Supporting information

Halide double perovskite Rb_2AgBiX_6 (X = Br, Cl) exhibits excellent stability and optical properties under high pressure

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Table S1. The lattice constant, bulk modulus B_0, pressure derivative B_0', volume V_0 and energy E_0 of $Rb_2AgBiCl_6$ and $Rb_2AgBiBr_6$ at zero pressure.

	a(Å)	B_0(eV/Å^3)	B_0'	V_0(Å^3)	E_0(eV)
$Rb_2AgBiCl_6$	10.866	0.144	5.970	1282.928	-130.176
$Rb_2AgBiBr_6$	11.405	0.127	6.004	1482.957	-117.052

Table S2. Lattice constant of $Rb_2AgBiCl_6$ at different high pressures (0-100 GPa).

$Rb_2AgBiCl_6$	Pressure（GPa）	10	20	30	40	50
	a(Å)	10.083	9.709	9.457	9.264	9.107
	Pressure（GPa）	60	70	80	90	100
	a(Å)	8.975	8.854	8.746	8.649	8.550

Table S3. Lattice constant of $Rb_2AgBiBr_6$ at different high pressures (0-100 GPa).

$Rb_2AgBiBr_6$	Pressure（GPa）	10	20	30	40	50
	a(Å)	10.518	10.112	9.835	9.625	9.455
	Pressure（GPa）	60	70	80	90	100
	a(Å)	9.312	9.193	9.087	8.982	8.890

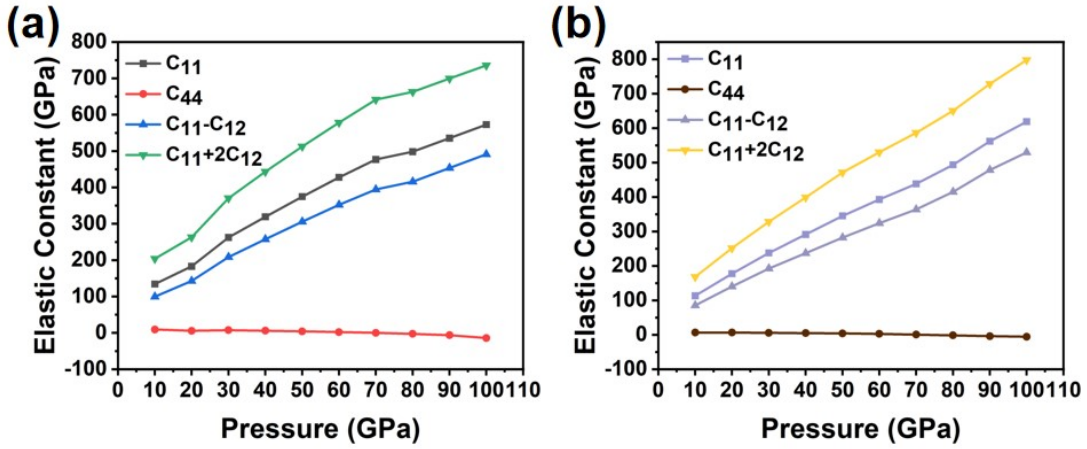

Figure S1. The elastic constants of $Rb_2AgBiCl_6$ (a) and $Rb_2AgBiBr_6$ (b) C_{11}, C_{44}, C_{11}-C_{12}, C_{11}+2C_{12} at different high pressures.

Table S4. The mechanical properties of $Rb_2AgBiCl_6$ under different high pressures include bulk modulus (B), Young's modulus (E), shear modulus (G), Poisson's ratio (ν), Pugh modulus (B/G), hardness (H).

Material name	Pressure (GPa)	B(GPa)	E(GPa)	G(GPa)	ν	B/G	H(GPa)
$Rb_2AgBiCl_6$	0	21.931	26.977	10.416	0.295	2.106	0.37
	10	67.957	53.756	19.645	0.368	3.459	1.21
	20	87.730	57.153	20.537	0.391	4.272	1.66
	30	123.511	80.539	28.944	0.391	4.267	2.92
	40	147.749	90.084	32.210	0.398	4.587	3.53
	50	170.922	98.937	35.246	0.404	4.849	4.12
	60	192.722	106.156	37.692	0.408	5.113	4.63
	70	213.751	111.737	39.542	0.413	5.406	5.00
	80	220.956	114.328	40.434	0.414	5.465	5.14
	90	233.223	119.006	42.053	0.415	5.546	5.54
	100	245.214	123.096	43.456	0.416	5.643	5.51

Table S5. The mechanical properties of $Rb_2AgBiBr_6$ under different high pressures include bulk modulus (B), Young's modulus (E), shear modulus (G), Poisson's ratio (ν), Pugh modulus (B/G), hardness (H).

Material name	Pressure (GPa)	B(GPa)	E(GPa)	G(GPa)	ν	B/G	H(GPa)
$Rb_2AgBiBr_6$	0	21.564	18.805	6.941	0.355	3.107	0.26
	10	56.101	42.568	15.496	0.374	3.620	0.77
	20	83.904	58.051	20.962	0.385	4.003	1.87
	30	109.444	71.242	25.599	0.392	4.275	2.77
	40	132.986	81.603	29.191	0.398	4.556	3.34
	50	157.071	92.123	32.848	0.402	4.782	3.87
	60	176.687	99.252	35.286	0.406	5.007	4.37
	70	195.548	104.653	37.090	0.411	5.272	4.76
	80	216.792	112.323	39.728	0.414	5.457	5.42
	90	242.708	122.869	43.397	0.414	5.593	6.24
	100	265.852	132.140	46.622	0.417	5.702	6.80

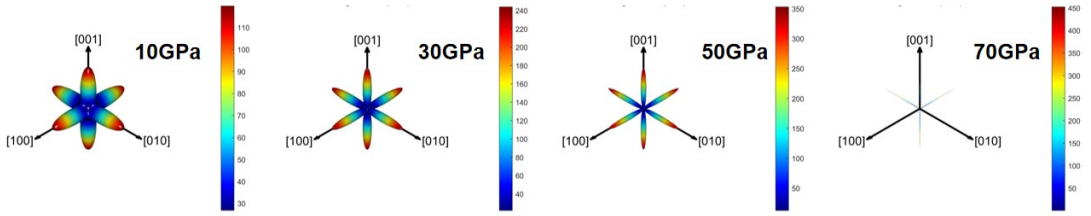

Figure S2. 3D plots of $Rb_2AgBiCl_6$ Young's modulus (E) under high pressures of 10GPa, 30GPa, 50GPa, and 70GPa (001, 100, and 010 represent different crystal planes of the crystal).

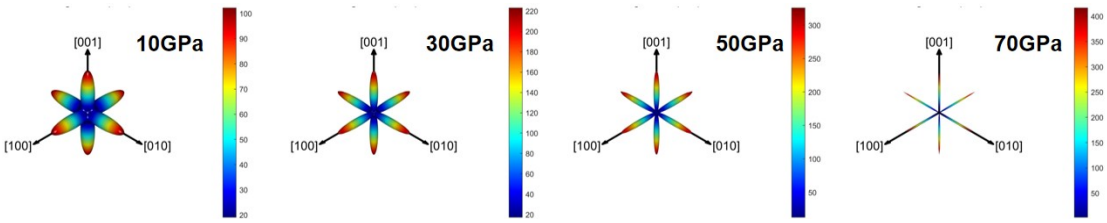

Figure S3. 3D plots of $Rb_2AgBiBr_6$ Young's modulus (E) under high pressures of 10GPa, 30GPa, 50GPa, and 70GPa (001, 100, and 010 represent different crystal planes of the crystal).

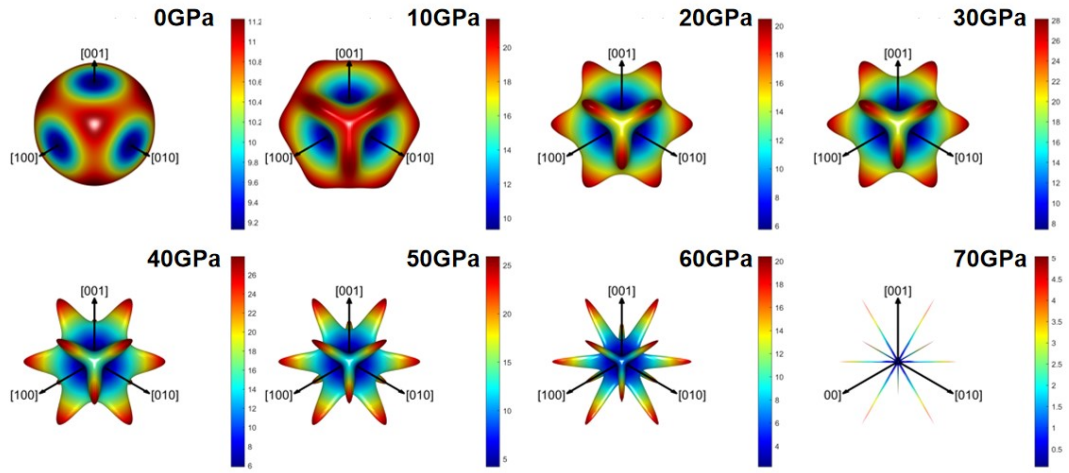

Figure S4. 3D diagram of the shear modulus (G) of $Rb_2AgBiCl_6$ at different high pressures (001, 100, and 010 represent different crystal planes of the crystal).

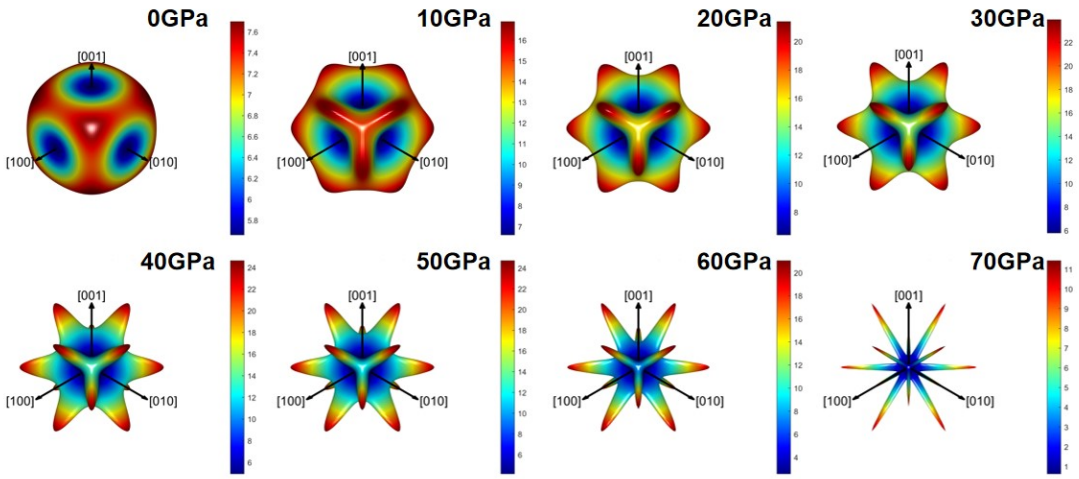

Figure S5. 3D diagram of the shear modulus (G) of $Rb_2AgBiBr_6$ at different high pressures (001, 100, and 010 represent different crystal planes of the crystal).

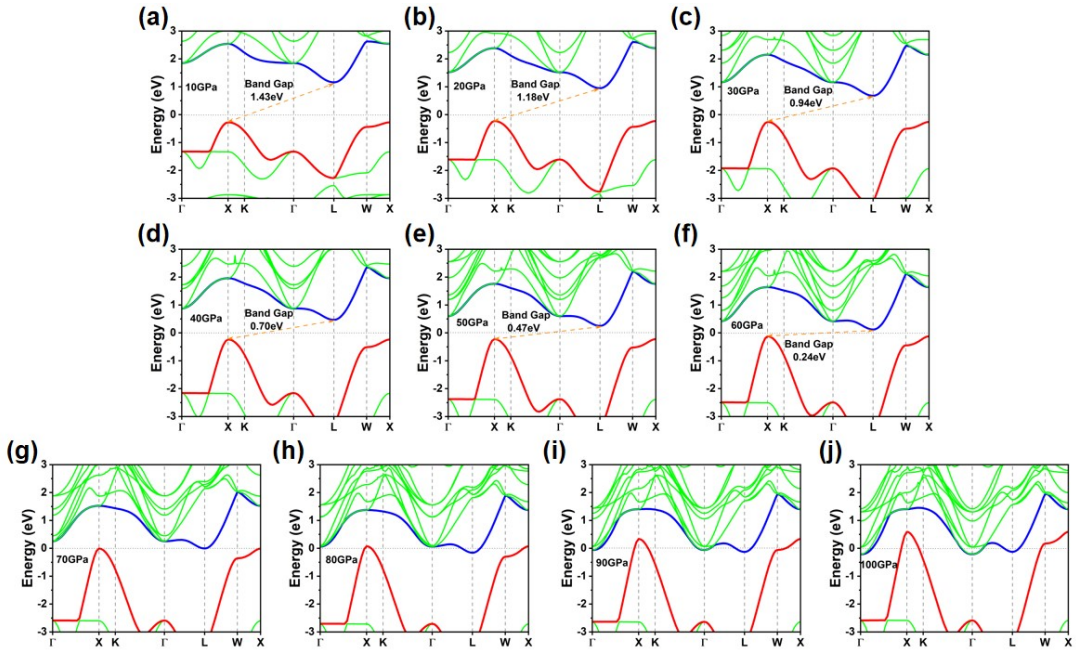

Figure S6. Electronic band structure and band gap value (a-j) of $Rb_2AgBiCl_6$ at different high pressures (0-100 GPa).

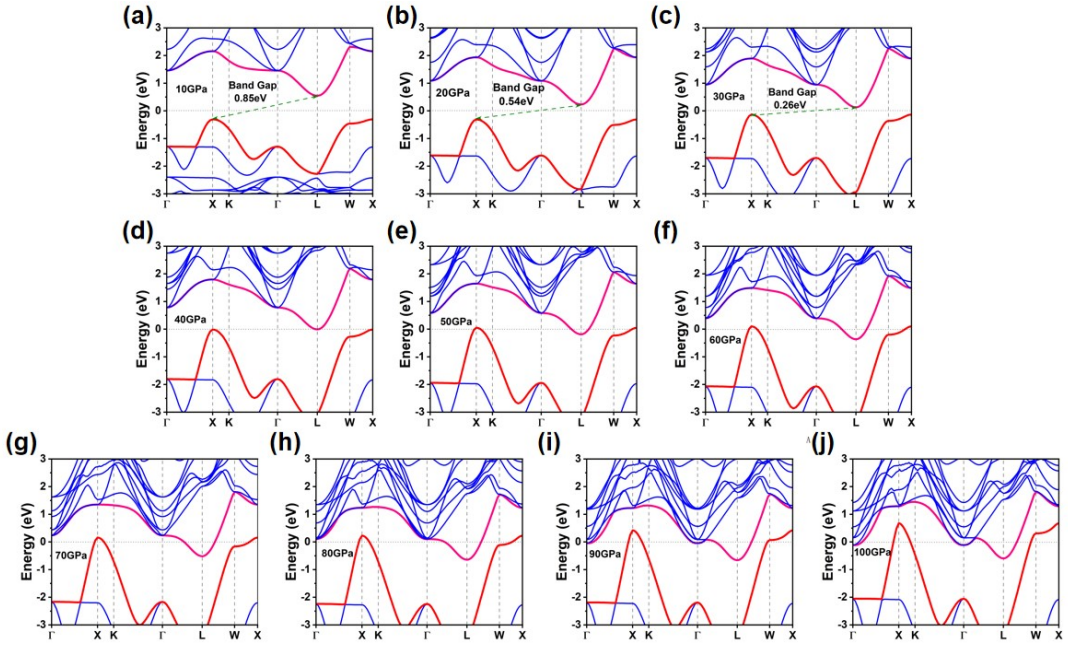

Figure S7. Electronic band structure and band gap value (a-j) of $Rb_2AgBiBr_6$ at different high pressures (0-100 GPa).

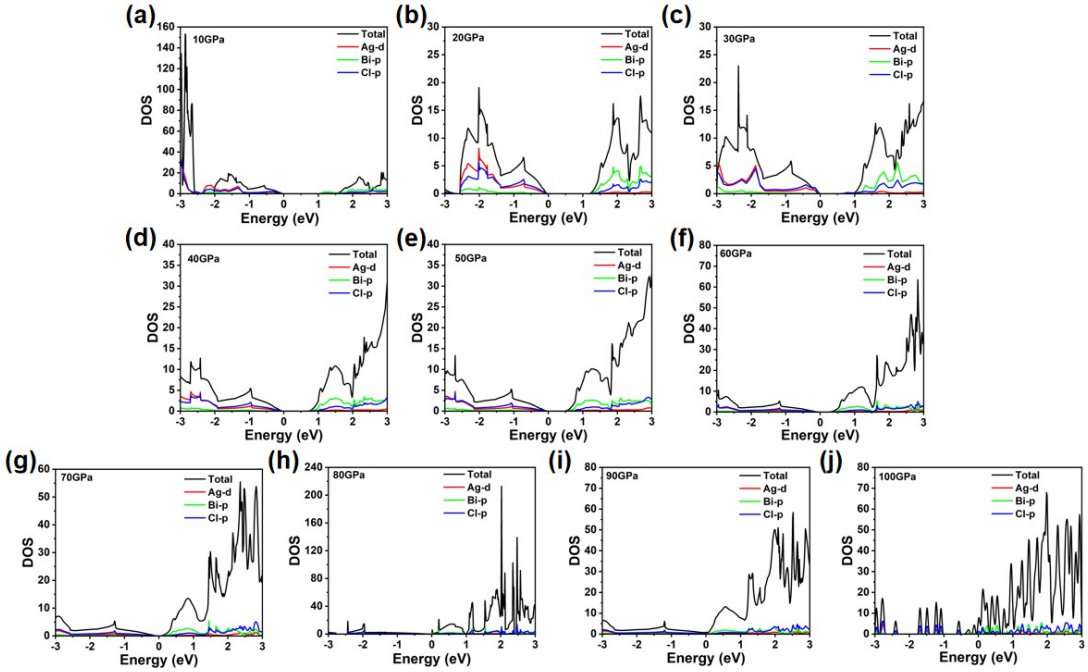

Figure S8. DOS (a-j) of $Rb_2AgBiCl_6$ at different high pressures (0-100 GPa).

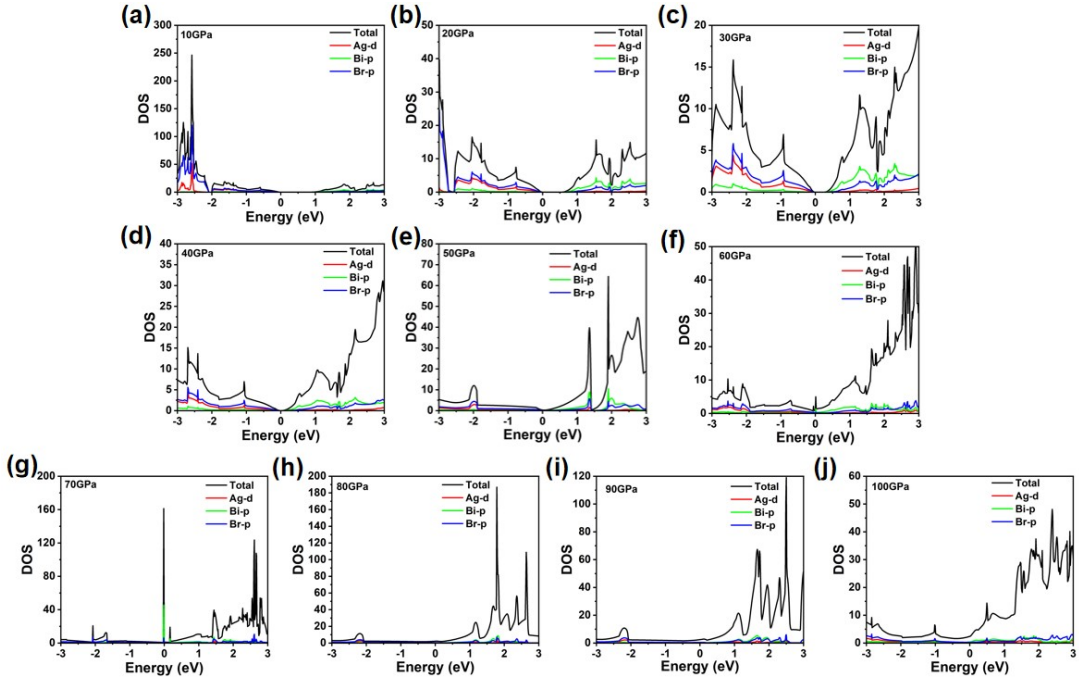

Figure S9. DOS (a-j) of $Rb_2AgBiBr_6$ at different high pressures (0-100 GPa).

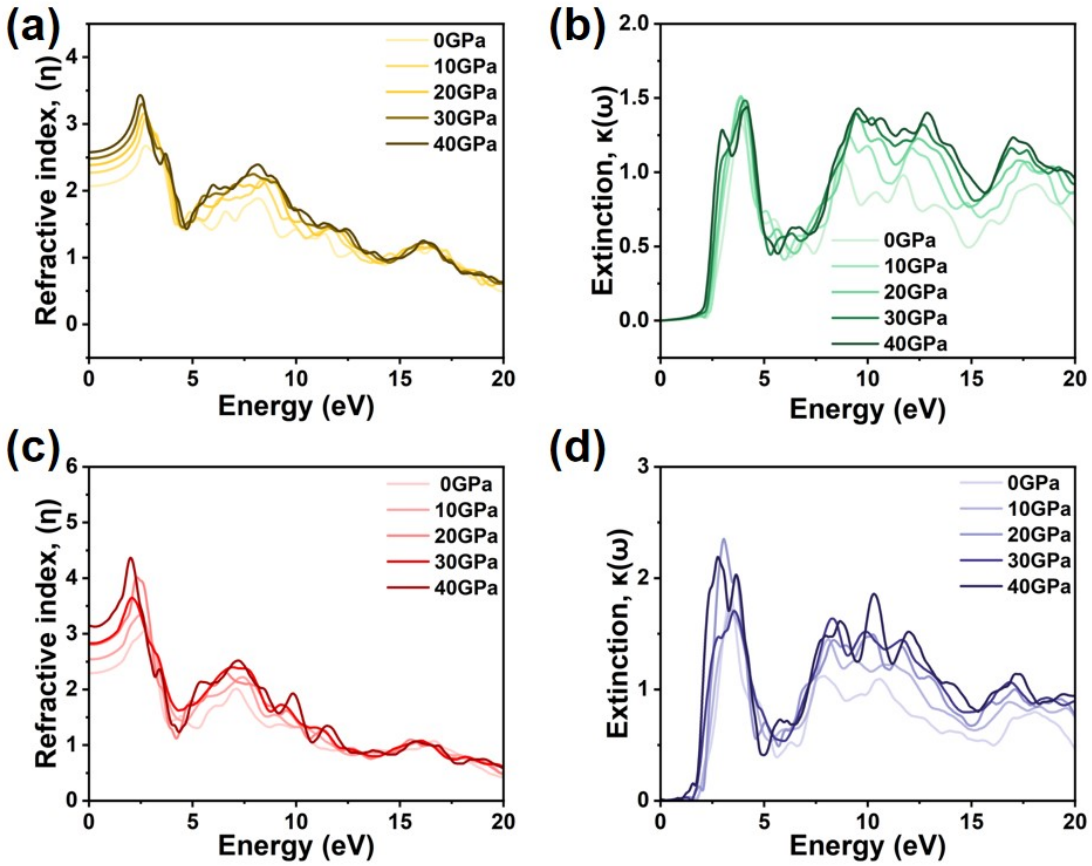

Figure S10. Refractive index (a) and extinction coefficient (b) of $Rb_2AgBiCl_6$ at different high pressures. Refractive index (c) and extinction coefficient (d) of $Rb_2AgBiBr_6$ at different high pressures.

Table S6. The electron effective mass and hole effective mass of $Rb_2AgBiCl_6$ at 0 GPa and 30 GPa.

$Rb_2AgBiCl_6$	**Pressure(GPa)**	**0**	**30**
	Electron effective mass(m_0)	**0.266**	**0.214**
	hole effective mass(m_0)	**0.189**	**0.158**

Table S7. The electron effective mass and hole effective mass of $Rb_2AgBiBr_6$ at 0 GPa and 30 GPa.

$Rb_2AgBiBr_6$	Pressure(GPa)	0	30
	Electron effective mass(m_0)	0.218	0.168
	hole effective mass(m_0)	0.163	0.139

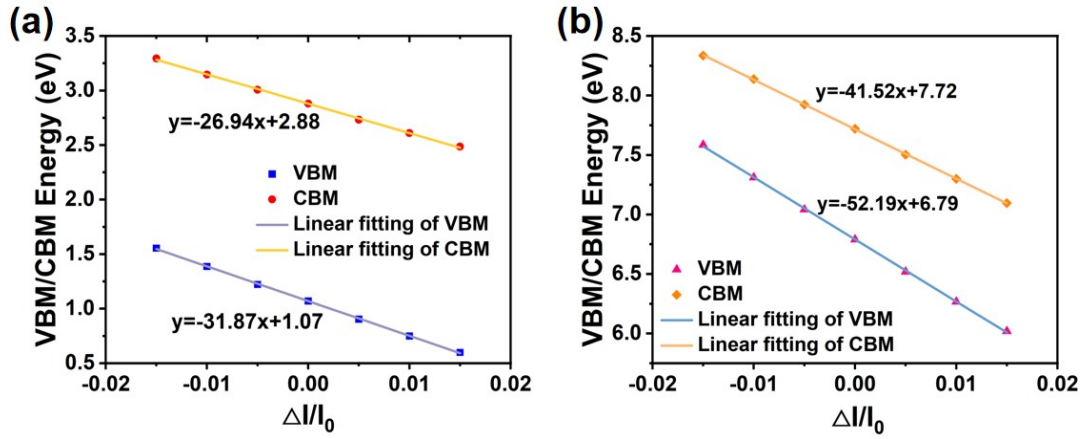

Figure S11. The edge positions of the valence and conduction bands of $Rb_2AgBiCl_6$ under different strains at 0 GPa (a) and 30 GPa (b) are linearly fitted by solid lines, which determine the deformation potential.

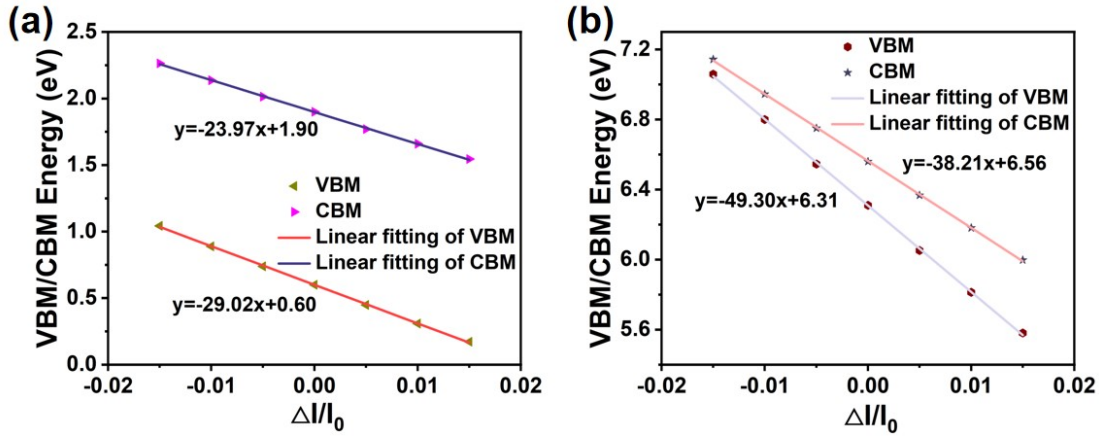

Figure S12. The edge positions of the valence and conduction bands of $Rb_2AgBiBr_6$ under different strains at 0 GPa (a) and 30 GPa (b) are linearly fitted by solid lines, which determine the deformation potential.

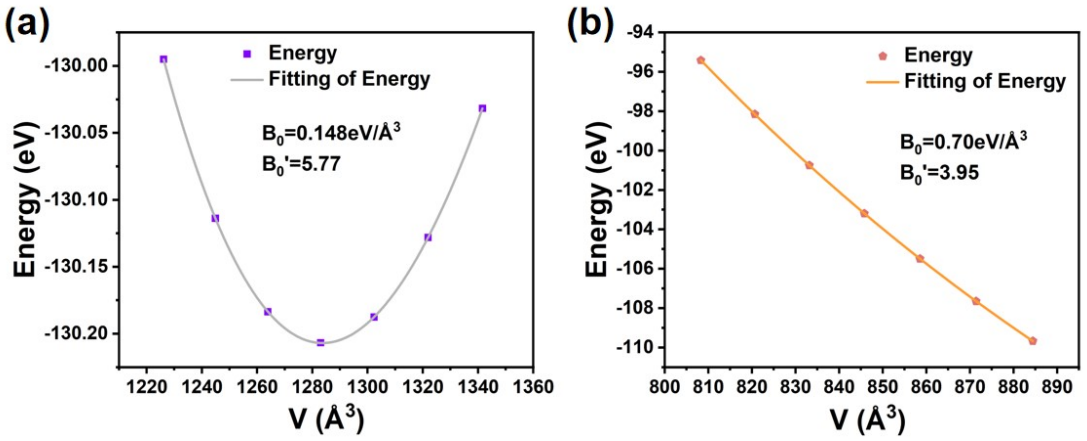

Figure S13. The parabolic fit between the total energy and volume of $Rb_2AgBiCl_6$ at 0 GPa (a) and 30 GPa (b) determines the elastic constant.

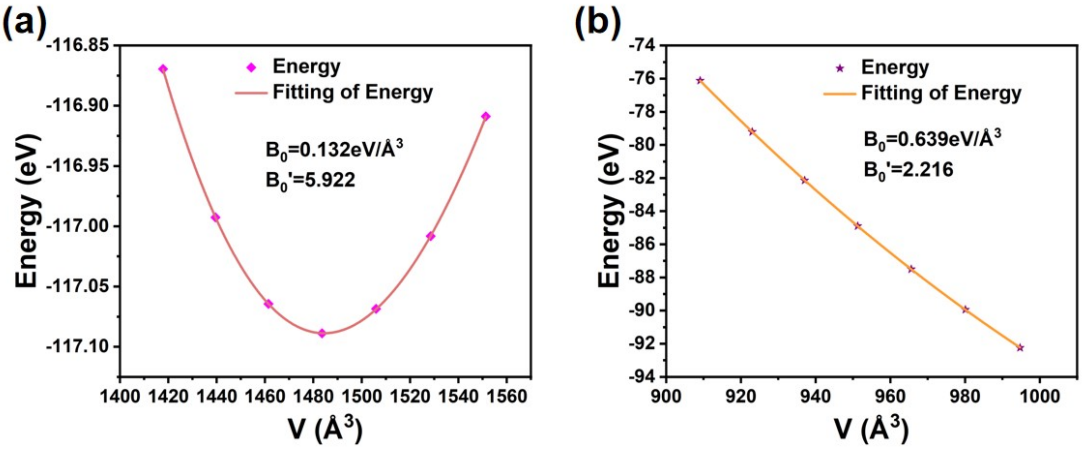

Figure S14. The parabolic fit between the total energy and volume of $Rb_2AgBiBr_6$ at 0 GPa (a) and 30 GPa (b) determines the elastic constant.

Table S8. The deformation potential E of $Rb_2AgBiCl_6$ and $Rb_2AgBiBr_6$ is at 0 GPa and 30 GPa.

$Rb_2AgBiCl_6$		**E_{VBM} (eV)**	**E_{CBM} (eV)**
	0GPa	**31.87**	**26.94**
	30GPa	**52.19**	**41.52**
$Rb_2AgBiBr_6$		**E_{VBM} (eV)**	**E_{CBM} (eV)**
	0GPa	**29.02**	**23.97**

	30GPa	**49.30**	**38.21**

Table S9. The elastic constant C_{ii} of Rb2AgBiCl6 and Rb2AgBiBr6 is at 0 GPa and 30 GPa.

$Rb_2AgBiCl_6$		**C_{ii} (GPa)**
	0GPa	**23.70**
	30GPa	**111.29**
$Rb_2AgBiBr_6$		**C_{ii} (GPa)**
	0GPa	**21.11**
	30GPa	**102.17**