Supplementary Information

Investigating Pressure-Driven Semiconductor-to-Metal Transition in Lead-Free Perovskites $AlGeX_3$ (X= F, Cl, and Br): Insights from First-Principles Calculations

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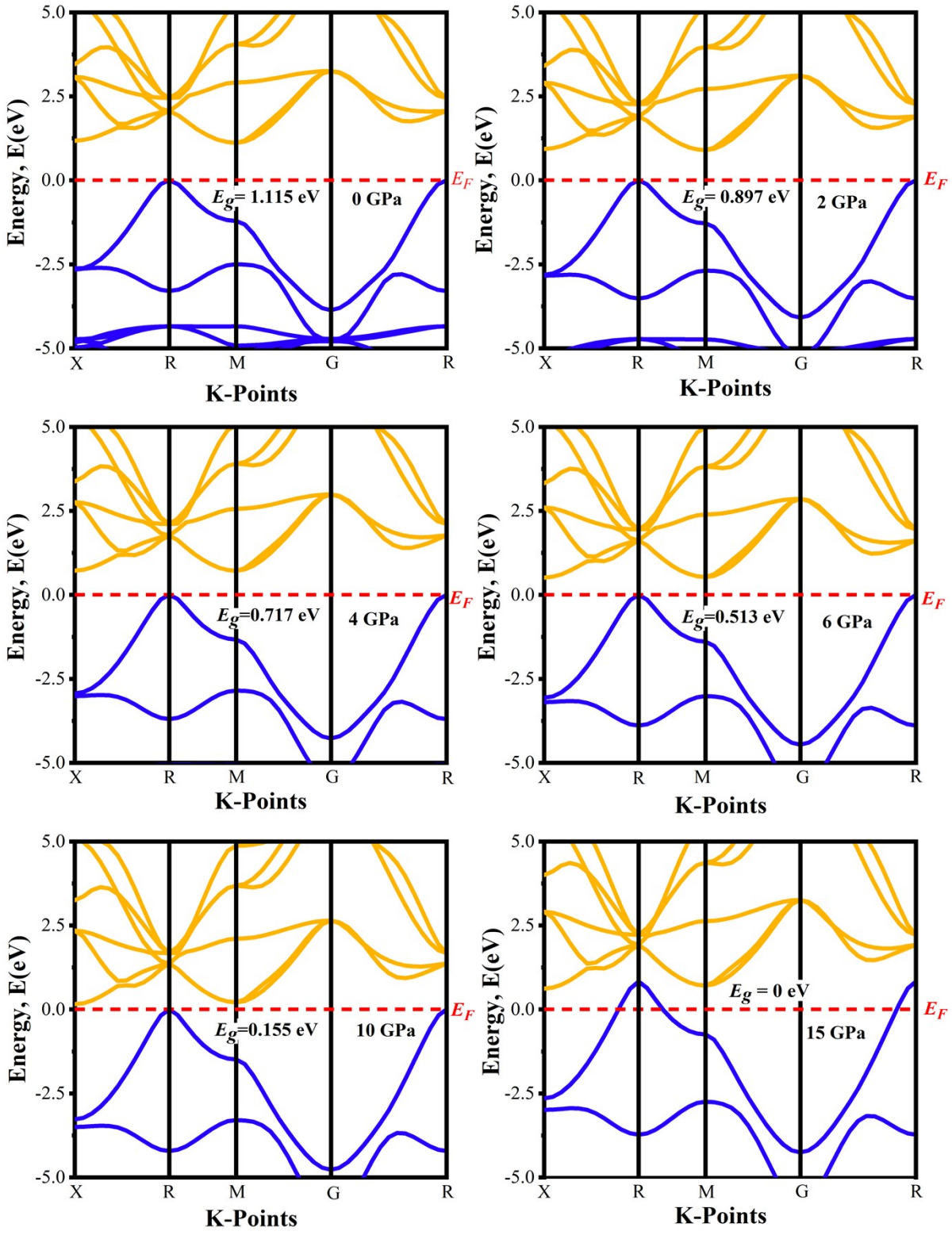

Fig. S1 Band structure of $AlGeF_3$ under hydrostatic pressure.

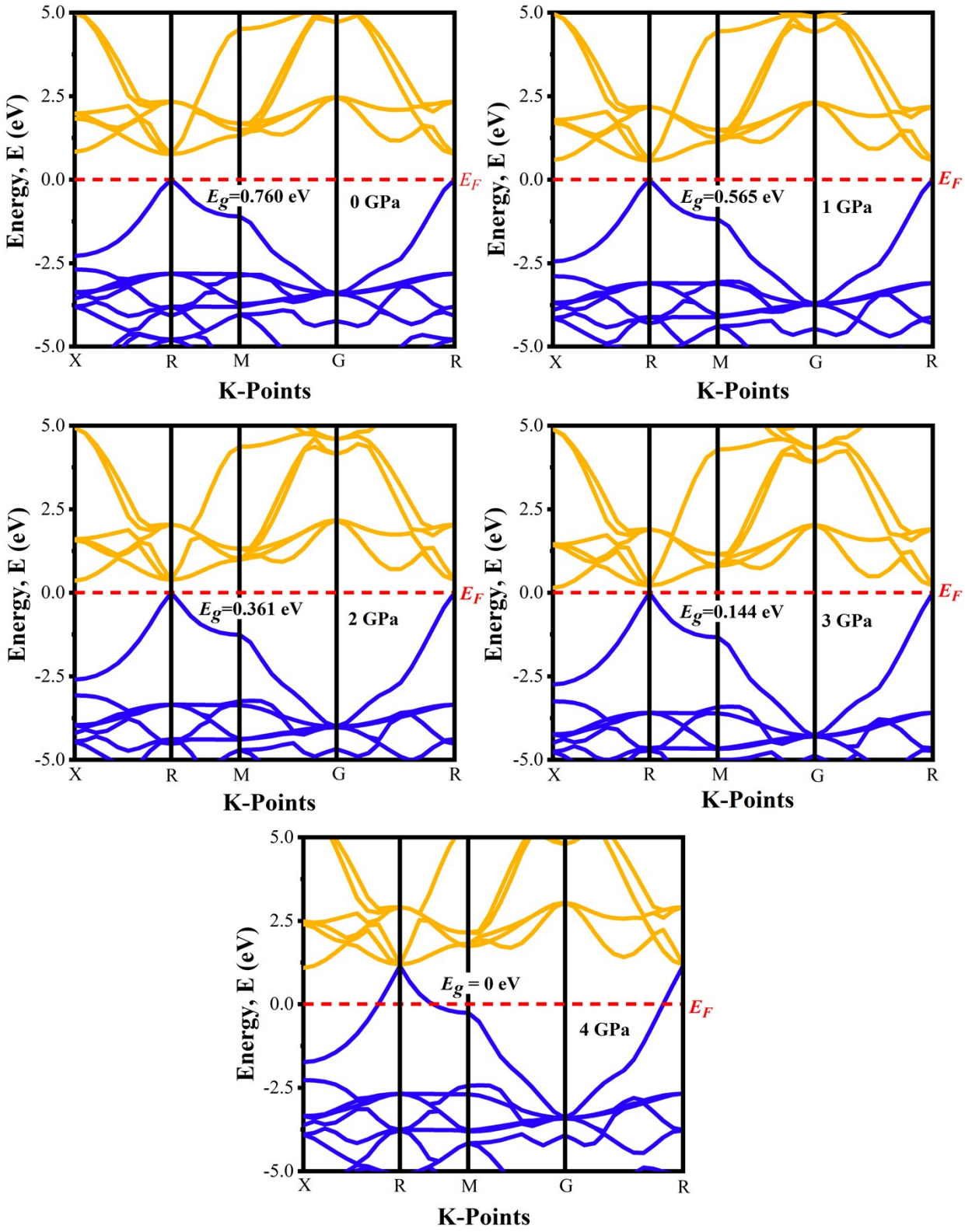

Fig. S2 Band structure of $AlGeCl_3$ under hydrostatic pressure.

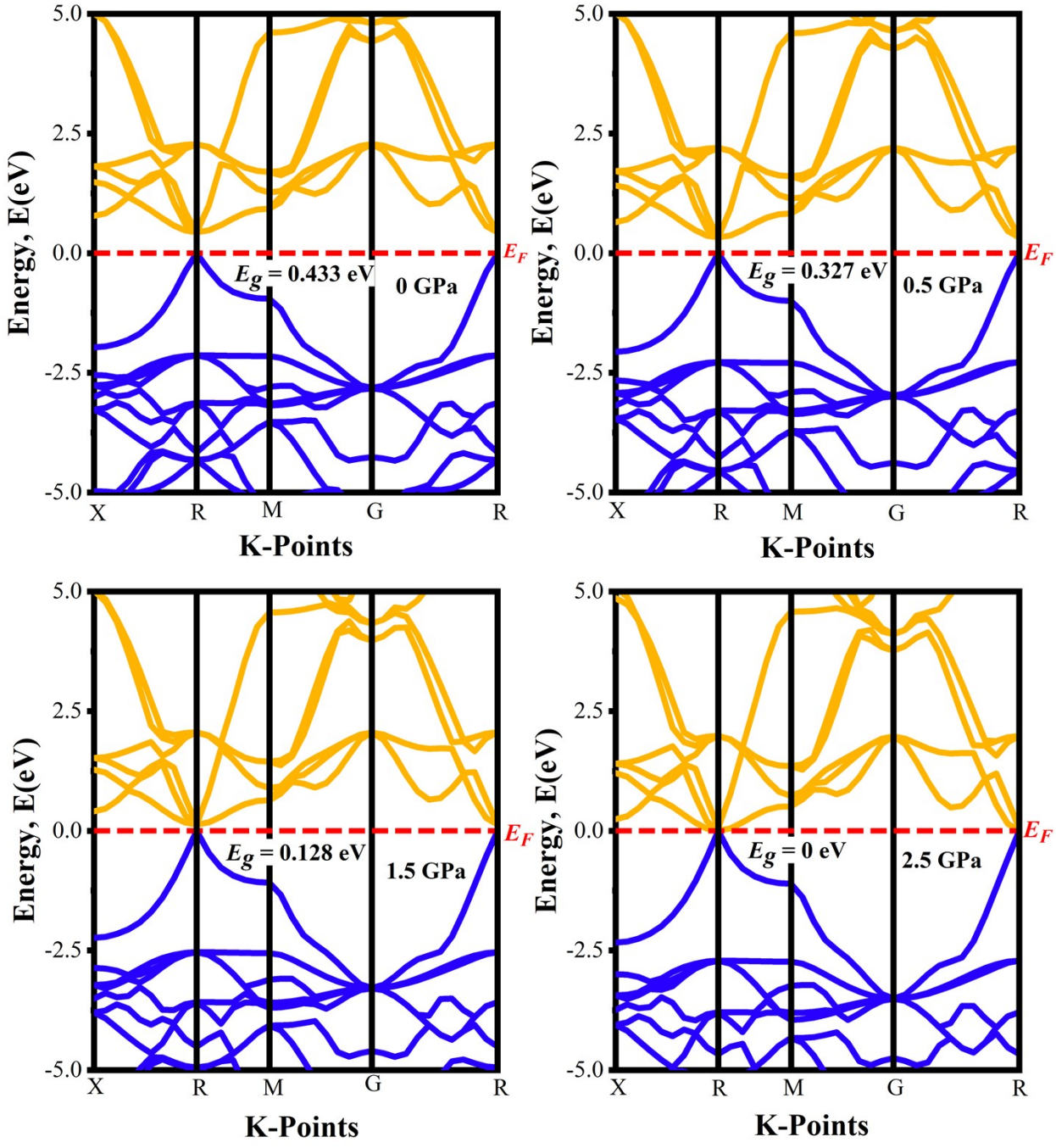

Fig. S3 Band structure of $AlGeBr_3$ under hydrostatic pressure.

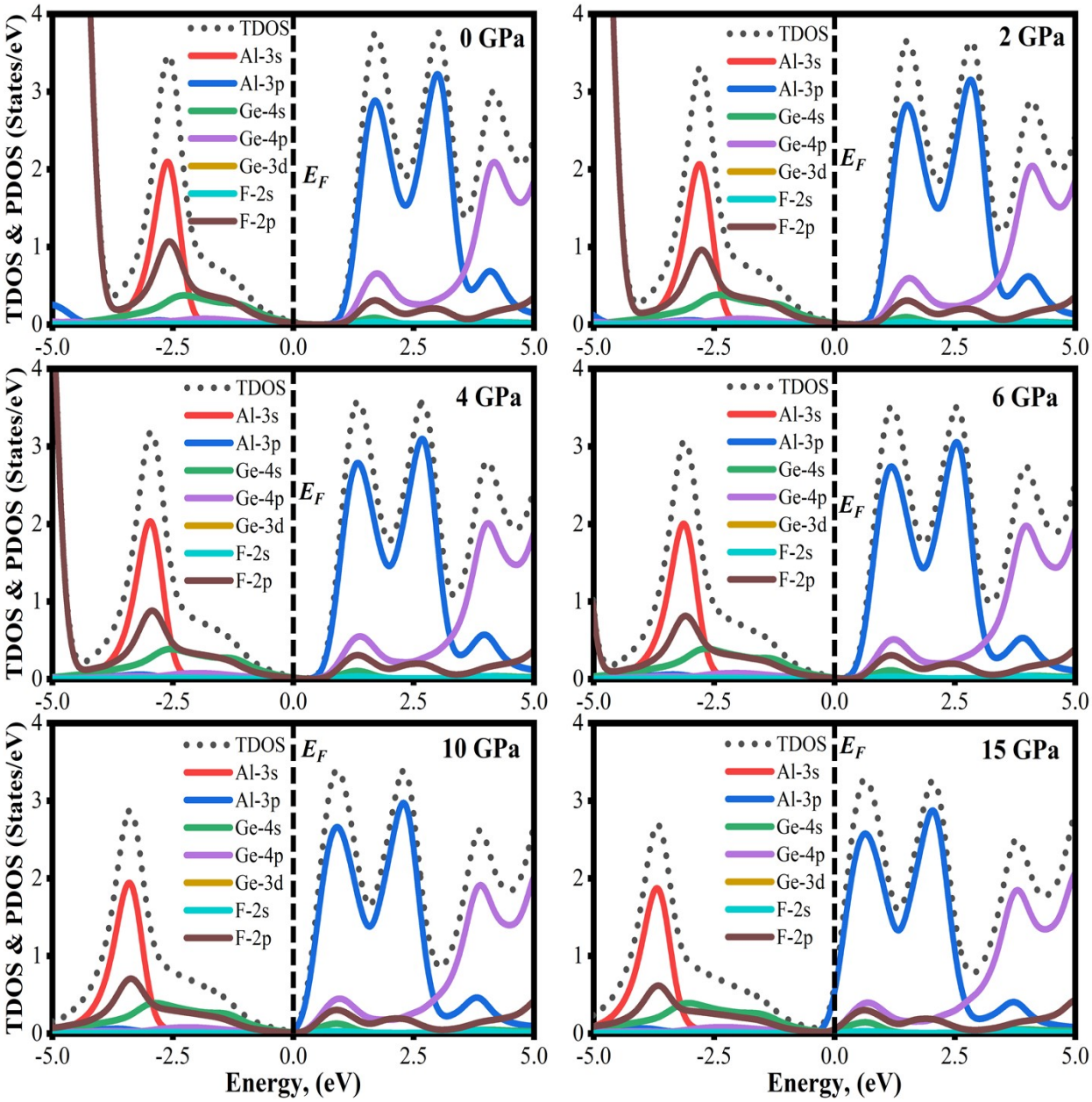

Fig. S4 The calculated TDOS and PDOS of cubic $AlGeF_3$ perovskites under pressure.

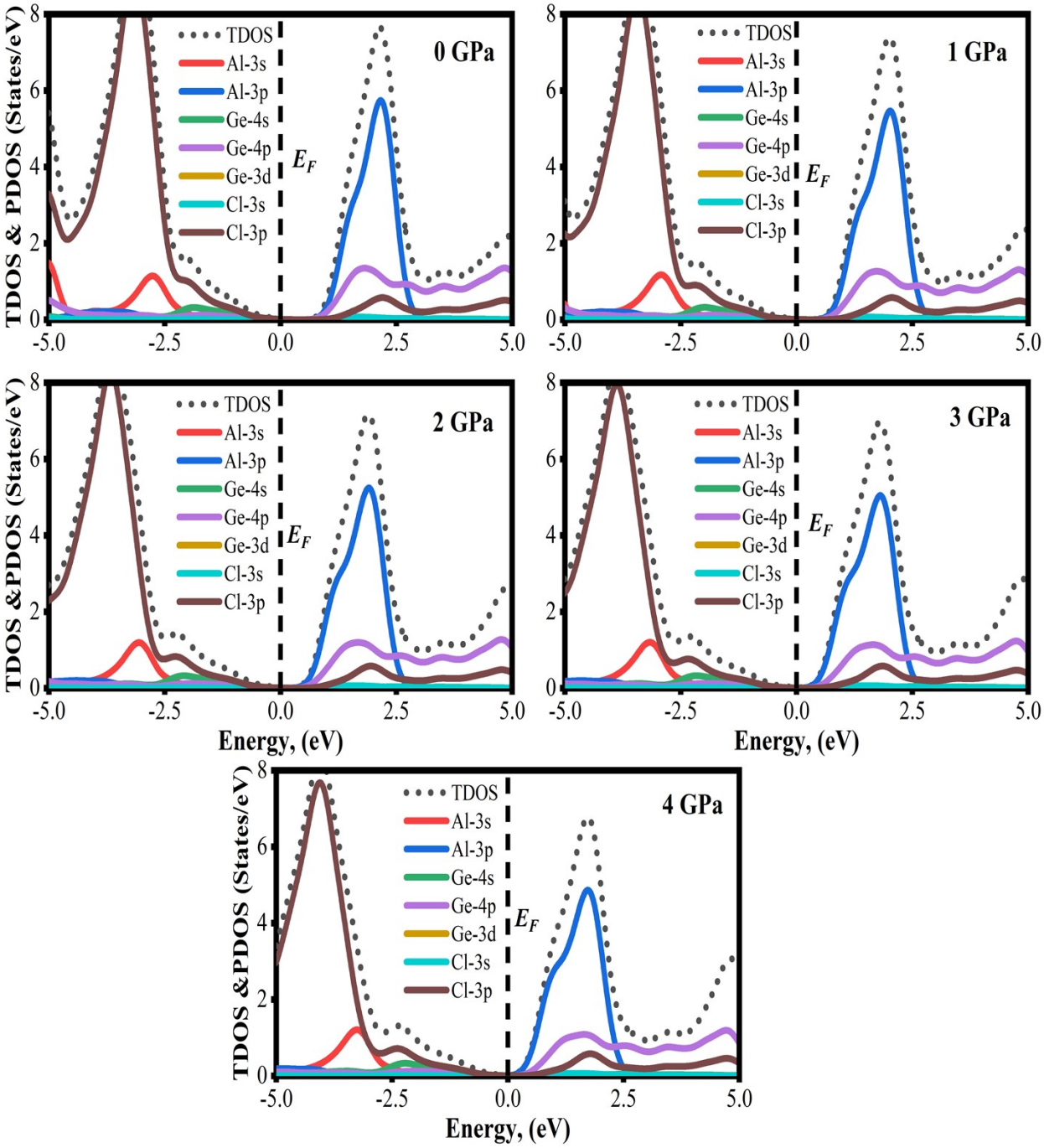

Fig. S5 The calculated TDOS and PDOS of cubic $AlGeCl_3$ perovskites under pressures.

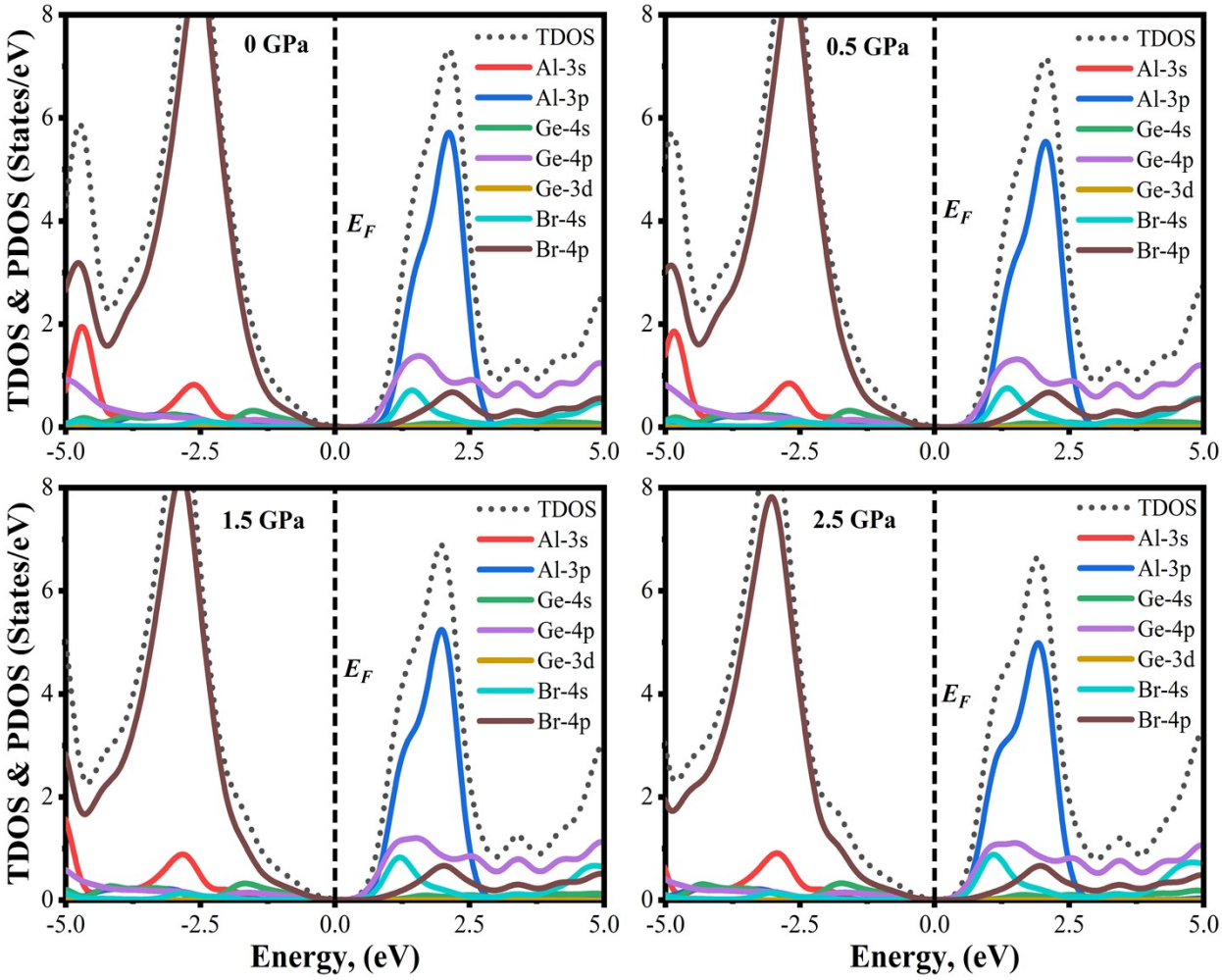

Fig. S6 The calculated TDOS and PDOS of cubic $AlGeBr_3$ perovskites under pressures.

Table S1: The calculated lattice parameters (a), cell volume (V), formation energy (ΔH_f), and band gap (E_g) of $AlGeX_3$ (X = F, Cl, and Br) at different pressures.

(a) $AlGeF_3$

Pressure (GPa)	**a(Å)**	**V(Å^3)**	**ΔH_f (eV/atom)**	**E_g(eV)**
0	4.456	88.48	-4.455	1.115
2	4.401	85.24	-4.308	0.897
4	4.355	82.61	-4.108	0.717
6	4.315	80.34	-3.908	0.513
10	4.245	76.48	-3.508	0.155
15	4.173	72.69	-2.908	0

(b) $AlGeCl_3$

Pressure (GPa)	**a(Å)**	**V(Å^3)**	**ΔE_f (eV/atom)**	**E_g(eV)**
0	5.215	141.83	-3.370	0.760
1	5.156	137.10	-3.295	0.565
2	5.106	133.16	-3.095	0.361
3	5.061	129.61	-2.895	0.144
4	5.019	126.41	-2.695	0

(c) $AlGeBr_3$

Pressure (GPa)	**a(Å)**	**V(Å^3)**	**ΔE_f (eV/atom)**	**E_g(eV)**
0	5.471	163.72	-3.045	0.433
0.5	5.434	160.44	-2.968	0.327
1.5	5.370	154.80	-2.768	0.128
2.5	5.313	149.99	-2.568	0

Table S2: Variation in bond length of cubic $AlGeX_3$ (X = F, Cl, and Br) at different pressure

$AlGeF_3$			**$AlGeCl_3$**			**$AlGeBr_3$**		
Pressure (GPa)		**Bond length (Å)**	**Pressure (GPa)**		**Bond length (Å)**	**Pressure (GPa)**		**Bond length (Å)**
0GPa	Ge-F	2.22797	0GPa	Ge-Cl	2.60752	0GPa	Ge-Br	2.73528
	Al-F	3.15083		Al-Cl	3.68759		Al-Br	3.86827
	Al-Ge	3.85897		Al-Ge	4.51636		Al-Ge	4.73764
2GPa	Ge-F	2.20052	1GPa	Ge-Cl	2.57817	0.5GPa	Ge-Br	2.71692
	Al-F	3.11200		Al-Cl	3.64608		Al-Br	3.84231
	Al-Ge	3.81141		Al-Ge	4.46552		Al-Ge	4.70585
4GPa	Ge-F	2.17765	2GPa	Ge-Cl	2.55327	1.5GPa	Ge-Br	2.68466
	Al-F	3.07967		Al-Cl	3.61087		Al-Br	3.79668
	Al-Ge	3.77180		Al-Ge	4.42239		Al-Ge	4.64997
6GPa	Ge-F	2.15747	3GPa	Ge-Cl	2.53033	2.5GPa	Ge-Br	2.65663
	Al-F	3.05113		Al-Cl	3.57843		Al-Br	3.75704
	Al-Ge	3.73686		Al-Ge	4.38266		Al-Ge	4.60141
10GPa	Ge-F	2.12233	4GPa	Ge-Cl	2.50934			
	Al-F	3.00142		Al-Cl	3.54874			
	Al-Ge	3.67598		Al-Ge	4.34630			
15GPa	Ge-F	2.08669						
	Al-F	2.95103						
	Al-Ge	3.61426						

Table S3(a): The calculated elastic constants, bulk modulus (B), shear modulus (G), Young's modulus (E), Pugh's ration, Poisson's ratio (υ), hardness (H_v), and machinability index (μ_M) of $AlGeF_3$ under hydrostatic pressure.

Pressure (GPa)	**C_{11}**	**C_{12}**	**C_{44}**	**C_{12}-C_{44}**	**B (Gpa)**	**G (Gpa)**	**E**	**B/G**	**υ**	**H_v**	**μ_M**
0	72.41	26.32	9.17	17.15	41.68	13.40	36.31	3.11	0.3548	1.5907	4.5436
2	84.94	25.48	4.48	21.00	45.30	10.68	29.72	4.24	0.3907	0.9525	10.1113
4	101.82	32.64	5.04	27.60	55.70	12.25	34.25	4.55	0.3975	0.9696	11.0523
6	122.13	38.75	8.05	30.70	66.54	16.70	46.22	3.99	0.3842	1.4017	8.2661
10	152.74	50.38	7.03	43.35	84.50	17.71	49.66	4.77	0.4021	1.1911	12.0201
15	174.11	61.93	8.09	53.84	99.32	19.79	55.68	5.02	0.4066	1.2166	12.2774

Table S3(b): Changes in anisotropy of cubic $AlGeF_3$ under hydrostatic pressure.

Pressure (GPa)	**A_1**	**A_2**	**A_3**	**A**	**A_G**	**A_B**	**A^U**	**A^{eq}**
0	0.3981	0.3981	0.3981	0.3981	0.1970	0	1.0924	2.5123
2	0.1507	0.1507	0.1507	0.1507	0.7296	0	5.7428	6.6350
4	0.1456	0.1456	0.1456	0.1456	0.7513	0	6.0168	6.8684
6	0.1931	0.1931	0.1931	0.1931	0.5761	0	4.0462	5.1788
10	0.1374	0.1374	0.1374	0.1374	0.7880	0	6.5010	7.2801
15	0.1442	0.1442	0.1442	0.1442	0.7574	0	6.0953	6.9352

Table S4(a): The calculated elastic constants, bulk modulus (B), shear modulus (G), Young's modulus (E), Pugh's ration, Poisson's ratio (**υ**), hardness (H_v), and machinability index (μ_M) of $AlGeCl_3$ under hydrostatic pressure.

Pressure (GPa)	C_{11}	C_{12}	C_{44}	C_{12}-C_{44}	**B (Gpa)**	**G (Gpa)**	**Y**	**B/G**	**υ**	H_v	μ_M
0	60.47	11.78	6.15	5.63	28.01	11.10	29.41	2.52	0.3250	1.7641	4.5581
1	70.28	13.91	6.16	7.75	32.70	11.97	32.00	2.73	0.3369	1.7009	5.3084
2	77.04	13.46	6.18	7.28	34.65	12.77	34.13	2.71	0.3359	1.7957	5.6070
3	83.50	12.67	6.19	6.48	36.28	13.56	36.17	2.68	0.3338	1.9031	5.8610
4	99.11	21.11	6.21	14.9	47.11	14.34	39.06	3.29	0.3618	1.5681	7.5864

Table S4(b): Changes in anisotropy of cubic $AlGeCl_3$ under hydrostatic pressure.

Pressure (GPa)	A_1	A_2	A_3	**A**	A_G	A_B	A^U	A^{eq}
0	0.2524	0.2524	0.2524	0.2524	0.4198	0	2.6570	3.9618
1	0.2187	0.2187	0.2187	0.2187	0.5019	0	3.3504	4.5733
2	0.1944	0.1944	0.1944	0.1944	0.5720	0	4.0057	5.1436
3	0.1748	0.1748	0.1748	0.1748	0.6373	0	4.6765	5.7224
4	0.1593	0.1593	0.1593	0.1593	0.6950	0	5.3259	6.2790

Table S5(a): The calculated elastic constants, bulk modulus (B), shear modulus (G), Young's modulus (E), Pugh's ration, Poisson's ratio (**υ**), hardness (H_v), and machinability index (μ_M) of $AlGeBr_3$ under hydrostatic pressure.

Pressure (GPa)	**C_{11}**	**C_{12}**	**C_{44}**	**C_{12}-C_{44}**	**B (Gpa)**	**G (Gpa)**	**Y**	**B/G**	**υ**	**H_v**	**μ_M**
0	53.85	9.77	5.60	4.17	24.46	10.08	26.59	2.43	0.3188	1.7242	4.3661
0.5	58.32	10.09	5.71	4.38	26.16	10.65	28.12	2.46	0.3209	1.7659	4.5822
1.5	67.40	11.18	5.92	5.26	29.92	11.73	31.12	2.55	0.3267	1.8125	5.0540
2.5	76.07	12.10	6.13	5.97	33.42	12.76	33.96	2.62	0.3307	1.8678	5.4524

Table S5(b): Changes in anisotropy of cubic $AlGeBr_3$ under hydrostatic pressure.

Pressure (GPa)	**A_1**	**A_2**	**A_3**	**A**	**A_G**	**A_B**	**A^U**	**A^{eq}**
0	0.2542	0.2542	0.2542	0.2542	0.4160	0	2.6260	3.9341
0.5	0.2367	0.2367	0.2367	0.2367	0.4560	0	2.9530	4.2241
1.5	0.2107	0.2107	0.2107	0.2107	0.5237	0	3.5470	4.7451
2.5	0.1915	0.1915	0.1915	0.1915	0.5811	0	4.0958	5.2217

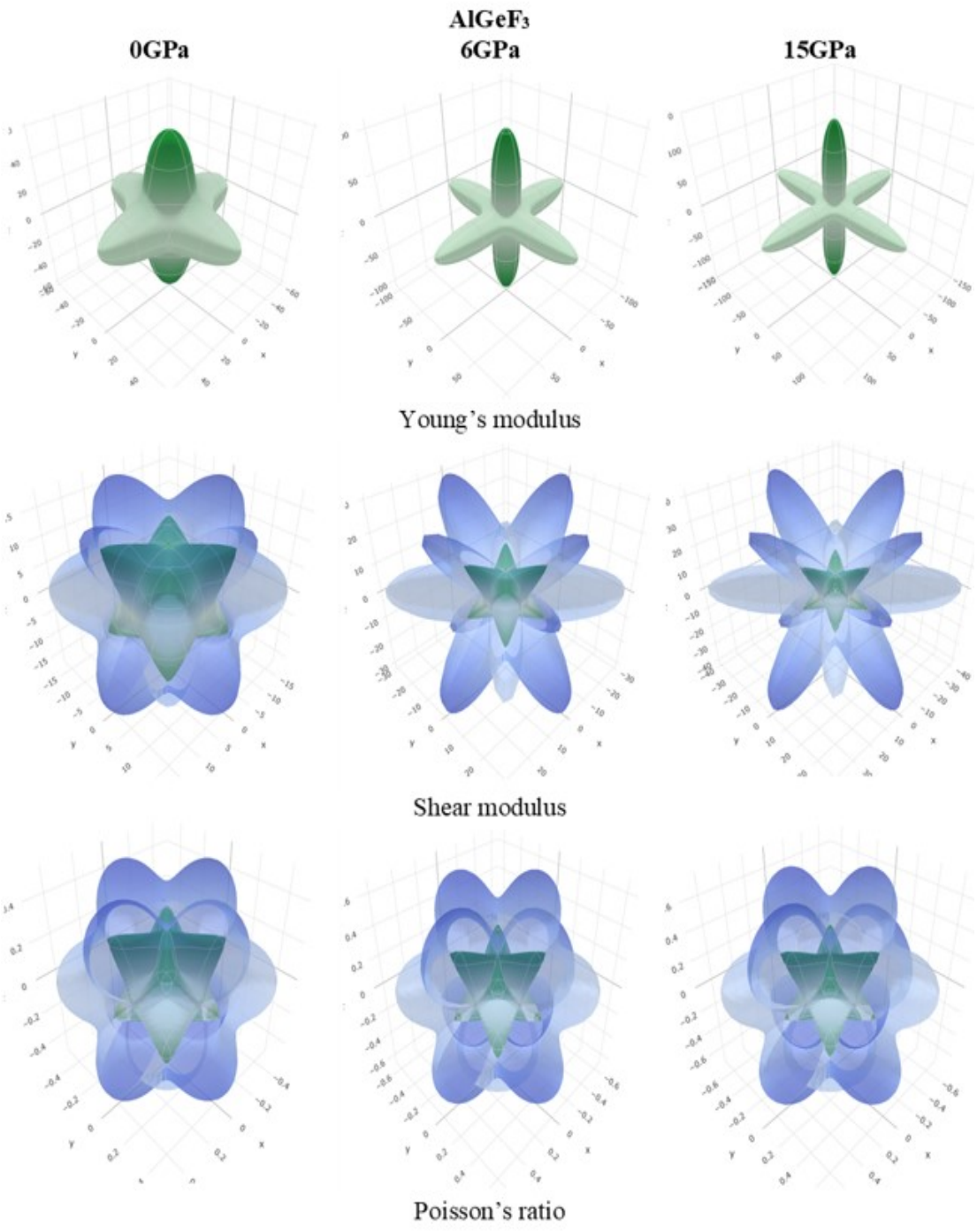

Fig. S7 Anisotropic 3D representation of Young's modulus, shear modulus, and Poisson's ratio of $AlGeF_3$ at different pressures.

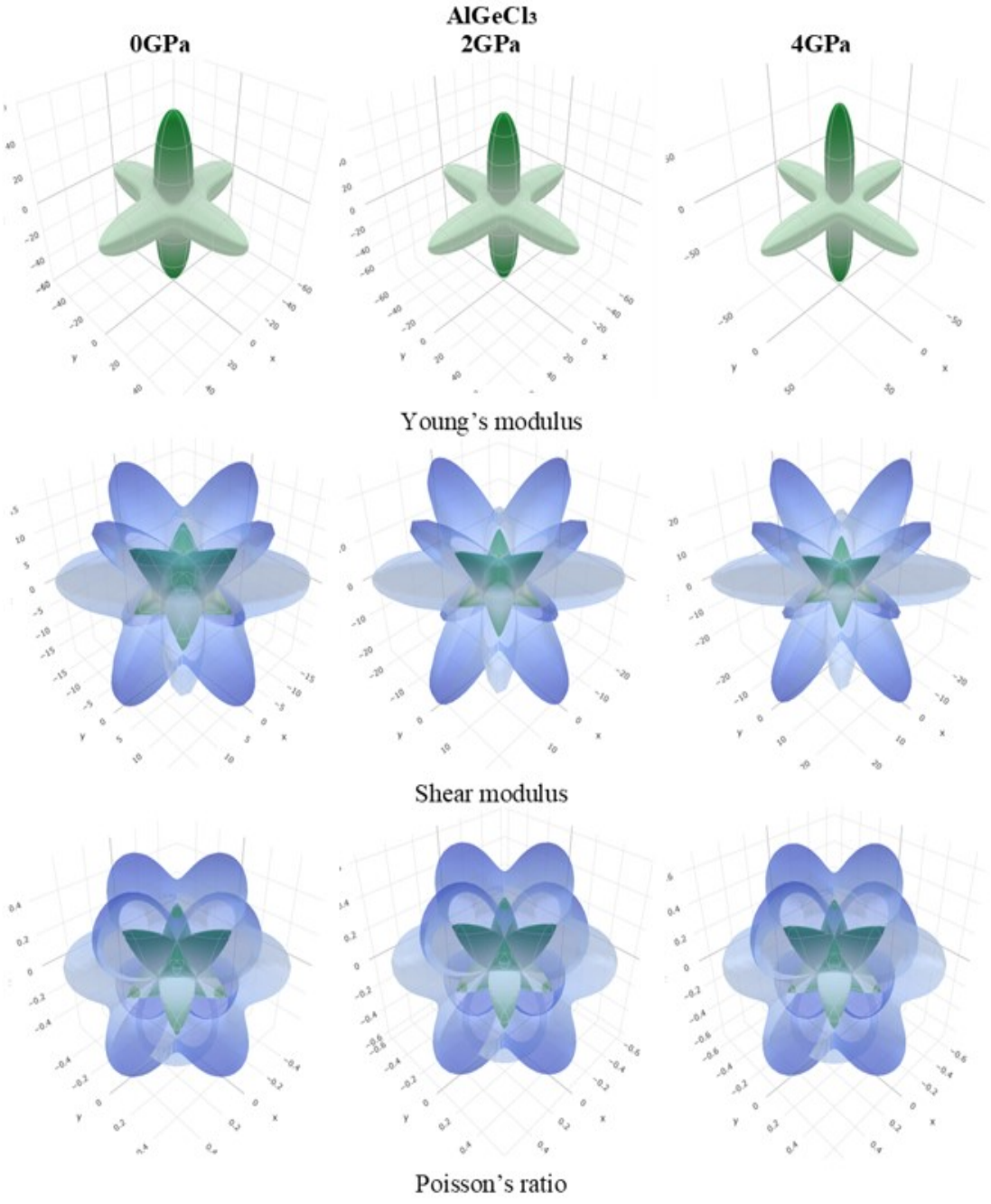

Fig. S8 Anisotropic 3D representation of Young's modulus, shear modulus, and Poisson's ratio of $AlGeCl_3$ at different pressures.

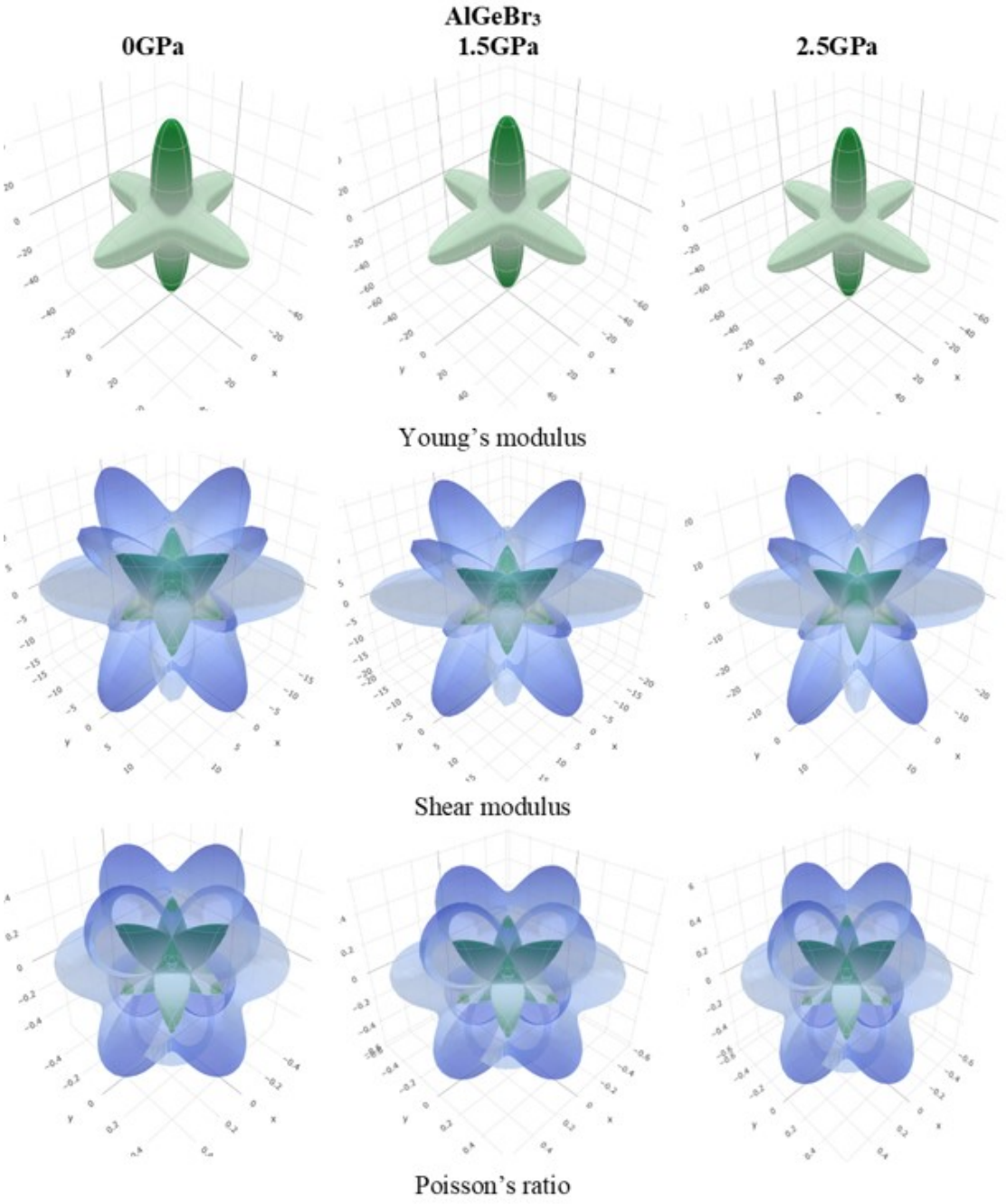

Fig. S9 Anisotropic 3D representation of Young's modulus, shear modulus, and Poisson's ratio of $AlGeBr_3$ at different pressure.