Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information

Chemical Bonding within $A^{III}B^{VI}$ Materials under Uniaxial Compression

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Table S1: Topological parameters at the BCP for GaTe: δ, electron density; γ, Laplacian of electron density; ξ, Virial energy; ζ, Kinetic energy; η, Hamiltonian; λ, Bond degree parameters.

Pres. /GPa	ρ_b^δ / $(e \cdot Bohr^{-3})$	$\nabla^2\rho_b^\gamma$ / $(e \cdot Bohr^{-5})$	$\lvert V_b\rvert^\xi$ / $(a.u.)$	G_b^ζ / $(a.u.)$	H_b^η / $(a.u.)$	$\lvert V_b\rvert/G_b$	${H_b/\rho_b}^\lambda$ / $\frac{(a.u.)}{(e \cdot Bohr^{-3})}$
0	6.54E-02	-1.40E-02	-6.44E-02	2.81E-02	-3.40E-02	2.29	-0.52
	5.69E-02	1.30E-02	-4.51E-02	2.63E-02	-2.09E-02	1.71	-
8	7.24E-02	-2.26E-03	-7.28E-02	3.58E-02	-3.67E-02	2.04	-0.51
	5.64E-02	5.81E-03	-4.62E-02	2.48E-02	-2.24E-02	1.86	-
10	4.03E-02	3.06E-02	-1.95E-02	1.87E-02	-5.92E-03	1.04	-
	4.15E-02	2.06E-02	-2.35E-02	1.77E-02	-9.15E-03	1.32	-
	4.09E-02	2.97E-02	-2.05E-02	1.89E-02	-6.55E-03	1.08	-
	5.94E-02	-3.58E-04	-5.19E-02	2.59E-02	-2.60E-02	2.01	-0.44
	5.89E-02	-3.59E-03	-5.21E-02	2.50E-02	-2.65E-02	2.08	-0.45
30	7.77E-02	4.41E-03	-8.02E-02	4.14E-02	-3.95E-02	1.94	-
	4.59E-02	2.50E-02	-2.75E-02	2.11E-02	-1.06E-02	1.31	-
	3.05E-02	2.27E-02	-1.14E-02	1.23E-02	-2.87E-03	0.93	-
	3.14E-02	2.21E-02	-1.24E-02	1.27E-02	-3.44E-03	0.98	-
	7.91E-02	1.04E-02	-8.10E-02	4.35E-02	-3.92E-02	1.86	-
	4.97E-02	3.72E-02	-2.93E-02	2.55E-02	-9.98E-03	1.15	-

Table S2: Topological parameters at the BCP for InSe: δ, electron density; γ, Laplacian of electron density; ξ, Virial energy; ζ, Kinetic energy; η, Hamiltonian; λ, Bond degree parameters.

Pres. /GPa	ρ_b^δ / $(e \cdot Bohr^{-3})$	$\nabla^2\rho_b^\gamma$ / $(e \cdot Bohr^{-5})$	$\lvert V_b\rvert^\xi$ / $(a.u.)$	G_b^ζ / $(a.u.)$	H_b^η / $(a.u.)$	$\lvert V_b\rvert/G_b$	${H_b/\rho_b}^\lambda$ / $\frac{(a.u.)}{(e \cdot Bohr^{-3})}$
0	4.90E-02	1.34E-02	-3.43E-02	2.11E-02	-1.55E-02	1.63	-
	5.82E-02	8.57E-02	-2.87E-02	3.93E-02	-3.65E-03	0.73	-
4	5.25E-02	2.00E-02	-3.73E-02	2.45E-02	-1.61E-02	1.52	-
	5.80E-02	8.79E-02	-2.80E-02	3.96E-02	-3.00E-03	0.71	-
6	5.20E-02	1.93E-02	-3.67E-02	2.40E-02	-1.60E-02	1.53	-
	4.15E-02	6.21E-02	-1.30E-02	2.46E-02	1.24E-03	0.53	-
	3.90E-02	5.66E-02	-1.16E-02	2.23E-02	1.27E-03	0.52	-
	6.51E-02	8.77E-02	-3.85E-02	4.48E-02	-8.29E-03	0.86	-
	2.60E-02	4.45E-02	-2.00E-03	1.40E-02	4.56E-03	0.14	-
30	6.64E-02	5.67E-02	-4.84E-02	4.08E-02	-1.71E-02	1.19	-
	2.97E-02	4.44E-02	-5.30E-03	1.56E-02	2.90E-03	0.34	-
	2.66E-02	3.79E-02	-4.12E-03	1.31E-02	2.68E-03	0.31	-
	3.13E-02	5.13E-02	-4.97E-03	1.75E-02	3.93E-03	0.28	-
	3.22E-02	5.15E-02	-5.79E-03	1.79E-02	3.54E-03	0.32	-
	8.45E-02	7.64E-02	-7.44E-02	5.95E-02	-2.76E-02	1.25	-
	5.22E-02	6.76E-02	-2.50E-02	3.22E-02	-4.03E-03	0.77	-

Table S3: Topological parameters at the BCP for GaSe: δ, electron density; γ, Laplacian of electron density; ξ, Virial energy; ζ, Kinetic energy; η, Hamiltonian; λ, Bond degree parameters.

Pres. /GPa	ρ_b^δ / $(e \cdot Bohr^{-3})$	$\nabla^2\rho_b^\gamma$ / $(e \cdot Bohr^{-5})$	$\lvert V_b\rvert^\xi$ / $(a.u.)$	G_b^ζ / $(a.u.)$	H_b^η / $(a.u.)$	$\lvert V_b\rvert/G_b$	${H_b/\rho_b}^\lambda$ / $\frac{(a.u.)}{(e \cdot Bohr^{-3})}$
0	6.65E-02	-1.37E-02	-6.61E-02	2.90E-02	-3.47E-02	2.27	-0.52
	6.92E-02	4.29E-02	-5.63E-02	4.06E-02	-2.28E-02	1.38	-
11	7.58E-02	-1.27E-02	-8.12E-02	3.69E-02	-4.22E-02	2.20	-0.56
	6.84E-02	4.23E-03	-6.46E-02	3.35E-02	-3.18E-02	1.93	-
14	4.36E-02	5.59E-02	-1.70E-02	2.48E-02	-1.51E-03	0.69	-
	8.05E-02	4.61E-02	-7.47E-02	5.08E-02	-3.16E-02	1.47	-
	5.21E-02	4.91E-02	-2.94E-02	2.90E-02	-8.58E-03	1.01	-
	4.30E-02	4.78E-02	-1.83E-02	2.31E-02	-3.18E-03	0.79	-
	4.35E-02	4.74E-02	-1.90E-02	2.33E-02	-3.58E-03	0.81	-
	6.73E-02	-6.04E-03	-6.55E-02	3.10E-02	-3.35E-02	2.11	-0.50
30	4.53E-02	6.97E-02	-1.56E-02	2.81E-02	9.19E-04	0.55	-
	4.62E-02	4.28E-02	-2.35E-02	2.42E-02	-6.38E-03	0.97	-
	6.08E-02	4.42E-02	-4.29E-02	3.44E-02	-1.59E-02	1.25	-
	9.35E-02	5.68E-02	-9.65E-02	6.48E-02	-4.11E-02	1.49	-
	8.08E-02	1.43E-03	-8.64E-02	4.36E-02	-4.30E-02	1.98	-

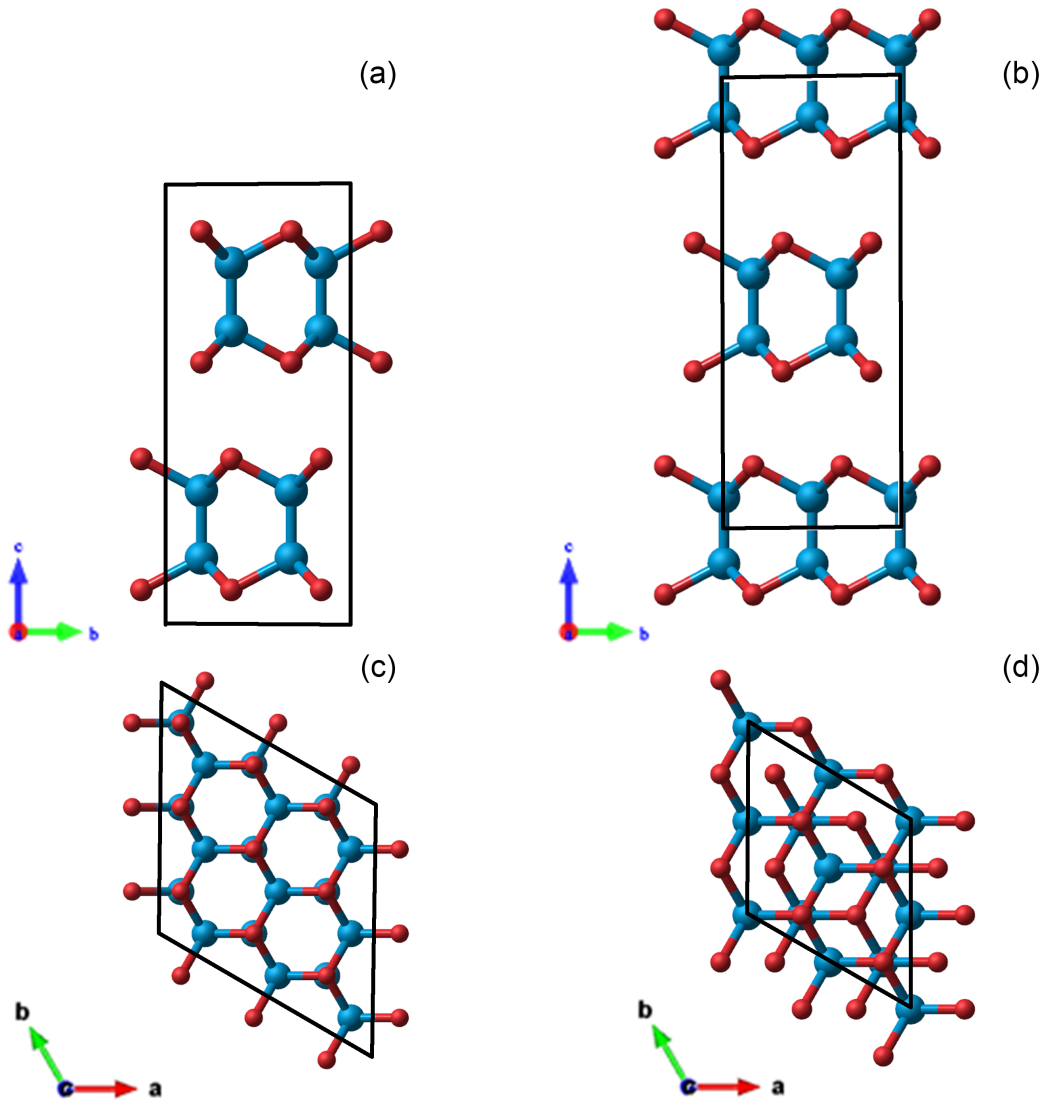

Figure S1: The polymorphs of GaSe: (a) β-phase side view; (b) ε-phase side view; (c-d) top view respectively

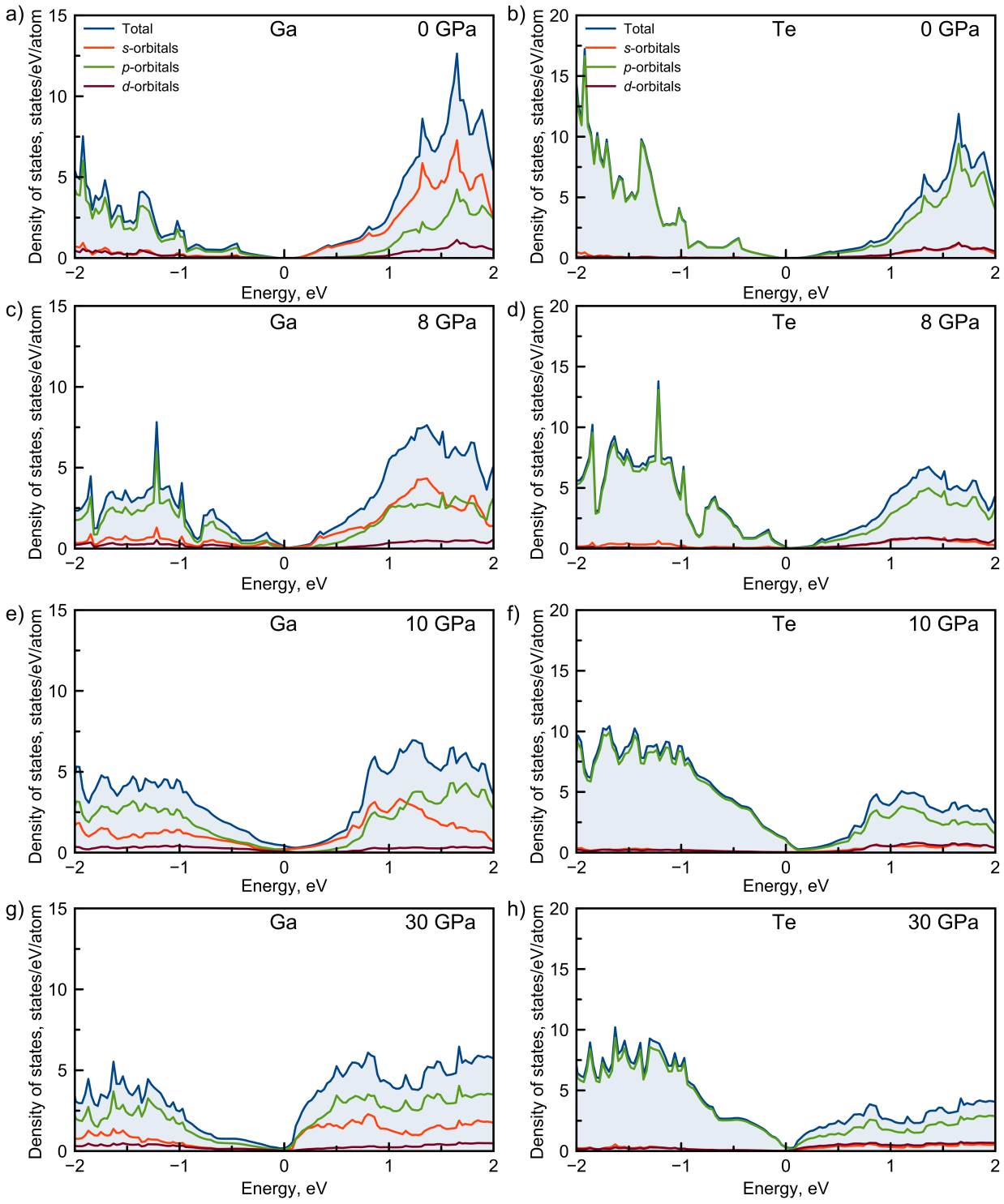

Figure S2: Density of electronic states projected to each atomic orbital of Ga and Te atoms GaTe under pressure: (a)-(b) 0 GPa; (c)-(d) 8 GPa; (e)-(f) 10 GPa; (g)-(h) 30 GPa

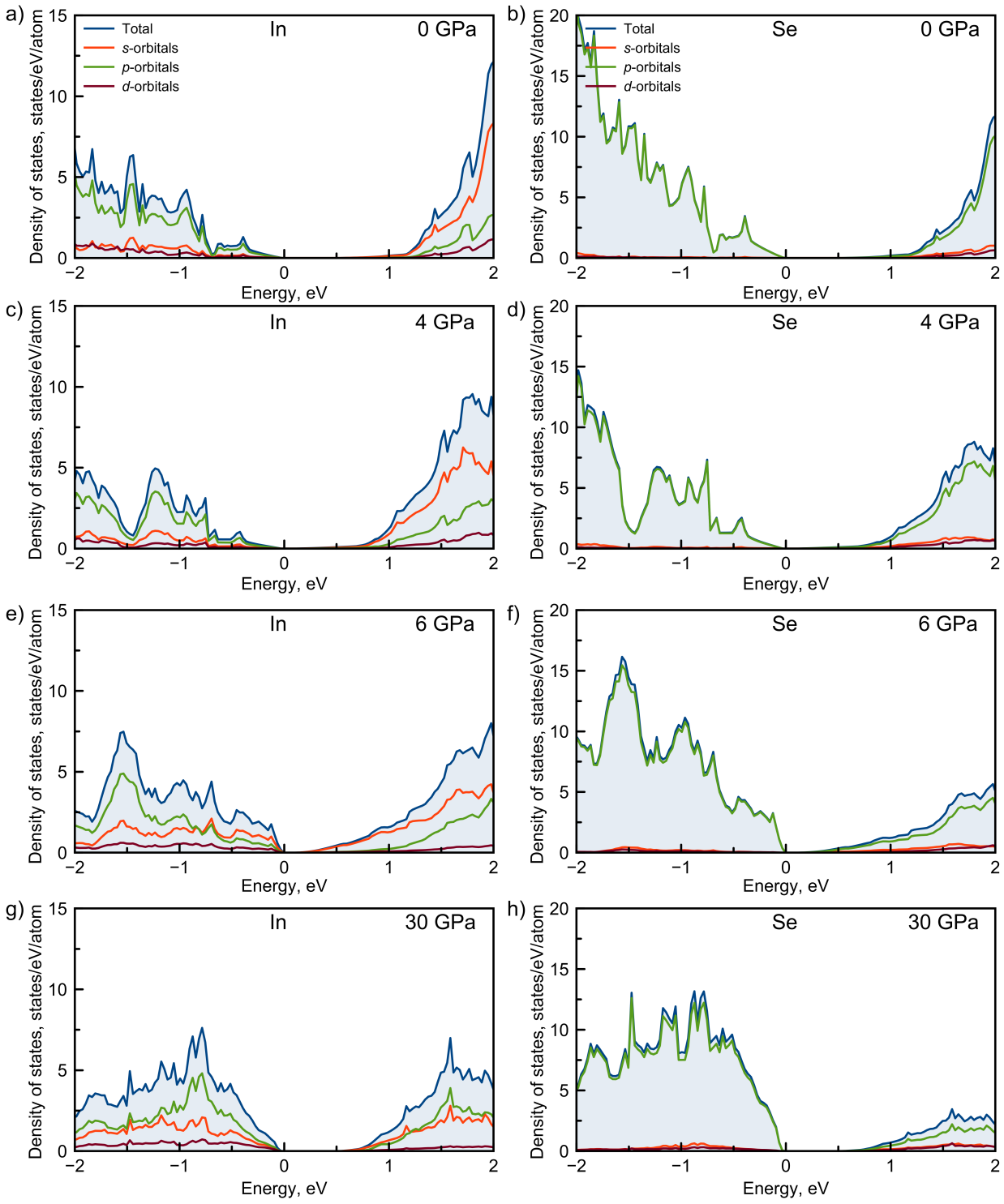

Figure S3: Density of electronic states projected to each atomic orbital of In and Se atoms InSe under pressure: (a)-(b) 0 GPa; (c)-(d) 4 GPa; (e)-(f) 6 GPa; (g)-(h) 30 GPa

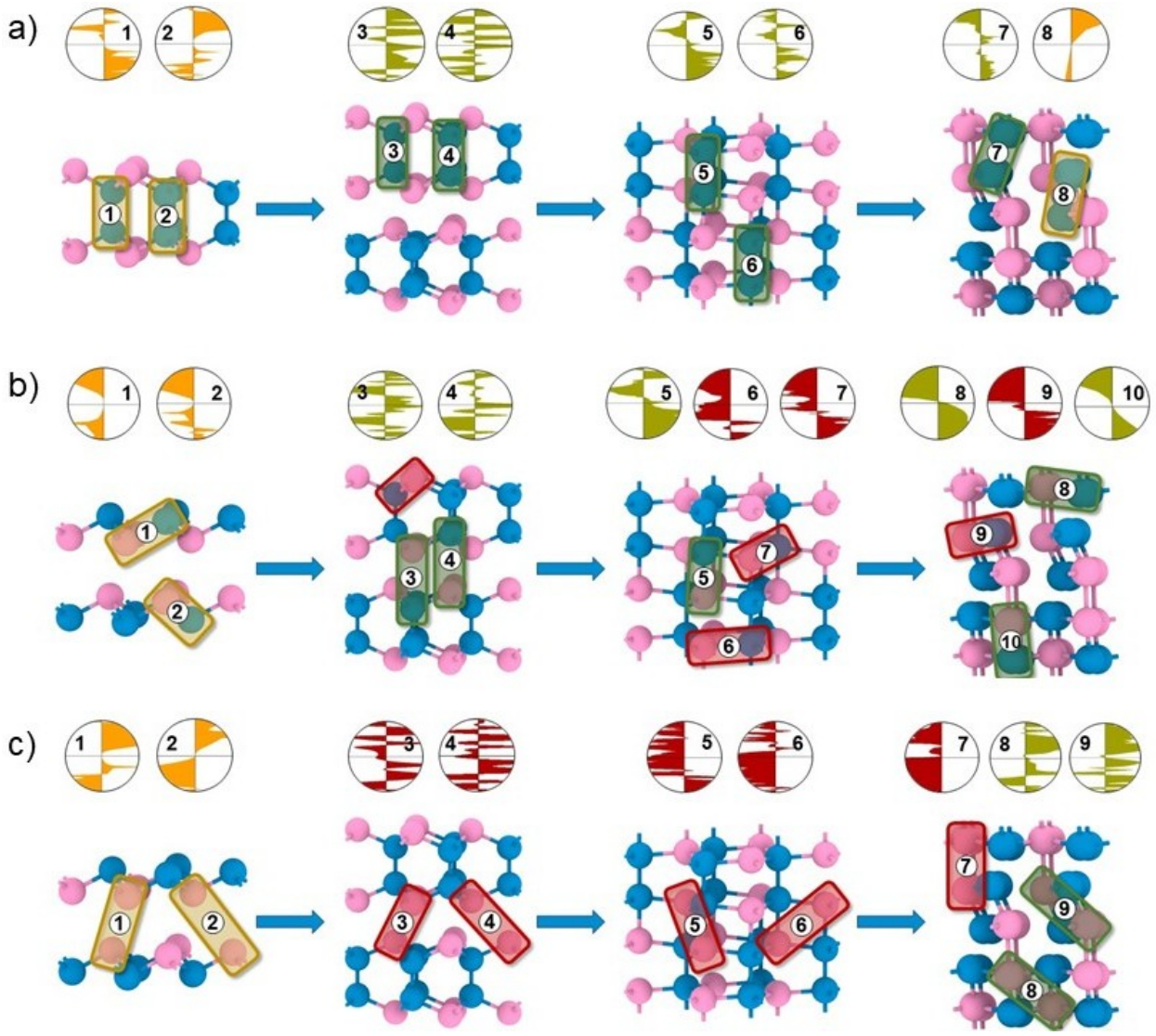

Figure S4: The changes in (a) Ga-Ga; (b) Ga-Te; (c) Te-Te bonds under pressure (Te – orange circle, Ga – blue circle). The bonding, antibonding, and neutral states between the atoms are marked by the green, red and yellow color of the background, respectively. The small circles above the structures represent the pCOHP near the Fermi level. The assigned numbers correspond to the bonds labelled on the structures.

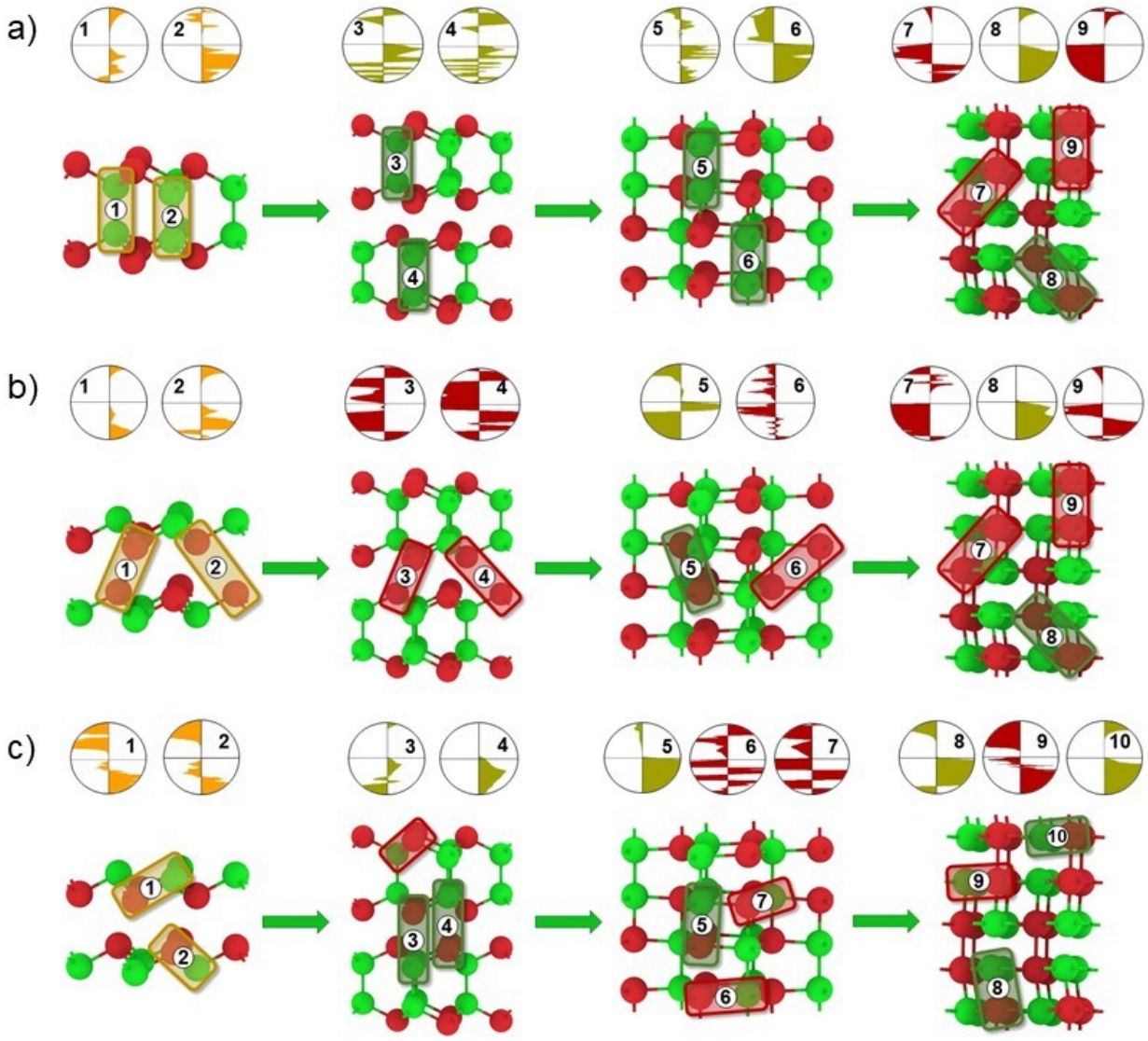

Figure S5: The changes in (a) In-In; (b) Se-Se; (c) In-Se bonds under pressure (Se – red circle, In – green circle). The bonding, antibonding, and neutral states between the atoms are marked by the green, red and yellow color of the background, respectively. The small circles above the structures represent the pCOHP near the Fermi level. The assigned numbers correspond to the bonds labelled on the structures.

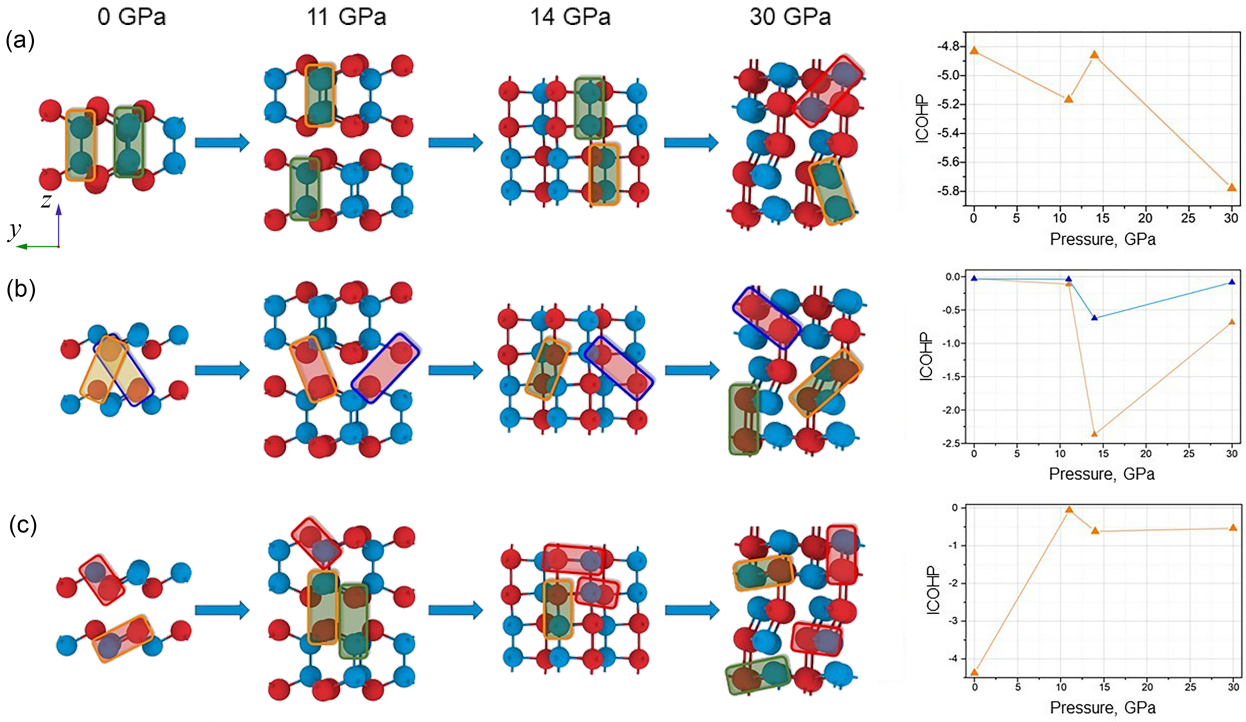

Figure S6: The changings in (a) Ga-Ga; (b) Se-Se; (c) Ga-Se bonds under the pressure (Se – red circle, Ga – blue circle). The bonding, antibonding, and neutral states between the atoms are marked with green, red and yellow color of the background, respectively. The bonds on the ICOHP diagram have the color of the dependence, the other bonds are similar to the marked ones. Different colors in ICOHP dependence of the Se-Se atoms indicate two different bonds that form the vdW gaps.