Supplementary material for

Pressure-induced band anticrossing in two adamantine ordered-vacancy compounds: $CdGa_2S_4$ and $HgGa_2S_4$

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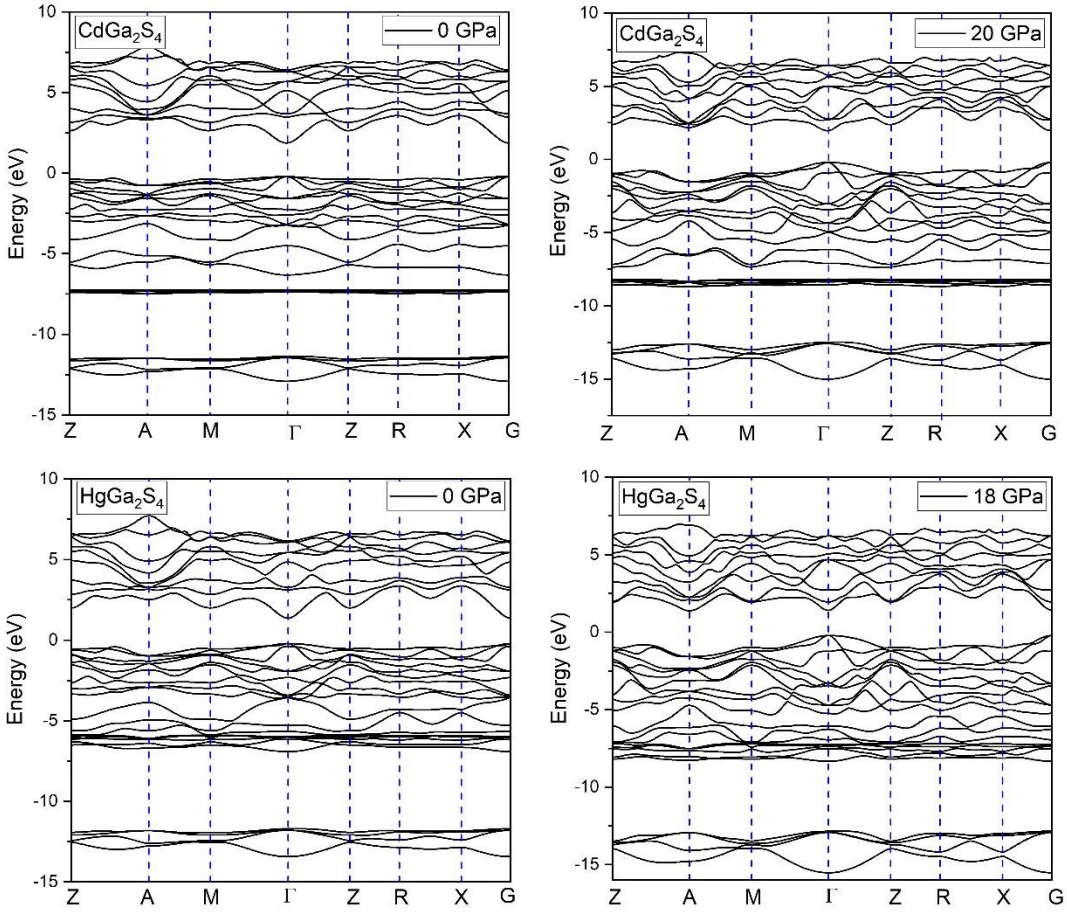

Figure S1. Theoretical calculated electronic band structure of $CdGa_2S_4$ and $HgGa_2S_4$ at low and high pressure.

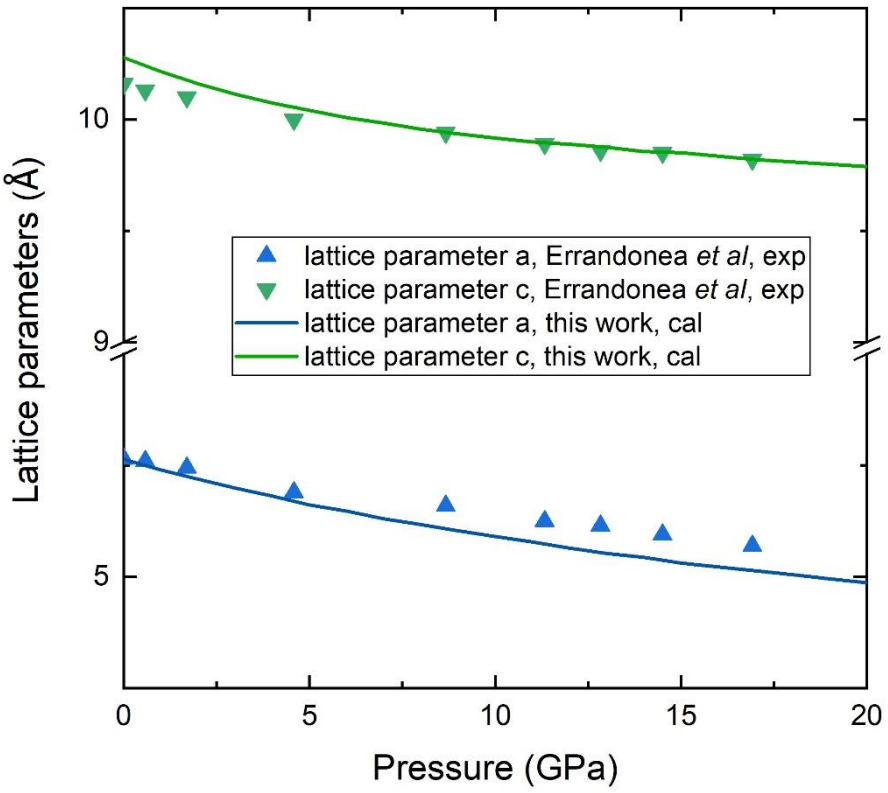

Figure S2. Pressure dependence of the lattice parameters of DC-$CdGa_2S_4$. Experimental data (symbols) correspond to Ref. [1] and theoretical data (solid lines) correspond to this work.

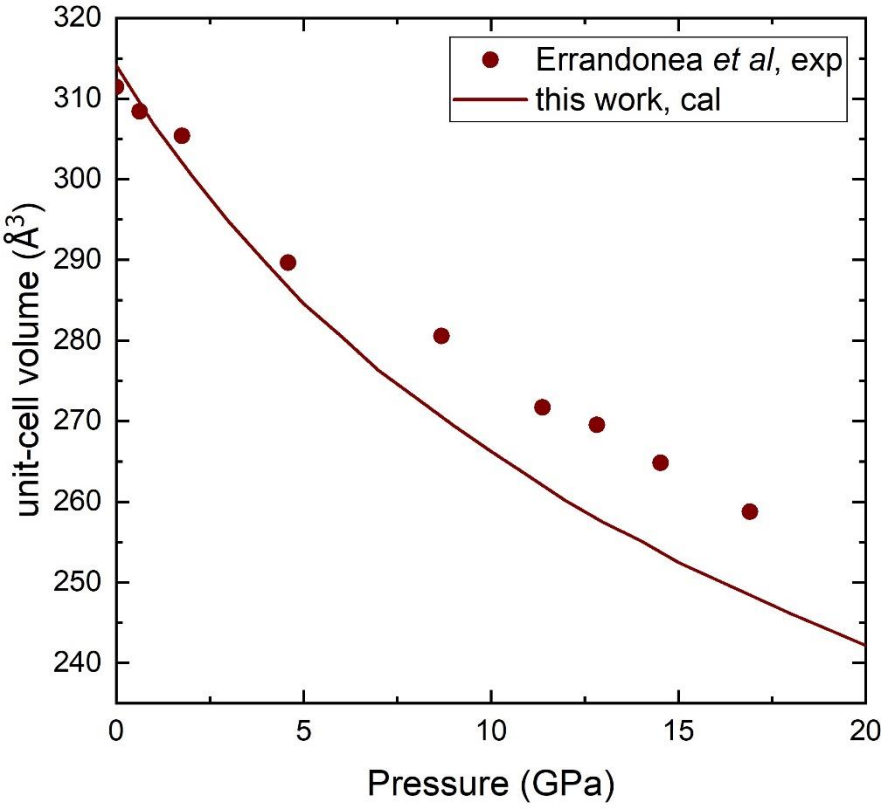

Figure S3. Pressure dependence of the unit-cell volume of DC-$CdGa_2S_4$. Experimental data (symbols) correspond to the work of Errandonea *et al.* [1] and theoretical data (solid lines) correspond to this work.

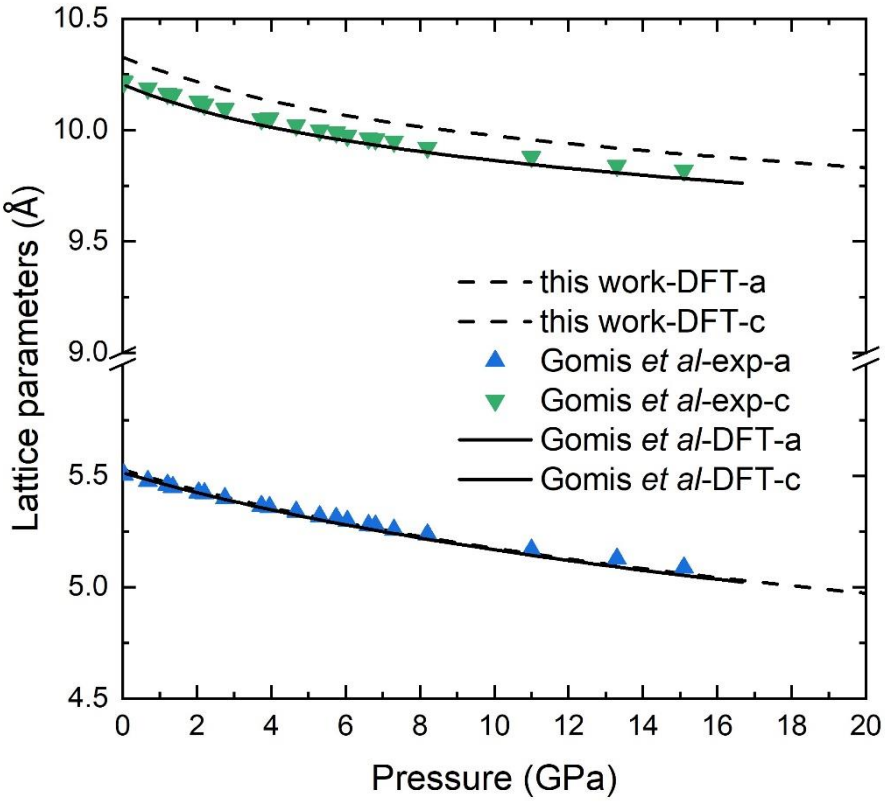

Figure S4. Pressure dependence of the lattice parameters of DC-$HgGa_2S_4$. Previous experimental and calculated data from Gomis *et al.* [2] are shown in triangles and solid lines. The calculated data from this work are shown in dashed line.

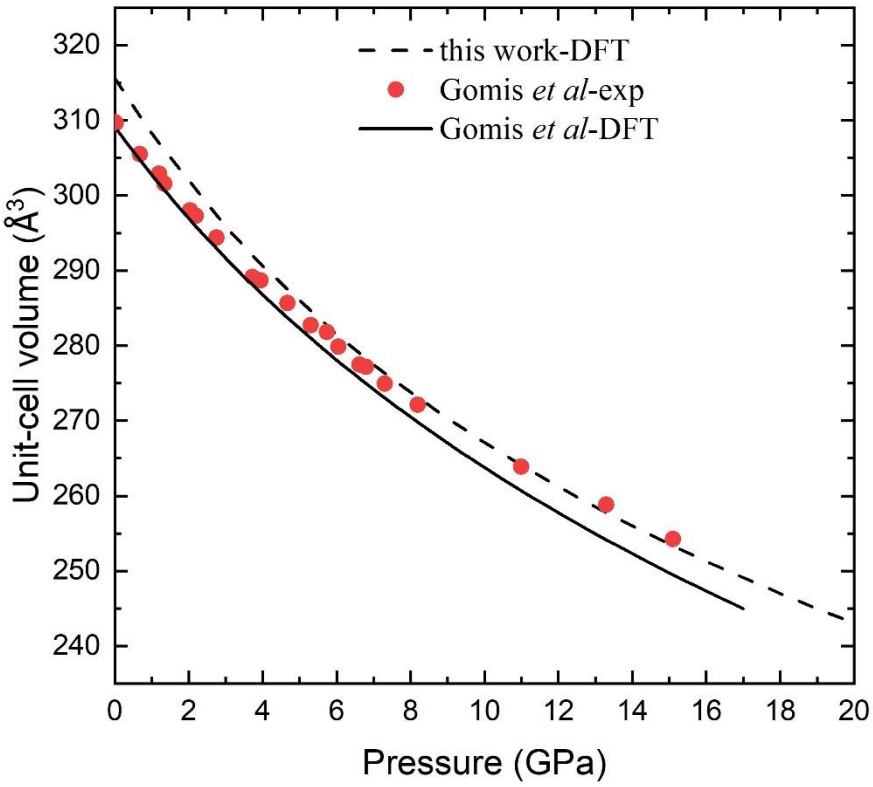

Figure S5. Theoretical pressure dependence of the unit-cell volume of DC-$HgGa_2S_4$ (dashed line). Experimental (symbols) and calculated (solid line) data from Gomis *et al*. [2] are also plotted for comparison.

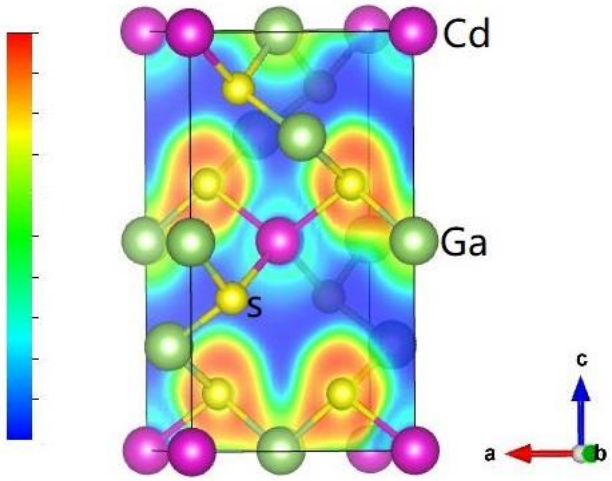

Figure S6. Theoretical calculated electron localization function of DC-$CdGa_2S_4$ in the (110) plane at 0 GPa.

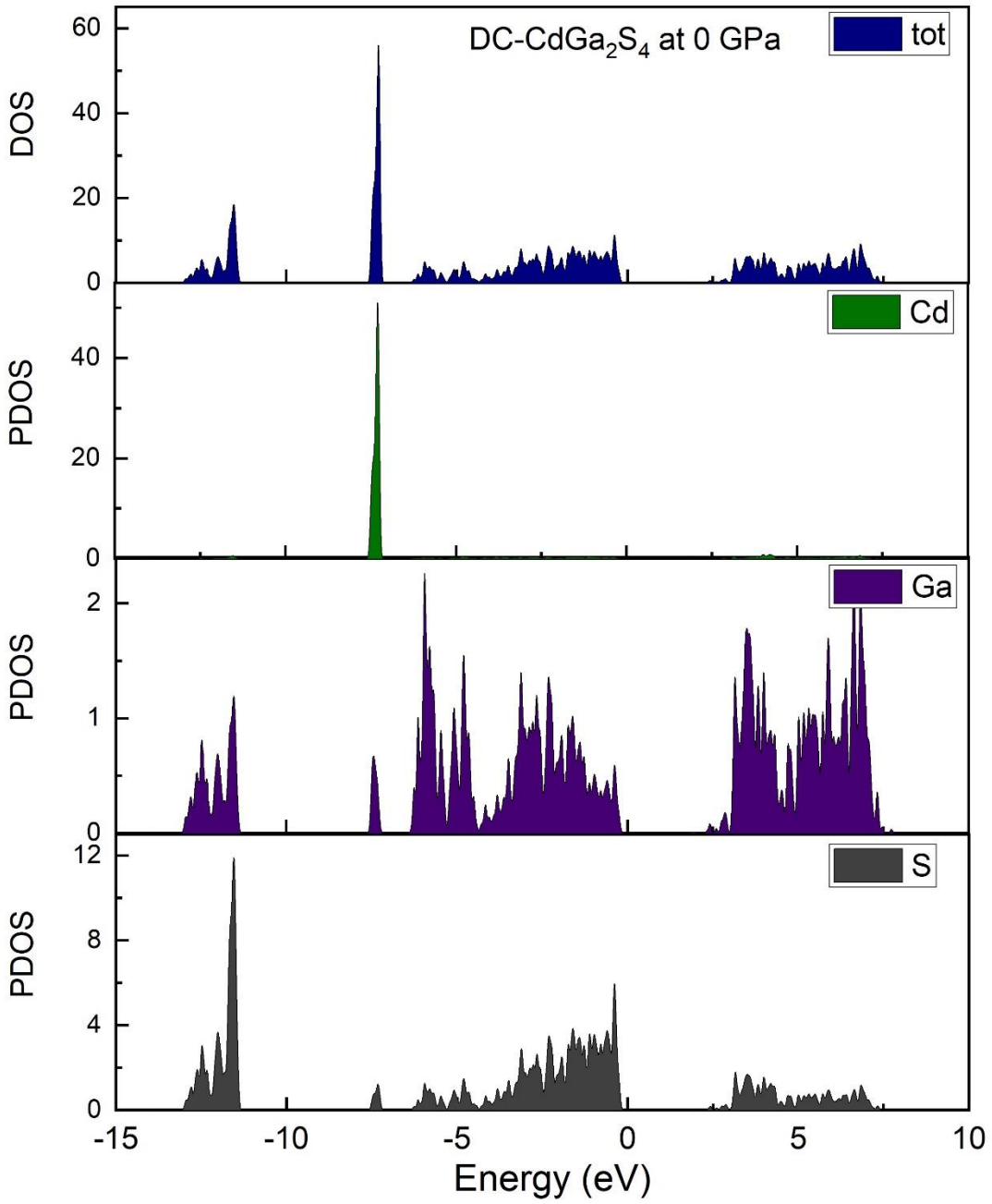

Figure S7. Theoretical calculated electronic density of state (DOS) and project density of state (PDOS) of DC-$CdGa_2S_4$ at 0 GPa.

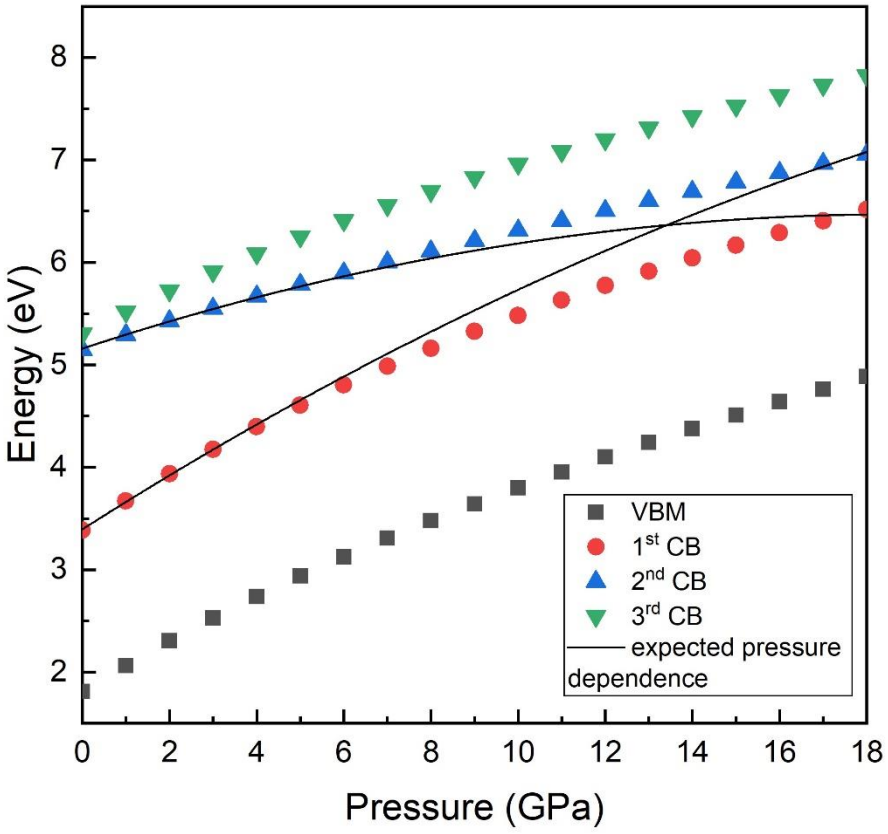

Figure S8. Pressure dependence of the theoretically calculated energy of the valence band maximum (VBM) and three lowest conduction bands (1st, 2nd and 3rd CB, the sequence is determined at 0 GPa) at the Γ point in DC-$HgGa_2S_4$. The solid lines show the expected pressure dependence of the 1st and 2nd CB energy in the absence of BAC.

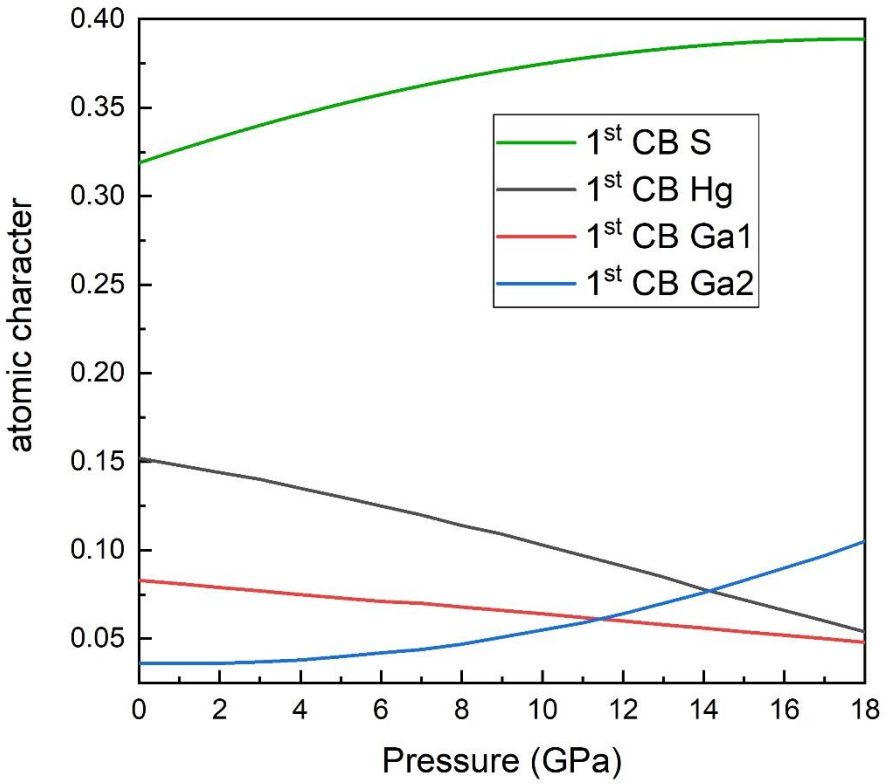

Figure S9. Pressure dependence of the calculated atomic character of the lowest conduction band (1st CB) at the Γ point of DC-$HgGa_2S_4$. Ga1 correspond to the Ga in 2b Wyckoff position while Ga2 is the Ga in 2c Wyckoff position, which is illustrated in figure 1.

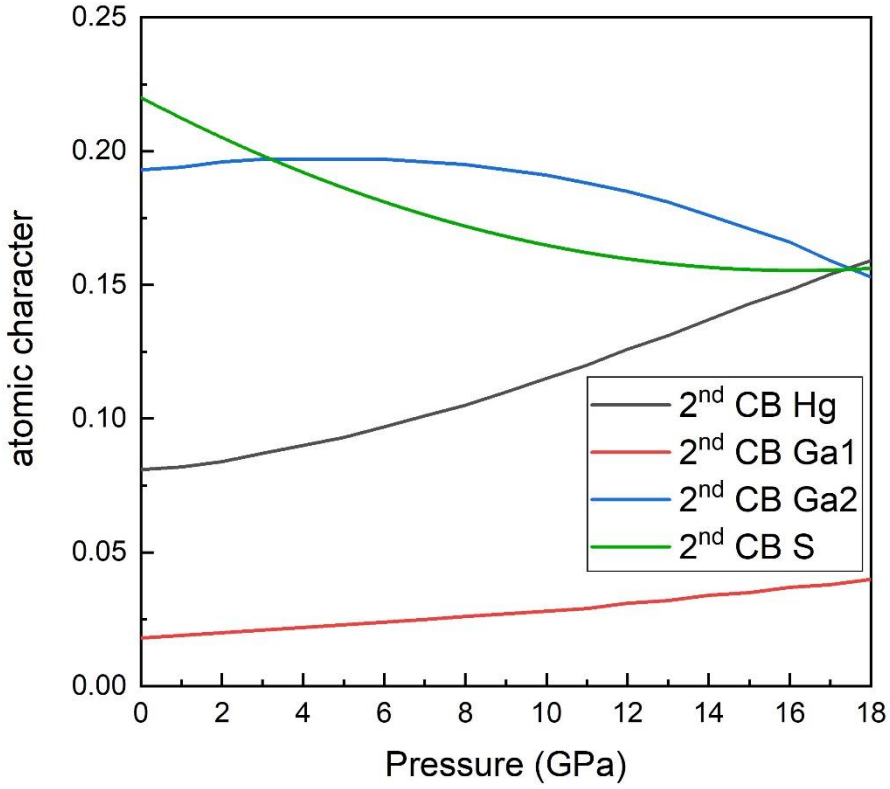

Figure S10. Pressure dependence of the calculated atomic character of the second-lowest conduction band (2^{nd} CB) at the Γ point of DC-$HgGa_2S_4$. Ga1 correspond to the Ga in 2b Wyckoff position while Ga2 is the Ga in 2c Wyckoff position, which is illustrated in figure 1.

References

[1] D. Errandonea, R.S. Kumar, F.J. Manjón, V. V. Ursaki, I.M. Tiginyanu, High-pressure x-ray diffraction study on the structure and phase transitions of the defect-stannite ZnGa2Se4 and defect-chalcopyrite CdGa2S4, J. Appl. Phys. 104 (2008) 063524.

[2] O. Gomis, D. Santamaría-Pérez, R. Vilaplana, R. Luna, J.A. Sans, F.J. Manjón, D. Errandonea, E. Pérez-González, P. Rodríguez-Hernández, A. Muñoz, I.M. Tiginyanu, V. V. Ursaki, Structural and elastic properties of defect chalcopyrite HgGa 2S4 under high pressure, J. Alloys Compd. 583 (2014) 70.