

Electronic Supplementary Information

Theoretical investigation on the promotion of second harmonic generation from chalcopyrite family $A^I\text{GaS}_2$ to $A^{II}\text{Ga}_2\text{S}_4$

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Table S2. Calculated results of bond angles and REDA index.

Fig. S1. Calculated results of bandgap.

Fig. S2. Calculated results of Birefringence.

Table. S1. Crystal data for A^IGaS₂ (A^I=Ag, Cu), A^{II}Ga₂S₄ (A^{II}=Hg, Zn)

Compound	Crystal system	Space group	a (Å)		b (Å)		c (Å)	
			Exp	cal.	Exp	cal.	Exp	cal.
AgGaS ₂	Tetragonal	$\bar{I}4_2d$	5.76	5.75	5.76	5.75	10.30	10.69
CuGaS ₂	Tetragonal	$\bar{I}4_2d$	5.35	5.47	5.35	5.47	10.47	10.47
HgGa ₂ S ₄	Tetragonal	$\bar{I}4$	5.51	5.59	5.51	5.59	10.24	10.50
ZnGa ₂ S ₄	Tetragonal	$\bar{I}4$	5.28	5.47	5.26	5.47	10.44	10.54

Table. S2. Bond angles and REDA index for AgGaS₂, CuGaS₂, HgGa₂S₄, ZnGa₂S₄

Compound	Bond	Bond angle	REDA
AgGaS ₂	Ag-S	106°-116°	0.330
	Ga-S	109°	0.031
	Total _{AgGaS2}	/	0.361
CuGaS ₂	Cu-S	109°-110°	0.062
	Ga-S	109°	-0.006
	Total _{CuGaS2}	/	0.056
HgGa ₂ S ₄	Hg-S	108°-111°	0.091
	Ga-S(1)(2)	104°-112°, 105°-117°	0.138
	Total _{HgGa2S4}	/	0.230
ZnGa ₂ S ₄	Zn-S	109°-110°	0.027
	Ga-S(1)(2)	106°-111°, 106°-115°	0.055
	Total _{ZnGa2S4}	/	0.083

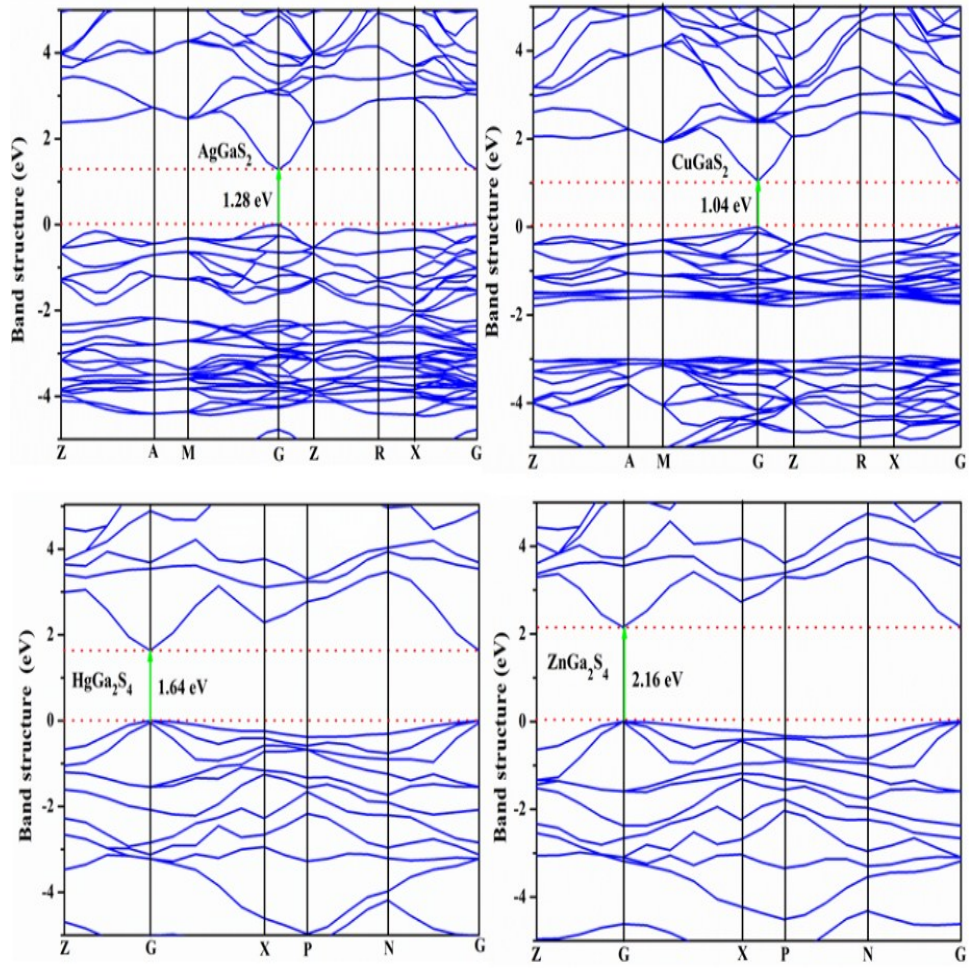


Fig. S1. Band structure of AgGaS₂, CuGaS₂, HgGa₂S₄, ZnGa₂S₄

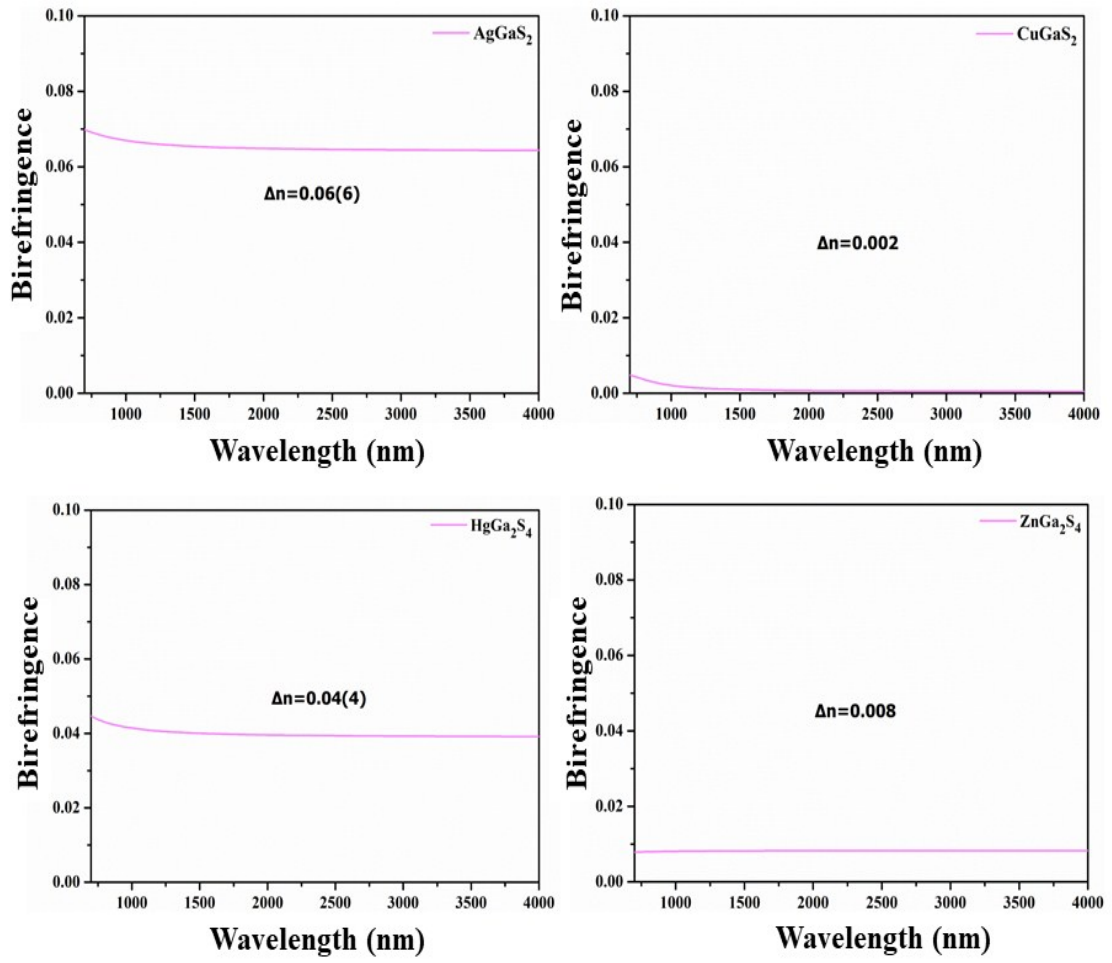


Fig. S2. Calculated Birefringence of AgGaS_2 , CuGaS_2 , HgGa_2S_4 , ZnGa_2S_4