Electronic Supplementary Material (ESI) for RSC Advances.

SUPPORTING INFORMATION

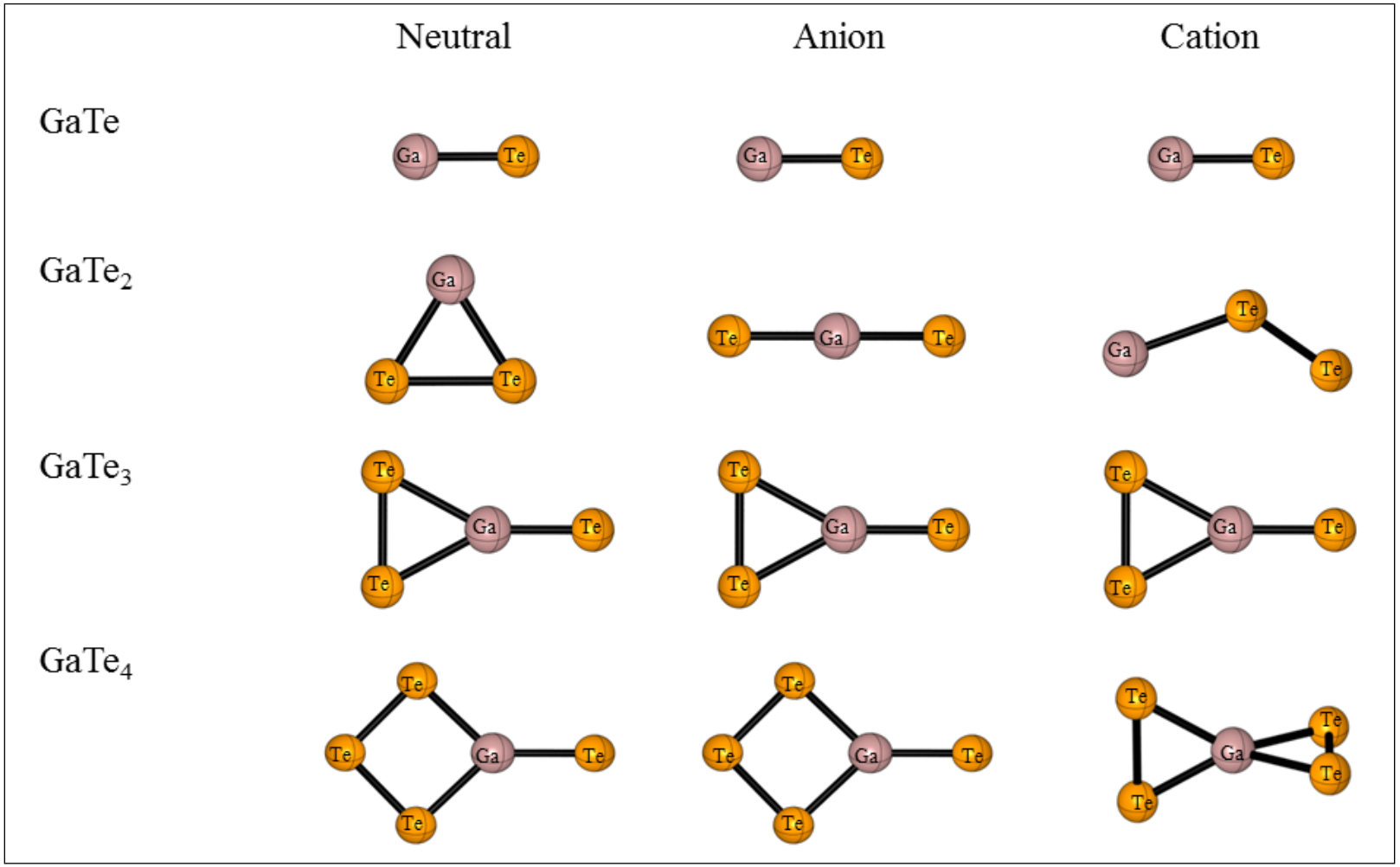

Fig. S1: Structural evolution from GaTe to $GaTe_4$.

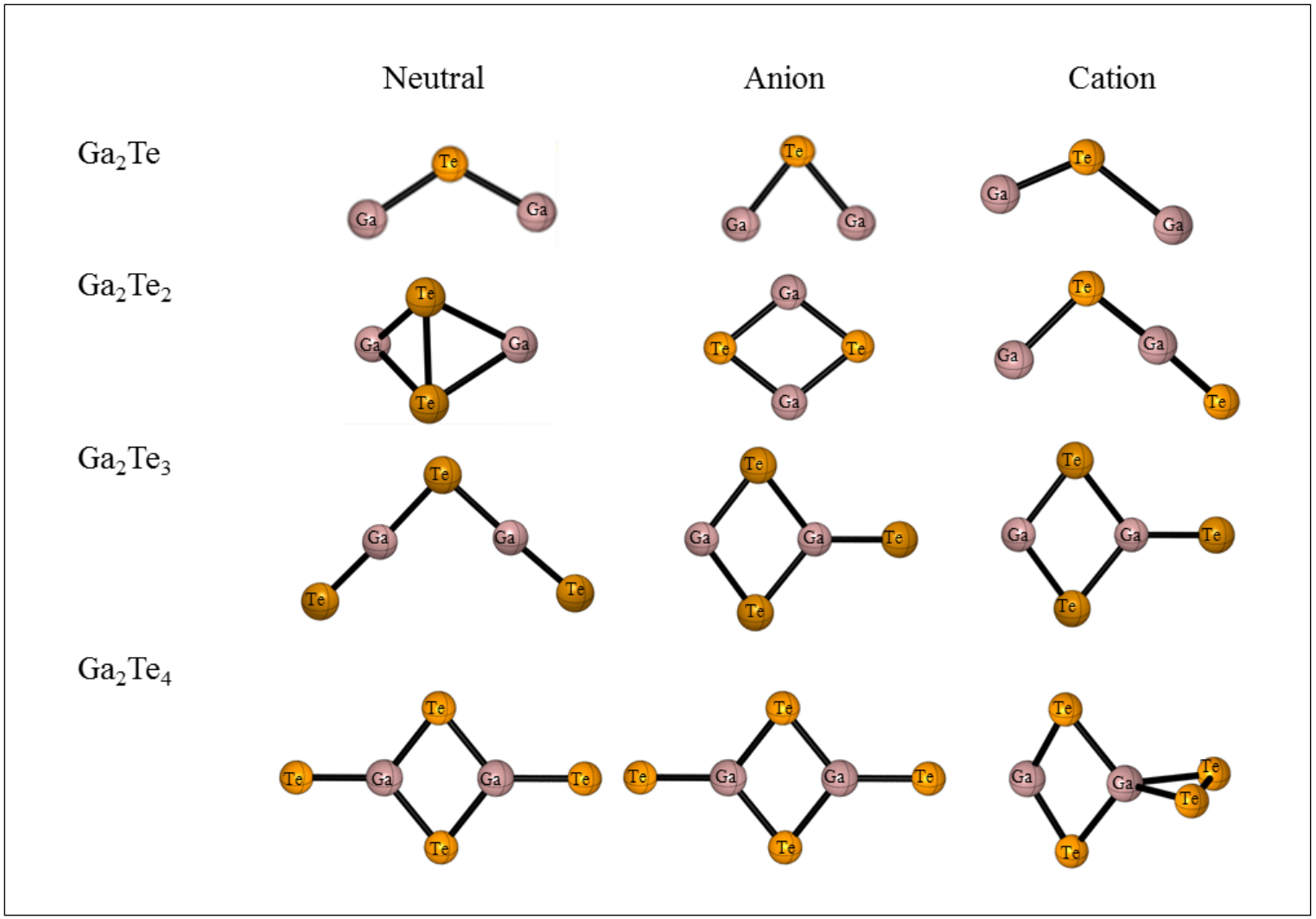

Fig. S2: Schematic diagram of the sequential addition of tellurium atom to Ga_2Te_n (n = 1–4).

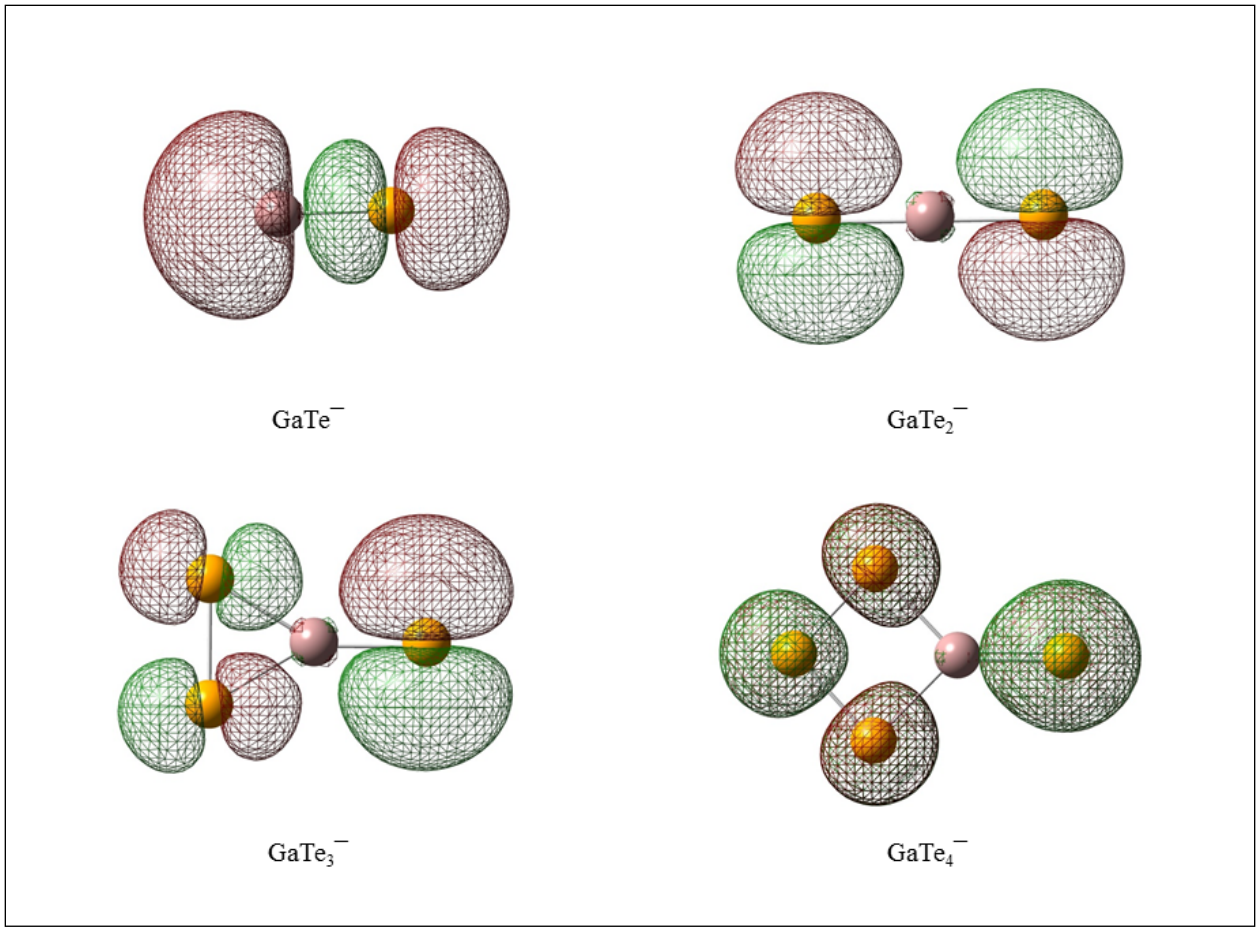

Fig. S3: Orbital accommodating the excess electron of anionic monogallium tellurides.

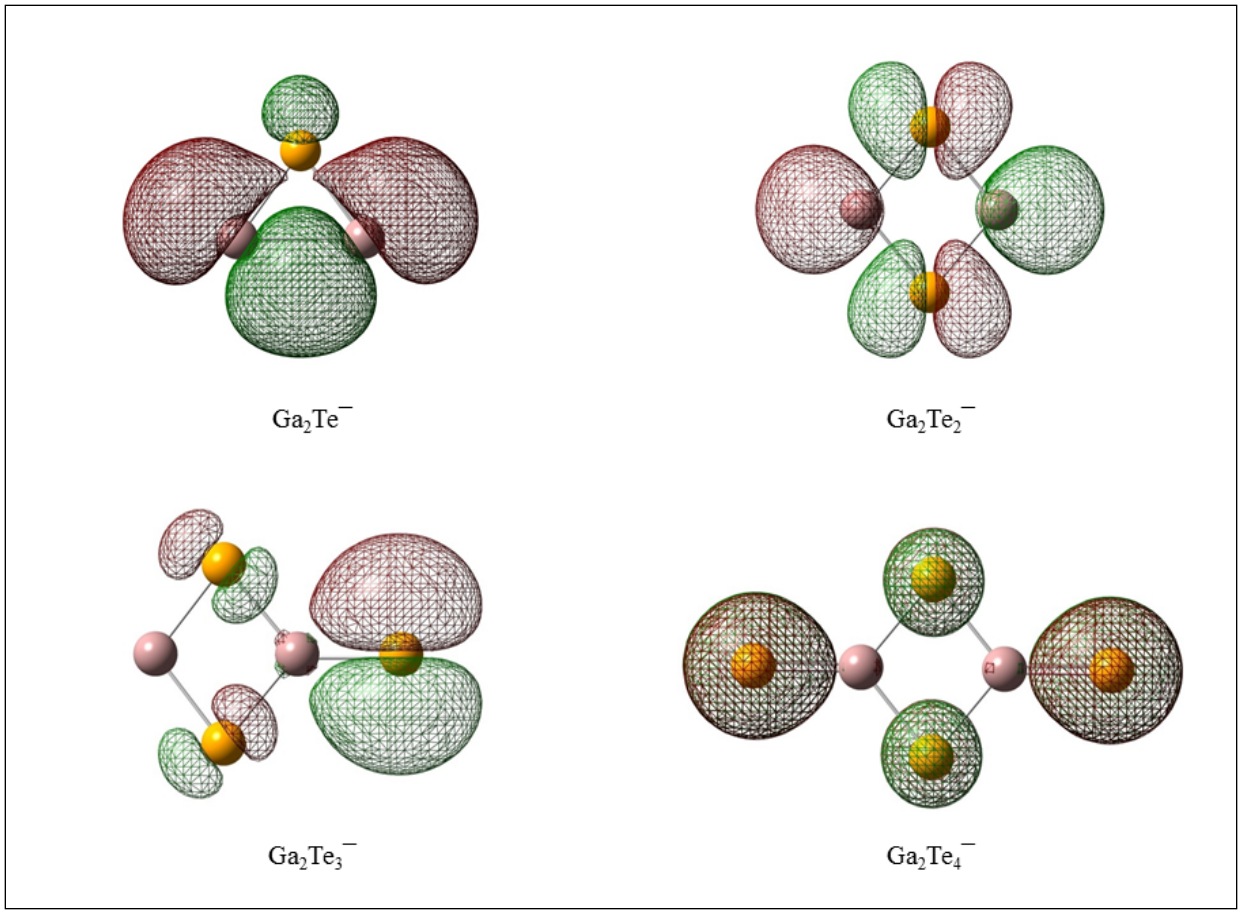

Fig. S4: Orbital accommodating the excess electron of anionic digallium tellurides.

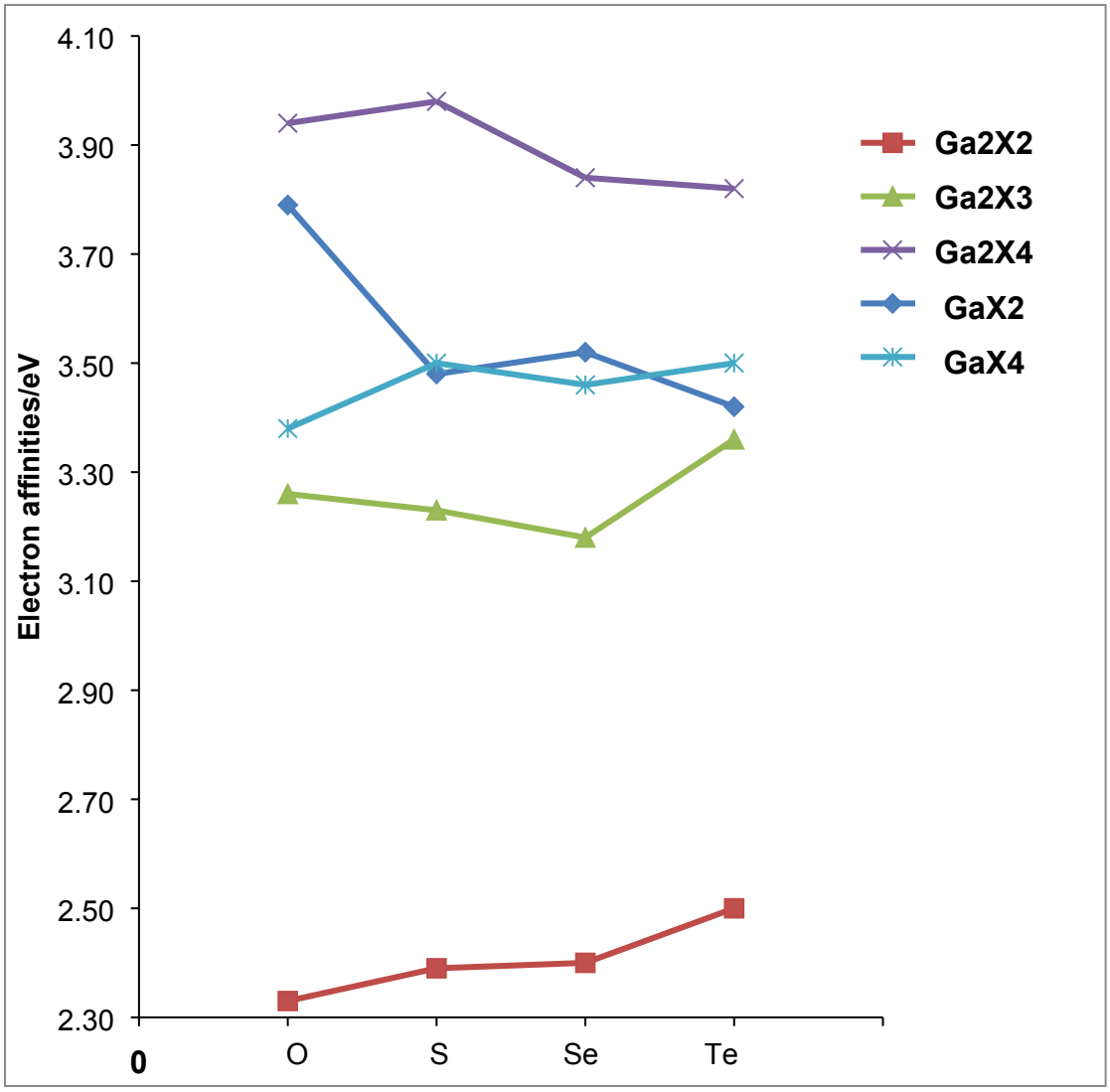

Fig. S5: Electron affinities of gallium chalcogenide (Ga_mX_n where X =O–Te; m =1,2 and n = 1–4) [Ref: 12–17,19–21,22] clusters with the B3LYP functional.

Table S1: Internal coordinates of the ground state geometries, harmonic vibrational wavenumbers (cm^{-1}), and energies (Hartree) at the B3P86 functional for $GaTe_n$ (n = 1–4) [Basis sets Ga: 6-311+G(2df) and Te: LANL2DZdp].

		$GaTe_n$		
		Neutral	**Anion**	**Cation**
***n* = 1**		Ga,0.,0.,-1.2595839389 Te,0.,0.,1.1453449389	Ga,0.,0.,-1.2994377662 Te,0.,0.,1.1851987662	Ga,0.,0.,-1.3813576298 Te,0.,0.,1.2671186298
	ν/cm^{-1}	257 (σ_g)	251 (σ_g)	149 (σ_g)
		***E* = –1933.762411**	***E* = –1933.879888**	***E* = –**1933.438318
***n* = 2**		Ga,0.0196844214,0.0087703118,0. Te,2.8581570318,-0.1835472564,0. Te,1.7748812491,2.2477872619,0.	Ga,0.,0.,0. Te,2.3958344846,0.,0. Te,-2.3958344846,0.,0.	Ga,1.9938714296,-1.0281499257,0. Te,-1.9299871135,0.3220848359,0. Te,0.1102446838,1.2666777616,0.
	ν/cm^{-1}	227 (a_1), 168 (a_1), 103 (b_2)	362 (σ_u), 168 (σ_g), 81 (π_u), 81 (π_u)	245 (a_1), 116 (a_1), 22 (a_1)
		***E* = – 1942.0140511**	***E* = –1942.15485**	***E* = –1941.706663**
***n* = 3**		Ga,-0.5703826342,-0.0889610235,0. Te,-2.8936172372,-0.4855113343,0. Te,1.4613495696,1.6325820535,0. Te,1.9191258619,-1.0314665456,0.	Ga,-0.1412926588,0.,-0.1381950146 Te,0.4140581793,0.,2.3962119782 Te,2.4048004821,0.,0.3608471441 Te,-1.8628317854,0.,-1.8219918003	Ga,0.,0.,0.53804178 Te,0.,0.,2.97550578 Te,0.,1.36168314,-1.64812498 Te,0.,-1.36168314,-1.64812498
	ν/cm^{-1}	324 (a'), 219 (a'), 126 (a'), 84(a'), 72 (a''), 47 (a')	330 (a_1), 185 (a_1), 144 (b_2), 127 (a_1), 82 (b_1), 60 (b_2)	327 (a_1), 209 (a_1), 147 (b_2), 130 (a_1), 67 (b_1), 40 (b_2)
		***E* = –1950.231676**	***E* = –1950.37661**	***E* = –1949.943481**
***n* = 4**		Ga,0.,0.,0.9039406391 Te,0.,1.9725938675,0.7578249608 Te,0.,0.,-2.6580566915 Te,0.,-1.9725938675,-0.7578249608 Te,0.,0.,3.341575874	Ga,0.,0.,0.9618547991 Te,0.,1.9652275408,-0.7664876197 Te,0.,0.,-2.7330345758 Te,0.,-1.9652275408,0.7664876197 Te,0.,0.,3.3759649162	Ga,0.,0.,0. Te,0.,1.3621366077,2.2010573856 Te,0.,-1.3621366077,2.2010573856 Te,1.3621366077,0.,-2.2010573856 Te,-1.3621366077,0.,-2.2010573856

ν/cm^{-1}	263 (a_1), 215 (b_2), 187 (b_2), 183 (a_1), 143 (a_1), 89 (a_1), 71 (b_1), 40 (b_2), 32 (b_1)	306 (a_1), 195 (b_2), 184 (a_1), 178 (b_2), 137 (a_1), 86 (a_1), 79 (b_1), 46 (b_2), 25 (b_1)	319 (b_2), 217 (a_1), 201 (b_2), 143 (e), 143 (e), 109 (a_1), 51 (e), 51 (e), 36 (b_1)
	***E* = –1958.471755**	***E* = –1958.611833**	***E* = –1958.190907**

Table S2: Internal coordinates of the ground state geometries, harmonic vibrational wavenumbers (cm^{-1}), and energies (Hartree) at the B3P86 functional for Ga_2Te_n (n = 1–4) [Basis sets Ga: 6-311+G(2df) and Te: LANL2DZdp].

		Ga_2Te_n		
		Neutral	**Anion**	**Cation**
***n* = 1**		Te,-0.0899180282,-0.1379848132,0. Ga,2.5309072261,0.0293016862,0. Ga,-0.9953104577,2.3271671771,0.	Te,-0.1648464147,-0.122581138,0. Ga,2.5125864398,0.1155020146,0. Ga,0.8339080402,2.3729788826,0.	Te,-0.0717970208,-0.1575930904,0. Ga,2.8422288477,0.046545608,0. Ga,-0.9614679469,2.1878048425,0.
	ν/cm^{-1}	204 (b_2), 195 (a_1), 37 (a_1)	205 (a_1), 141 (b_2), 104 (a_1)	159 (a_1), 123 (a_1), 39 (a_1)
		***E* = –3859.381883**	***E* = –3859.452615**	***E* = –3859.079897**
***n* = 2**		Ga,0.,2.0201678167,0.7525642224 Te,-1.3872637169,0.,-0.6930192224 Te,1.3872637169,0.,-0.6930192224 Ga,0.,-2.0201678167,0.7525642224	Ga,0.,0.,-1.6598399969 Te,0.,2.100675463,0. Te,0.,-2.100675463,0. Ga,0.,0.,1.6598399969	Ga,0.1481846634,-0.1771972945,0. Te,6.1850375779,-0.1824673134,0. Te,1.929502661,2.1265990662,0. Ga,4.0249634277,0.9540814717,0.
	ν/cm^{-1}	205 (a_1), 170 (b_2), 155 (a_1), 118 (b_1), 87 (a_2), 49 (a_1)	194 (b_{1u}), 176 (a_g), 150 (b_{3g}), 92 (a_g), 47 (b_{2u}), 39 (b_{3u})	336 (a'), 157 (a'), 134 (a'), 76 (a'), 60 (a''), 24 (a')
		***E* = –3867.625797**	***E* = –3867.734132**	***E* = –3867.323724**
***n* = 3**		Te,0.0430490165,0.,0.0491485273 Ga,-0.0544892855,0.,2.5613484797 Ga,2.546203716,0.,0.2834109273 Te,-0.2012191029,0.,4.8834988783 Te,4.8674455702,0.,0.4438739041	Ga,0.0000000002,0.,-0.1418949722 Ga,0.0000000002,0.,3.0239620179 Te,2.0790915951,0.,1.3945525318 Te,-2.0790915947,0.,1.3945525318 Te,0.0000000002,0.,5.4490507456	Ga,0.,0.,0.1600858976 Ga,0.,0.,2.9025740244 Te,2.1510641313,0.,1.3440684857 Te,-2.1510641313,0.,1.3440684857 Te,0.,0.,5.3694259636
	ν/cm^{-1}	372 (a_1), 361 (b_2), 162 (a_1), 151 (b_2), 84 (a_1), 68 (b_1), 62 (a_2), 55 (b_2), 14 (a_1)	293 (a_1), 235 (b_2), 190 (a_1), 158 (b_2), 131 (a_1), 91 (b_1), 81 (a_1), 43 (b_2), 32 (b_1)	310 (b_2), 295 (a_1), 209 (a_1), 166 (b_2), 123 (a_1), 109 (a_1), 84 (b_1), 50 (b_1), 38 (b_2)
		***E* = –3875.852304**	***E* = –3875.988792**	***E* = –3875.570983**

***n* = 4**		Ga,-1.5370608861,0.,0. Ga,1.5370608861,0.,0. Te,0.,2.0461473089,0. Te,0.,-2.0461473089,0. Te,-4.0376555072,0.,0. Te,4.0376555072,0.,0.	Ga,0.,0.,1.6018796304 Ga,0.,0.,-1.6018796304 Te,0.,2.0228529281,0. Te,0.,-2.0228529281,0. Te,0.,0.,4.0613319528 Te,0.,0.,-4.0613319528	Ga,0.0144054548,-0.0145097848, -0.0100877513 Te,2.70412703,0.0837678464, 0.0582385709 Te,-1.3980875036,2.1832731911, -0.1357697328 Ga,1.7519751144,-1.7646637859, -1.2268610431 Te,-0.6450035956,-2.1578044714, -1.500187319 Te,-1.3980874987, 0.6331531008, 2.0938558721
	ν/cm^{-1}	287 (a_g), 268 (b_{1u}), 255 (b_{2u}), 203 (b_{3g}), 157 (a_g), 129 (b_{1u}), 95 (b_{3u}), 80 (b_{2g}), 77 (a_g), 46 (b_{3g}), 32 (b_{2u}), 12 (b_{3u}) ***E* = –3884.093535**	297 (a_g), 237 (b_{2u}) , 236 (b_{1u}), 187 (b_{3g}), 157 (a_g), 123 (b_{1u}), 97 (b_{3u}), 85 (b_{2g}), 78 (a_g), 51 (b_{3g}), 31 (b_{2u}), 16 (b_{3u}) ***E* = –3884.243145**	317 (b_2), 282 (a_1), 216 (a_1), 198 (a_1), 155 (a_1), 138 (b_1), 120 (a_1), 92 (a_1), 68 (b_1), 43 (b_2), 41 (b_1), 35 (a_2) ***E* = –3883.816615**

Table S3: Internal coordinates of the ground state geometries, harmonic vibrational wavenumbers (cm^{-1}), and energies (Hartree) at the B3PW91 functional for $GaTe_n$ (n = 1–4) [Basis sets Ga: 6-311+G(2df) and Te: LANL2DZdp].

		$GaTe_n$		
		Neutral	**Anion**	**Cation**
***n* = 1**		Ga,0.,0.,-1.2612328796 Te,0.,0.,1.1469938796	Ga,0.,0.,-1.302035904 Te,0.,0.,1.187796904	Ga,0.,0.,-1.3845514819 Te,0.,0.,1.2703124819
	ν/cm^{-1}	257 (σ_g)	250 (σ_g)	147 (σ_g)
		***E* = –1932.923074**	***E* = –1933.02045**	***E* = –1932.620031**
***n* = 2**		Ga,0.0157619826,0.0070226778,0. Te,2.8604717989,-0.183466952,0. Te,1.7764889207,2.2494545916,0.	Ga,0.,0.,0. Te,2.4004966503,0.,0. Te,-2.4004966503,0.,0.	Ga,2.0203758826,-1.0285085396,0. Te,-1.9527134144,-0.3109684262,0. Te,0.1064665319,1.2559199658,0.
	ν/cm^{-1}	227 (a_1), 168 (a_1), 103 (b_2)	360 (σ_u), 167 (σ_g), 81 (π_u), 81 (π_u)	245 (a_1), 114 (a_1), 22 (a_1)
		***E* = –1941.0617802**	***E* = –1941.182666**	***E* = –1940.775193**
***n* = 3**		Ga,0,-0.5722543721,-0.0887133288,0. Te,0,-2.8998354976,-0.4845375999,0. Te,0,1.4659119818,1.6329244108,0. Te,0,1.922653448,-1.033030332,0.	Ga,0,-0.1424849099,0.,-0.1393611272 Te,0,0.4164553095,0.,2.3993693864 Te,0,2.4080102444,0.,0.363173705 Te,0,-1.8672464268,0.,-1.8263096568	Ga,0,0.,0.,-0.5387115679 Te,0,0.,0.,-2.9814906072 Te,0,0.,1.3622119398,1.6512349076 Te,0,0.,-1.3622119398,1.6512349076
	ν/cm^{-1}	340 (a'), 219 (a'), 126 (a'), 84(a''), 72 (a'), 47 (a')	329(a_1), 185 (a_1), 143 (b_2), 126 (a_1), 82 (b_1), 60 (b_2)	326 (a_1), 210 (a_1), 146 (b_2), 130 (a_1), 66 (b_1), 40 (b_2)
		***E* = –1949.166763**	***E* = –1949.291842**	***E* = –1948.898948**
***n* = 4**		Ga,0.,0.,0.9035962431 Te,0.,1.9759128156,-0.7599022274 Te,0.,0.,-2.6597336602 Te,0.,-1.9759128156,-0.7599022274 Te,0.,0.,3.3477517718	Ga,0.,0.,0.9634209388 Te,0.,1.9684966417,-0.7695837605 Te,0.,0.,-2.7345659914 Te,0.,-1.9684966417,-0.7695837605 Te,0.,0.,3.3821224737	Ga,0.,0.,0. Te,0.,1.3628261869,2.2059428792 Te,0.,-1.3628261869,2.2059428792 Te,1.3628261869,0.,-2.2059428792 Te,-1.3628261869,0.,-2.2059428792

ν/cm^{-1}	260 (a_1), 215 (b_2), 188 (b_2), 182 (a_1), 142 (a_1), 89 (a_1), 71 (b_1), 40 (b_2), 32 (b_1)	304 (a_1), 194 (b_2), 184 (a_1), 178 (b_2), 136 (a_1), 85 (a_1), 79 (b_1), 46 (b_2), 25 (b_1)	318 (b_2), 217 (a_1), 200 (b_2), 142 (e), 142 (e), 109 (a_1), 51 (e), 51 (e), 36 (b_1)
	***E* = –1957.293459**	***E* = –1957.413757**	***E* = –1957.033446**

Table S4: Internal coordinates of the ground state geometries, harmonic vibrational wavenumbers (cm^{-1}), and energies (Hartree) at the B3PW91 functional for Ga_2Te_n (n = 1–4) [Basis sets Ga: 6-311+G(2df) and Te: LANL2DZdp].

		Ga_2Te_n		
		Neutral	**Anion**	**Cation**
***n* = 1**		Ga,0.0157619826,0.0070226778,0. Te,2.8604717989,0.183466952,0. Te,1.7764889207,2.2494545916,0.	Ga,0.,0.,0. Te,2.4004966503,0.,0. Te,-2.4004966503,0.,0.	Ga,2.0203758826,-1.0285085396,0. Te,-1.9527134144,-0.3109684262,0. Te,0.1064665319,1.2559199658,0.
	ν/cm^{-1}	202 (b_2), 194 (a_1), 37 (a_1)	203 (a_1), 140 (b_2), 103 (a_1)	159 (a_1), 127 (a_1), 39 (a_1)
		E* = *–3857.813688	***E* = *–3857.864815***	***E* = *–3857.532582***
***n* = 2**		Ga,0.,2.0234047861,0.7557533179 Te,-1.3882895013,0.,-0.6962083179 Te,1.3882895013,0.,-0.6962083179 Ga,0.,-2.0234047861,0.7557533179	Ga,0.,0.,-1.6629136436 Te,0.,2.1050849619,0. Te,0.,-2.1050849619,0. Ga,0.,0.,1.6629136436	Ga,0.1355335239,-0.1779061694,0. Te,6.1956609906,-0.1825957521,0. Te,1.9285989788,2.1275351909,0. Ga,4.0278948367,0.9539826606,0.
	ν/cm^{-1}	205 (a_1), 170 (b_2), 155 (a_1), 118 (b_1), 87 (a_2), 49 (a_1)	193 (b_{1u}), 178 (a_g), 149 (b_{3g}), 92 (a_g), 40 (b_{2u}),40 (b_{3u})	342 (a'), 158 (a'), 126 (a'), 73 (a'), 64 (a''), 28 (a')
		E* = *–3865.944712	***E* = *–3866.033037***	***E* = *–3865.663509***
***n* = 3**		Te,0.0459928506,0.,0.0525094661 Ga,-0.0600717752,0.,2.5698512671 Ga,2.5553678212,0.,0.2789972258 Te,-0.2219904599,0.,4.8951096133 Te,4.8816914777,0.,0.4248131444	Ga,0.0000000002,0.,-0.1445644472 Ga,0.0000000002,0.,3.0258167605 Te,2.08315598,0.,1.391798191 Te,-2.0831559797,0.,1.391798191 Te,0.0000000002,0.,5.4553741846	Ga,0.,0.,0.1565191042 Ga,0.,0.,2.9042381996 Te,2.1546952717,0.,1.3413701381 Te,-2.1546952717,0.,1.3413701381 Te,0.,0.,5.3767252843
	ν/cm^{-1}	370 (a_1), 360 (b_2), 161 (a_1), 151 (b_2), 84 (a_1), 68 (b_1), 62 (a_2), 55 (b_2), 14 (a_1)	292 (a_1), 234 (b_2), 190 (a_1), 157 (b_2), 130 (a_1), 91 (b_1), 81 (a_1), 44 (b_2), 32 (a_1)	309 (b_2), 294 (a_1), 209 (a_1), 165 (b_2), 123 (a_1), 108 (a_1), 84 (b_1), 49 (b_1), 38 (b_2)
		E* = *–3874.058469	***E* = *–3874.175275***	***E* = *–3873.797546***

***n* = 4**		Ga,-1.5375504669,0.,0. Ga,1.5375504669,0.,0. Te,0.,2.0511740011,0. Te,0.,-2.0511740011,0. Te,-4.0446988693,0.,0. Te,4.0446988693,0.,0.	Ga,0.,0.,1.6034629475 Ga,0.,0.,-1.6034629475 Te,0.,2.0275162757,0. Te,0.,-2.0275162757,0. Te,0.,0.,4.0683324907 Te,0.,0.,-4.0683324907	Ga,0.014167858,-0.0142704672, -0.0099213686 Te,2.7093840324,0.0834449452, 0.0580140778 Te,-1.401584011,2.187180148, -0.1338751711 Ga,1.7547464538,-1.7674551968, -1.2288017376 Te,-0.6456780572,-2.1620973, -1.5031718559 Te,-1.4015840062,0.6362898057, 2.0968583307
	ν/cm^{-1}	277 (a_g), 239 (b_{2u}), 236 (b_{1u}), 199 (b_{3g}), 158 (a_g), 126 (b_{1u}), 94 (b_{3u}), 78 (a_g), 69 (b_{2g}), 48 (b_{3g}), 23 (b_{2u}), 19 (b_{3u}) ***E* = –3882.187574**	295 (a_g), 237 (b_{2u}) , 233 (b_{1u}), 187 (b_{3g}), 156 (a_g), 123 (b_{1u}), 97 (b_{3u}), 85 (b_{2g}), 77 (a_g), 51 (b_{3g}), 31 (b_{2u}), 16 (b_{3u}) ***E* = –3882.316546**	316 (b_2), 282 (a_1), 216 (a_1), 198 (a_1), 154 (b_2), 137 (b_1), 120 (a_1), 92 (a_1), 68 (b_1), 43 (b_2), 41 (b_1), 35 (a_2) ***E* = –3881.93023**

Table S5: Internal coordinates of the ground state geometries, harmonic vibrational wavenumbers (cm^{-1}), and energies (Hartree) at the B3LYP functional for $GaTe_n$ (n = 1–4) [Basis sets Ga: 6-311+G(2df) and Te: LANL2DZdp].

		$GaTe_n$		
		Neutral	**Anion**	**Cation**
***n* = 1**		Ga,0,0.,0.,-1.2733650397 Te,0,0.,0.,1.1591260397	Ga,0,0.,0.,-1.3091934505 Te,0,0.,0.,1.1949544505	Ga,0,0.,0.,-1.4200131681 Te,0,0.,0.,1.3057741681
	ν/cm^{-1}	242 (σ_g)	242 (σ_g)	125 (σ_g)
		***E* = –1932.937167**	***E* = –1933.035322**	***E* = –1932.636996**
***n* = 2**		Ga,0,-0.0041576161,-0.0018524559,0. Te,0,2.8738124499,-0.1866174633,0. Te,0,1.7830678684,2.2614802366,0.	Ga,0,0.,0.,0. Te,0,2.4127294192,0.,0. Te,0,-2.4127294192,0.,0.	Ga,0,2.1044479558,1.0323353362,0. Te,0,-2.0256524641,0.2784119926,0. Te,0,0.0953335083,1.2271903288,0.
	ν/cm^{-1}	218 (a_1), 160 (a_1), 94 (b_2)	351 (σ_u), 162 (σ_g), 79 (π_u), 79 (π_u)	236 (a_1), 110 (a_1), 28 (a_1)
		***E* = –1941.0504531**	***E* = –1941.169292**	***E* = –1940.769161**
***n* = 3**		Ga,0,0.0506596149,0.0299569366, 0.0199197691 Te,0,2.6203100804,0.1727901517, 0.0141674593 Te,0,-2.077620005,1.1479296097, -0.0074266011 Te,0,1.258767979,-2.293033048, -0.2314836523	Ga,0,-0.0144304653,-0.00879102,0. Te,0,2.6020278327,-0.0982342433,0. Te,0,1.1061492657,2.3572510722,0. Te,0,-2.086159209,-1.2708855659,0.	Ga,0,0.0096988147,0.0043395032,0. Te,0,2.5831378016,-0.3463701434,0. Te,0,1.4631581853,2.1567895801,0. Te,0,-2.2322735814, -0.9987780207,0.
	ν/cm^{-1}	278 (a'), 165 (a'), 147 (a''), 94 (a'), 71 (a'), 47 (a'')	318 (a_1), 176 (a_1), 135 (b_2), 121 (a_1), 81 (b_1), 59 (b_2)	315 (a_1), 201 (a_1), 137 (b_2), 125 (a_1), 66 (b_1), 40 (b_2)
		***E* = –1949.128321**	***E* = –1949.249973**	***E* = –1948.85986**

***n* = 4**		Ga,0,0.,0.,0.9172107419 Te,0,0.,1.9858667992,-0.7669890476 Te,0,0.,0.,-2.6854436915 Te,0,0.,-1.9858667992,-0.7669890476 Te,0,0.,0.,3.3740209447	Ga,0,0.,0.,0.9766748764 Te,0,0.,1.9818553213,-0.7761903516 Te,0,0.,0.,-2.7603587707 Te,0,0.,-1.9818553213,-0.7761903516 Te,0,0.,0.,3.4078744975	Ga,0,0.,0.,0. Te,0,0.,1.3722590855,2.222151623 Te,0,0.,-1.3722590855,2.222151623 Te,0,1.3722590855,0.,-2.222151623 Te,0,-1.3722590855,0.,-2.222151623
	ν/cm^{-1}	252 (a_1), 205 (b_2), 179 (b_2), 175 (a_1), 137 (a_1), 89 (a_1), 70 (b_1), 40 (b_2), 31 (b_1)	295 (a_1), 184 (b_2), 175 (a_1), 170 (b_2), 131 (a_1), 85 (a_1), 78 (b_1), 46 (b_2), 24 (b_1)	306 (b_2), 208 (a_1), 193 (b_2), 133 (e), 133 (e), 105 (a_1), 51 (e), 51 (e), 35 (b_1)
		***E* = –1957.22703**	***E* = –1957.34623**	***E* = –1956.964773**

Table S6: Internal coordinates of the ground state geometries, harmonic vibrational wavenumbers (cm^{-1}), and energies (Hartree) at the B3LYP functional for Ga_2Te_n (n = 1–4) [Basis sets Ga: 6-311+G(2df) and Te: LANL2DZdp].

		Ga_2Te_n		
		Neutral	**Anion**	**Cation**
***n* = 1**		Te,0,-0.0855373005,-0.1312623137,0. Ga,0,2.5609213319,0.0049543413,0. Ga,0,-1.0297052913,2.3447920224,0.	Te,0,-0.1705117925,-0.1267939596,0. Ga,0,2.5374240494,0.088016337,0. Ga,0,0.8147358084,2.4046773817,0.	Te,0,-0.0463084024,-0.1321450033,0. Ga,0,2.9171255201,-0.0172310404,0. Ga,0,-1.0618532378,2.2261334037,0.
	ν/cm^{-1}	196 (b_2), 187 (a_1), 37 (a_1)	194 (a_1), 133 (b_2), 91 (a_1)	159 (a_1), 123 (a_1), 30 (a_1)
		***E* = –3857.866157**	***E* = –3857.911955**	***E* = –3857.586191**
***n* = 2**		Ga,0,0.,2.0584358799,0.7585660949 Te,0,-1.3992351736,0.,-0.6990210949 Te,0,1.3992351736,0.,-0.6990210949 Ga,0,0.,-2.0584358799,0.7585660949	Ga,0,0.,0.,-1.6875503794 Te,0,0.,2.1264916151,0. Te,0,0.,-2.1264916151,0. Ga,0,0.,0.,1.6875503794	Ga,0,0.0689974265,-0.17378416,0. Te,0,6.2371699912,-0.1722248249,0. Te,0,1.9327159006,2.1184963302,0. Ga,0,4.0488050117,0.9485285848,0.
	ν/cm^{-1}	195 (a_1), 162 (b_2), 148 (a_1), 109 (b_1), 77 (a_2), 48 (a_1)	179 (b_{1u}), 170 (a_g), 136 (b_{3g}), 90 (a_g), 52 (b_{2u}), 42 (b_{3u})	324 (a'), 151 (a'), 126 (a'), 75 (a'), 59 (a''), 24 (a')
		***E* = –3865.966584**	***E* = –3866.053104**	***E* = –3865.690747**
***n* = 3**		Te,0,0.0792146787,0.,0.0904384145 Ga,0,-0.0972181165,0.,2.6205665117 Ga,0,2.6105346262,0.,0.2488557209 Te,0,-0.3427510497,0.,4.9491905626 Te,0,4.9512097755,0.,0.3122295071	Ga,0,0.0000000002,0.,-0.1820130873 Ga,0,0.0000000002,0.,3.0417422927 Te,0,2.0951428101,0.,1.3874523221 Te,0,-2.0951428097,0.,1.3874523221 Te,0,0.0000000002,0.,5.4855890189	Ga,0,0.,0.,0.129110857 Ga,0,0.,0.,2.9197501446 Te,0,2.1637007314,0.,1.3322375037 Te,0,-2.1637007314,0.,1.3322375037 Te,0,0.,0.,5.4068868397
	ν/cm^{-1}	359 (a_1), 350 (b_2), 154 (a_1), 147 (b_2), 84 (a_1), 66 (b_1), 61 (a_2), 56 (b_2), 15 (a_1)	281 (a_1), 219 (b_2), 178 (a_1), 144 (b_2), 125 (a_1), 89 (b_1), 80 (a_1), 41 (b_2), 32 (b_1)	298 (b_2), 284 (a_1), 200 (a_1), 154 (b_2), 118 (a_1), 104 (a_1), 83 (b_1), 49 (b_1), 38 (b_2)
		***E* = –3874.054184**	***E* = –3874.165272**	***E* = –3873.788824**

***n* = 4**		Ga,0,-1.563132217,0.,0. Ga,0,1.563132217,0.,0. Te,0,0.,2.0548853409,0. Te,0,0.,-2.0548853409,0. Te,0,-4.0841802999,0.,0. Te,0,4.0841802999,0.,0.	Ga,0,0.,0.,1.6278342852 Ga,0,0.,0.,-1.6278342852 Te,0,0.,2.0332956281,0. Te,0,0.,-2.0332956281,0. Te,0,0.,0.,4.1064751857 Te,0,0.,0.,-4.1064751857	Ga,0,0.0075895135,-0.007644479, -0.0053147308 Te,0,2.7276120555,0.0774188814, 0.0538245302 Te,0,-1.4192642398,2.2102757456, -0.1290992345 Ga,0,1.7757527746,-1.7886136558, -1.2435118989 Te,0,-0.6421636218,-2.1779711644, -1.5142079671 Te,0,-1.4192642348,0.6488107635, 2.1168443712
	ν/cm^{-1}	276 (a_g), 258 (b_{1u}), 244 (b_{2u}), 193 (b_{3g}), 152 (a_g), 124 (b_{1u}), 94 (b_{3u}), 79 (b_{2g}), 77 (a_g), 47 (b_{3g}), 33 (b_{2u}), 13 (b_{3u})	286 (a_g), 227 (b_{2u}) , 226 (b_{1u}), 177 (b_{3g}), 151 (a_g), 118 (b_{1u}), 96 (b_{3u}), 84 (b_{2g}), 77 (a_g), 52 (b_{3g}), 33 (b_{2u}), 16 (b_{3u})	305 (b_2), 271 (a_1), 207 (a_1), 190 (a_1), 143 (a_1), 128 (b_1), 116 (a_1), 89 (a_1), 67 (b_1), 43 (b_2), 41 (b_1), 34 (a_2)
		***E* = –3882.152755**	***E* = –3882.281229**	***E* = –3881.891928**

Table S7: Internal coordinates of the ground state geometries, harmonic vibrational wavenumbers (cm^{-1}), and energies (Hartree) with the MP2 level for $GaTe_n$ (n = 1–4) [Basis sets Ga: 6-311+G(2df) and Te: LANL2DZdp].

		$GaTe_n$		
		Neutral	**Anion**	**Cation**
***n* = 1**		Ga,0.,0.,-1.2366563355 Te,0.,0.,1.1224173355	Ga,0.,0.,-1.2840715309 Te,0.,0.,1.1698325309	Ga,0.,0.,-1.3658114171 Te,0.,0.,1.2515724171
	ν/cm^{-1}	301 (σ_g)	270 (σ_g)	148 (σ_g)
		***E* = –1931.407474**	***E* = –1931.498509**	***E* = –1931.11059**
***n* = 2**		Ga,0.0603215288,0.0268760863,0. Te,2.8418201883,-0.2015368058,0. Te,1.7505809851,2.2476710369,0.	Ga,0.,0.,0. Te,2.380792447,0.,0. Te,-2.380792447,0.,0.	Ga,1.8884954872,-1.022829965,0. Te,-1.8397879234,-0.3635956037,0. Te,0.1254214362,1.3028685688,0.
	ν/cm^{-1}	299 (a_1), 226 (a_1), 178 (b_2)	383 (σ_u), 180 (σ_g), 83 (π_u), 83 (π_u)	285 (a_1), 145 (a_1), 29 (a_1)
		***E* = –1939.4200812**	***E* = –1939.550661**	***E* = –1939.135826**
***n* = 3**		Ga,0,0.3420671443,0.2025282795,0. Te,0,2.4610529228,1.4489846399,0. Te,0,-0.6640743927,-2.0771105412,0. Te,0,-2.1390456743,0.4255976218,0.	Ga,0,-0.5545250834,-0.0785795994,0. Te,0,-2.8671108016,-0.4480207436,0. Te,0,1.4535599688,1.6256139424,0. Te,0,1.8845514764,-1.0723704493,0.	Ga,0, -0.0000100377,0.5158544103,0. Te,0,-0.0000628096,2.9515408673,0. Te,0,-1.3793936337,-1.62955852,0. Te,0,1.3794665225,-1.6294987462,0.
	ν/cm^{-1}	348 (a'), 206 (a'), 176 (a'), 126 (a'), 76 (a''), 47 (a')	352 (a_1), 186 (a_1), 163 (b_2), 131 (a_1), 87 (b_1), 62 (b_2)	682 (b_2), 350 (a_1), 203 (a_1), 134 (a_1), 72 (b_1), 51 (b_2)
		***E* = –1947.4229709**	***E* = –1947.4223543**	***E* = –1947.1621088**
***n* = 4**		Ga,0,0.,0.,0. Te,0,0.,1.4084805584,2.1239748626 Te,0,0.,-1.4084805584,2.1239748626 Te,0,1.4084805584,0.,-2.1239748626 Te,0,-1.4084805584,0.,-2.1239748626	Ga,0,0.,0.,0.9380157547 Te,0,0.,1.964664822,-0.74288137 Te,0,0.,0.,-2.7152568217 Te,0,0.,-1.964664822,-0.74288137	Ga,0.,0.,0. Te,0.,1.37879942,2.1694783807 Te,0.,-1.37879942,2.1694783807 Te,1.37879942,0.,-2.1694783807 Te,-1.37879942,0.,-2.1694783807

		Te,0,0.,0.,3.3348137069	
ν/cm^{-1}	5026 (e), 5004 (e), 382 (b_2), 208 (b_2), 195 (a_1), 137 (e), 137 (e), 109 (a_1), 43 (b_1)	326 (a_1), 215 (b_2), 186 (a_1), 185 (b_2), 148 (a_1), 87 (a_1), 87 (b_1), 50 (b_2), 25 (b_1)	1415(e), 1415 (e), 334 (b_2), 207 (a_1), 189 (b_2), 112 (a_1), 62 (e), 62 (e), 37 (b_1)
	***E* = –1955.4271886**	***E* = –1955.537391**	***E* = –1955.181809**

Table S8: Internal coordinates of the ground state geometries, harmonic vibrational wavenumbers (cm^{-1}), and energies (Hartree) with the MP2 level for Ga_2Te_n (n = 1–4) [Basis sets Ga: 6-311+G(2df) and Te: LANL2DZdp].

		Ga_2Te_n		
		Neutral	**Anion**	**Cation**
***n* = 1**		Te,0,-0.1391006558,-0.2134586178,0. Ga,0,2.4462193,0.138250583,0. Ga,0,-0.861439904,2.2936920849,0.	Te,0,-0.1556299095,-0.1157276688,0. Ga,0,2.4887352519,0.1379530664,0. Ga,0,0.8485427228,2.3436743615,0.	Te,0,-0.14353379,-0.2087336516,0. Ga,0,2.7572154921,0.1469531086,0. Ga,0,0.8047178221,2.1385379029,0.
	ν/cm^{-1}	212 (b_2), 205 (a_1), 37 (a_1)	222 (a_1), 150 (b_2), 116 (a_1)	247 (a_1), 130 (a_1), 44 (a_1)
		***E* = –3854.89885**	***E* = –3854.947528**	***E* = –3854.621898**
***n* = 2**		Ga,0,0.,1.9479477762,0.7568236244 Te,0,-1.3986868761,0.,-0.6972786244 Te,0,1.3986868761,0.,-0.6972786244 Ga,0,0.,-1.9479477762,0.7568236244	Ga,0,0.,0.,-1.6127512738 Te,0,0.,2.0878788901,0. Te,0,0.,-2.0878788901,0. Ga,0,0.,0.,1.6127512738	Ga,0,0.3250113726,0.2154392632,0. Te,0,6.0888481489,-0.2306196551,0. Te,0,1.9133735242,2.1900769048,0. Ga,0,3.9604552843,0.9769979436,0.
	ν/cm^{-1}	209 (a_1), 178 (b_2), 158 (a_1), 134 (b_1), 95 (a_2), 52 (a_1)	914 (b_{2u}), 221 (b_{1u}), 196 (a_g), 167 (b_{3g}), 93 (a_g), 47 (b_{3u})	372 (a'), 167 (a'), 140 (a'), 80 (a'), 65 (a''), 24 (a')
		***E* = –3862.912699**	***E* = –3863.004325**	***E* = –3862.645467**
***n* = 3**		Te,-0.0462234305,0.,-0.0527727163 Ga,0.0460244149,0.,2.4444656026 Ga,2.4170981027,0.,0.3676507728 Te,0.0755461699,0.,4.7599818012 Te,4.7085446573,0.,0.7019552565	Ga,0,0.0000000002,0.,-0.0804628427 Ga,0,0.0000000002,0.,3.0028313233 Te,0,2.0738564649,0.,1.3958661484 Te,0,-2.0738564645,0.,1.3958661484 Te,0,0.0000000002,0.,5.4061220932	Ga,0,0.,0.,0.2146846017 Ga,0,0.,0.,2.8751447405 Te,0,2.1611541876,0.,1.3494178996 Te,0,-2.1611541876,0.,1.3494178996 Te,0,0.,0.,5.3315577077
	ν/cm^{-1}	394 (a_1), 380 (b_2), 176 (a_1), 155 (b_2), 83 (a_1), 73 (b_1), 66 (a_2), 55 (b_2), 18 (a_1)	307 (a_1), 249 (b_2), 204 (a_1), 162 (b_2), 135 (a_1), 93 (b_1), 85 (a_1), 50 (b_2), 29 (b_1)	328 (b_2), 317 (a_1), 220 (a_1), 171 (b_2), 130 (a_1), 114 (a_1), 87 (b_1), 53 (b_1), 40 (b_2)
		***E* = –3870.9370802**	***E* = –3871.038997**	***E* = –3870.682646**

***n* = 4**		Ga,0,-1.4833755382,0.,0. Ga,0,1.4833755382,0.,0. Te,0,0.,2.0616459329,0. Te,0,0.,-2.0616459329,0. Te,0,-3.9768912582,0.,0. Te,0,3.9768912582,0.,0.	Ga,0,0.,0.,1.5556482428 Ga,0,0.,0.,-1.5556482428 Te,0,0.,2.0346648431,0. Te,0,0.,-2.0346648431,0. Te,0,0.,0.,3.9893094887 Te,0,0.,0.,-3.9893094887	Ga,0,0.0204960588,-0.0206445, -0.0143528374 Te,0,2.7015085328,0.100904876, 0.0701528824 Te,0,-1.3667260559,2.1618310877, -0.1723255675 Ga,0,1.7059140185,-1.7182690927, -1.1946056967 Te,0,-0.6649190836,-2.1522443135, -1.4963216868 Te,0,1.366726051,0.5914180385, 2.0864885504
	ν/cm^{-1}	308 (a_g), 284 (b_{1u}), 274 (b_{2u}), 216 (b_{3g}), 166 (a_g), 134 (b_{1u}), 98 (b_{3u}), 87 (b_{2g}), 78 (a_g), 50 (b_{3g}), 36 (b_{2u}), 11 (b_{3u}) ***E* = –3878.951108**	346 (b_{1u}), 314 (a_g) , 250 (b_{2u}), 199 (b_{3g}), 165 (a_g), 140 (b_{1u}), 97 (b_{3u}), 90 (b_{2g}), 75 (a_g), 50 (b_{3g}), 29 (b_{2u}), 16 (b_{3u}) ***E* = –3879.066654**	968 (b_1), 333 (b_2), 303 (a_1), 221 (a_1), 192 (a_1), 158 (b_2), 125 (a_1), 97 (a_1), 72 (b_1), 52 (b_1), 44 (b_2), 36(a_2) ***E* = –3878.701154**

Table S9: Effective NAO electronic configurations (El.conf) and natural charges [q(M)] of gallium atoms in neutral, negatively and positively charged Ga_mTe_n (m = 1,2 and n = 1–4) clusters with the B3LYP functional [Basis sets Ga: 6-311+G(2df) and Te: LANL2DZdp]. [a]

	n			
	1	2	3	4
$GaTe_n$				
El.conf	$4s^{0.73}4p^{0.27}$	$4s^{0.98}4p^{0.35}$	$4s^{0.59}4p^{0.81}$	$4s^{0.59}4p^{0.84}$
q(Ga)	0.49	0.16	0.09	0.05
$GaTe_n^-$				
El.conf	$4s^{1.86}4p^{1.08}$	$4s^{1.17}4p^{1.37}$	$4s^{1.15}4p^{1.47}$	$4s^{1.16}4p^{1.50}$
q(Ga)	–0.006	0.43	0.33	0.29
$GaTe_n^+$				
El.conf	$4s^{0.83}4p^{0.08}$	$4s^{0.98}4p^{0.07}$	$4s^{0.61}4p^{0.81}$	$4s^{0.57}4p^{0.94}$
q(Ga)	0.58	0.40	0.06	–0.04
Ga_2Te_n				
El.conf	$4s^{1.93}4p^{0.57}$	$4s^{1.95}4p^{0.62}$	$4s^{1.20}4p^{1.31}$	$4s^{0.59}4p^{0.78}$
q(Ga)	0.48	0.41	0.46	0.11
$Ga_2Te_n^-$				
El.conf	$4s^{0.93}4p^{0.34}$	$4s^{0.82}4p^{0.49}$	$4s^{0.67}4p^{0.42}$ $4s^{0.58}4p^{0.75}$	$4s^{0.58}4p^{0.77}$
q(Ga)	0.21	0.17	(0.39, 0.15)	0.13
$Ga_2Te_n^+$				
El.conf	$4s^{0.99}4p^{0.12}$ $4s^{0.76}4p^{0.14}$	$4s^{0.99}4p^{0.12}$ $4s^{0.62}4p^{0.63}$	$4s^{0.64}4p^{0.54}$ $4s^{0.61}4p^{0.80}$	$4s^{0.58}4p^{0.93}$ $4s^{0.63}4p^{0.54}$
q(Ga)	(0.38, 0.59)	(0.38, 0.23)	(0.31, 0.08)	(–0.03, 0.31)

[a] All values are in *e*.

Table S10: ADEs, VDEs, VIPs (eV), HOMO–LUMO gaps (eV) and chemical hardness (η) of gallium telluride clusters with the B3LYP functional [Basis sets Ga: 6-311+G(2df) and Te: LANL2DZdp].

Clusters	**ADE/eV**	**VDE/eV**	**VIP/eV**	**HOMO–LUMO gaps/eV**	**η**
GaTe	2.67	2.69	8.16	3.99	2.74
$GaTe_2$	3.42	3.42	7.65	3.83	1.77
$GaTe_3$	3.31	3.52	7.36	2.97	1.92
$GaTe_4$	3.24	3.28	7.14	2.61	1.93
Ga_2Te	1.25	1.00	7.38	3.58	3.19
Ga_2Te_2	2.39	2.00	7.24	3.43	2.62
Ga_2Te_3	3.34	3.66	6.82	3.31	1.58
Ga_2Te_4	3.50	2.87	6.29	3.71	1.71