Supplementary information

Effect of stresses on the thermoelectric properties of In_4Se_3

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Table S1. Calculated lattice constants of In_4Se_3 at different Stresses

Stresses(GPa)	a=(Å)	b=(Å)	c=(Å)	V=(Å^3)	$\alpha=(°)$	β=(°)	γ=(°)
-2	29.655	23.874	7.613	5391.70	90	90	90
-1	16.373	12.767	4.185	874.81	90	90	90
0	15.605	12.563	4.162	815.94	90	90	90
1	15.377	12.438	4.150	793.73	90	90	90
2	15.114	12.319	4.134	769.71	90	90	90
3	14.929	12.225	4.115	751.06	90	90	90
4	14.759	12.142	4.098	734.45	90	90	90
5	14.632	12.064	4.081	720.46	90	90	90

Table S2. Calculated elastic constants of In_4Se_3 at different Stresses

Stresses(GPa)	C_{11}	C_{12}	C_{13}	C_{22}	C_{23}	C_{33}	C_{44}	C_{55}	C_{66}
-1	7.7	5.5	13.3	32.2	7.2	45.3	9.0	9.9	9.3
0	30.1	13.6	22.8	50.9	13.3	57.6	12.6	19.9	14.6
1	36.7	17.4	27.7	58.7	17.3	61.1	15.3	25.5	16.3
2	45.1	21.9	33.5	67.6	21.7	66.7	16.3	28.6	17.9
3	54.2	24.9	37.2	74.4	26.4	72.1	17.6	33.5	20.2
4	60.5	27.9	42.3	82.6	28.9	78.4	21.8	35.8	22.5
5	67.6	31.6	46.6	87.7	33.1	82.7	23.0	38.3	22.9

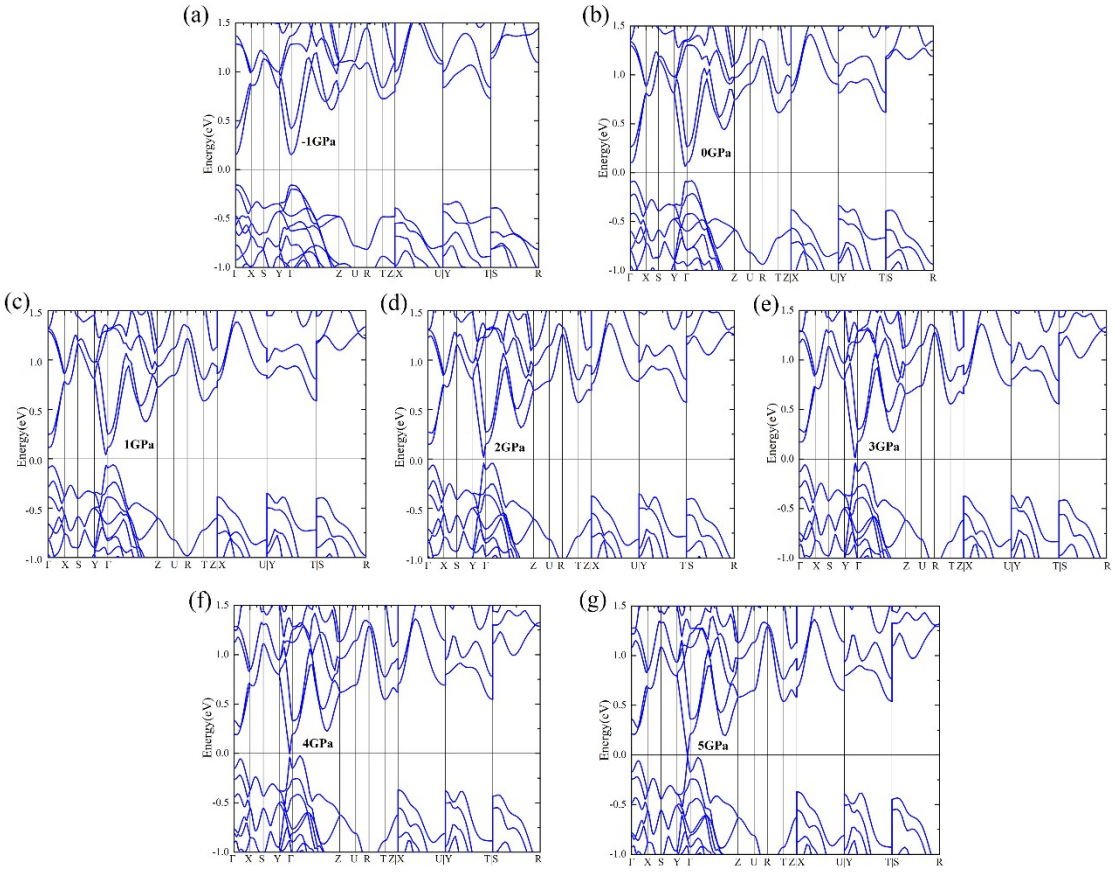

Fig. S1. Variation of the electronic band structure in the PBE potential with stresses.

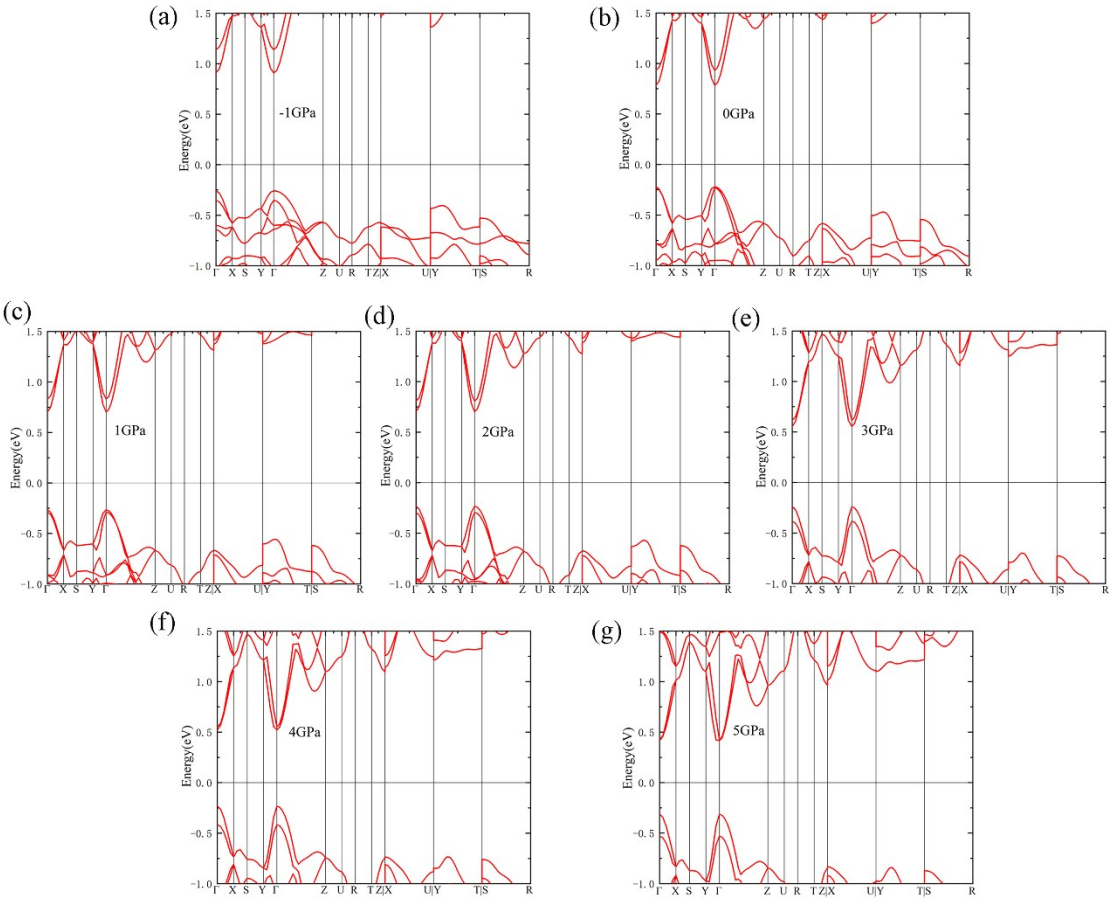

Fig. S2. Variation of the electronic band structure in the HSE06 potential with stresses.

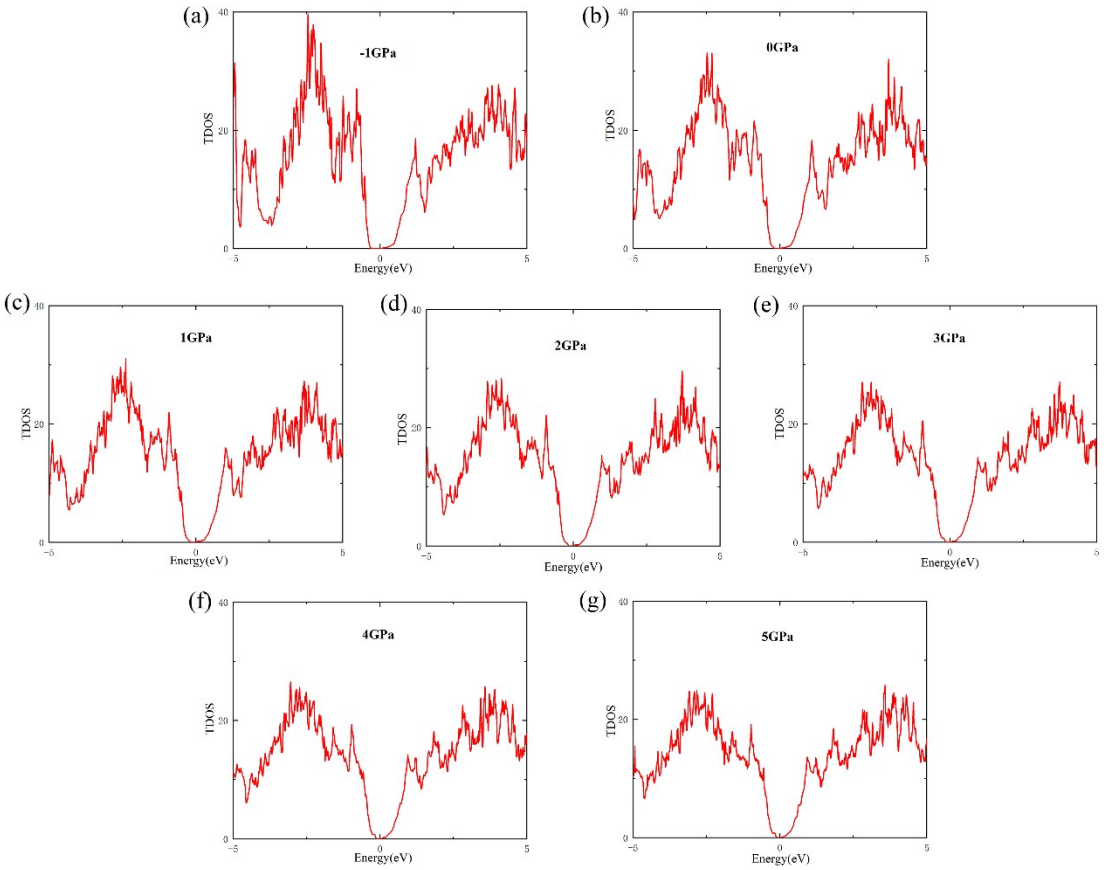

Fig. S3. Variation of the total density of states in the PBE potential with stresses.