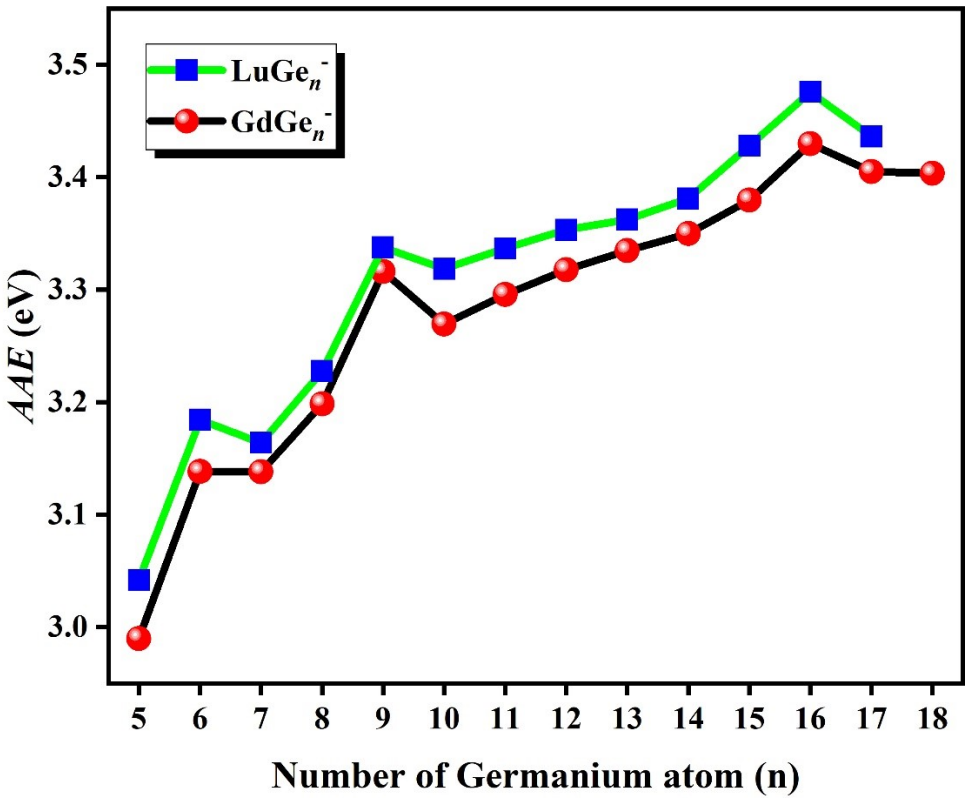

Figure S2. Size dependences of average atomization energy (AAE) for $GeGe_n^-$ and $LuGe_n^-$ (n=5-17) clusters. The values of $LuGe_n^-$ clusters are taken from Ref. 11.

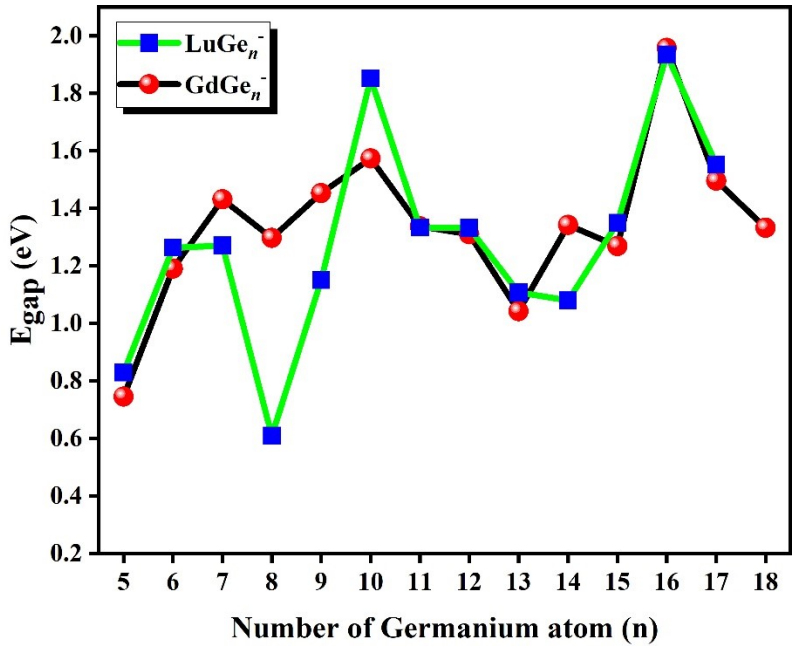

Figure S3. Size dependences of HOMO-LUMO energy gap (Egap) for $GeGe_n^-$ and $LuGe_n^-$ (n=5-17) clusters. The values of $LuGe_n^-$ clusters are taken from Ref. 11.

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Table S1. Total energies (a.u.) of $GdGe_n^-$ (n=5-18) clusters in octuplet and decuplet calculated by using mPW2PLYP/(aug-cc-pVTZ,def2-TZVP)//mPW2PLYP/(cc-pVTZ-PP,def2-TZPV) scheme.

	State			State	
Isomer	Octuplet	Decuplet	Isomer	Octuplet	Decuplet
5A1	-11148.59661	-11148.54910	**11A4**	-23609.02991	-23609.00713
5A2	-11148.58321	-11148.57607	**12A1**	-25685.78992	-25685.74058
6A1	-13225.35432	-13225.31848	**12A2**	-25685.78645	-25685.72747
6A2	-13225.32490	-13225.29891	**12A3**	-25685.77560	-25685.73268
6A3	-13225.31069	-13225.31720	**12A4**	-25685.77503	-25685.75326
7A1	-15302.07925	-15302.02559	**13A1**	-27762.53028	-27762.49715
7A2	-15302.07592	-15302.03822	**13A2**	-27762.52556	-27762.48418
7A3	-15302.07234	-15302.07213	**13A3**	-27762.52522	-27762.48141
7A4	-15302.06729	-15302.01301	**13A4**	-27762.51718	-27762.45367
8A1	-17378.82419	-17378.77772	**14A1**	-29839.27081	-29839.21985
8A2	-17378.82139	-17378.79228	**14A2**	-29839.26963	-29839.21702
8A3	-17378.82024	-17378.77767	**14A3**	-29839.25949	-29839.24956
8A4	-17378.81909	-17378.80639	**14A4**	-29839.24836	-29839.22125
8A5	-17378.81196	-17378.78227	**15A1**	-31916.02109	-31915.96955
9A1	-19455.59466	-19455.53751	**15A2**	-31916.01794	-31915.96750
9A2	-19455.57832	-19455.51909	**15A3**	-31916.00826	-31915.95910
9A3	-19455.57191	-19455.51415	**15A4**	-31916.00582	-31915.96282
9A4	-19455.55727	-19455.51576	**16A1**	-33992.78627	-33992.71106
10A1	-21532.30723	-21532.25069	**16A2**	-33992.76593	-33992.72447
10A2	-21532.30063	-21532.27283	**16A3**	-33992.72899	-33992.68894
10A3	-21532.29482	-21532.26481	**17A1**	-36069.50557	-36069.44537
10A4	-21532.27367	-21532.26768	**17A2**	-36069.47500	-36069.43183
11A1	-23609.04865	-23608.99830	**18A1**	-38146.23920	-38146.18444
11A2	-23609.04476	-23609.00664	**18A2**	-38146.23532	-38146.21333
11A3	-23609.03997	-23608.98703			

Table S2. Natural population analysis (NPA) charge (in a.u.), valence configuration, magnetic moment (μB) of 6*s*, 4*f*, 5*d*, 6*p*, and total of Gd atom, and total magnetic moment of the global minima $GdGe_n^-$ (*n*=5-18) compounds calculated at the mPW2PLYP level.

	Charge		Magnetic Moment of Gd Atom					Molecule
Compound	(a.u.)	Electron Configuration	6*s*	4*f*	5*d*	6*p*	Total	(μB)
$GdGe_5^-$	0.16	[core]$6s^{0.81}4f^{7.00}5d^{1.71}6p^{0.32}$	0.01	6.98	0.24	0.01	7.24	7
$GdGe_6^-$	0.25	[core]$6s^{0.70}4f^{7.00}5d^{1.72}6p^{0.32}$	0.00	6.98	0.24	0.00	7.22	7
$GdGe_7^-$	0.15	[core]$6s^{0.57}4f^{7.00}5d^{2.03}6p^{0.25}$	0.03	6.98	0.17	0.00	7.18	7
$GdGe_8^-$	0.15	[core]$6s^{0.50}4f^{7.00}5d^{2.03}6p^{0.33}$	0.01	6.98	0.25	0.01	7.25	7
$GdGe_9^-$	0.37	[core]$6s^{0.57}4f^{7.00}5d^{1.83}6p^{0.26}$	0.02	6.98	0.28	0.01	7.29	7
$GdGe_{10}^-$	-0.02	[core]$6s^{0.43}4f^{7.00}5d^{2.09}6p^{0.51}$	0.01	6.98	0.23	0.01	7.23	7
$GdGe_{11}^-$	0.11	[core]$6s^{0.39}4f^{7.00}5d^{1.85}6p^{0.65}$	0.01	6.98	0.18	0.01	7.18	7
$GdGe_{12}^-$	-0.26	[core]$6s^{0.36}4f^{7.00}5d^{2.11}6p^{0.78}$	0.00	6.98	0.17	0.01	7.16	7
$GdGe_{13}^-$	-0.04	[core]$6s^{0.46}4f^{7.00}5d^{2.10}6p^{0.49}$	0.01	6.98	0.22	0.01	7.22	7
$GdGe_{14}^-$	0.25	[core]$6s^{0.37}4f^{7.00}5d^{1.82}6p^{0.58}$	0.01	6.97	0.18	0.02	7.18	7
$GdGe_{15}^-$	-4.10	[core]$6s^{0.46}4f^{7.00}5d^{4.83}6p^{1.77}$	0.00	6.97	0.19	0.01	7.17	7
$GdGe_{16}^-$	-4.87	[core]$6s^{0.47}4f^{7.00}5d^{5.30}6p^{2.05}$	0.01	6.97	0.20	0.01	7.19	7
$GdGe_{17}^-$	-4.07	[core]$6s^{0.44}4f^{6.99}5d^{4.84}6p^{1.76}$	0.00	6.97	0.20	0.01	7.18	7
$GdGe_{18}^-$	-3.17	[core]$6s^{0.38}4f^{6.99}5d^{4.33}6p^{1.43}$	0.00	6.97	0.19	0.01	7.17	7