

Supplementary Information

AgGaGeSe₄: an Infrared Nonlinear Quaternary Selenide with Good Performance

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Figure S1. EDS analyses of AgGaGeSe₄.

Figure S2. XPS survey scan data of AgGaGeSe₄.

Figure S3. Tauc plot of direct band gap in AgGaGeSe₄.

Figure S4. The SHG intensity of a AgGaGeSe₄ sample compared to that of AgGaSe₂ using a 2.0 μm laser.

Figure S5. The calculated band structure of AgGaGeSe₄ using the local density approximation (LDA) Ceperley–Alder (CA) approach.

Figure S6. The real part ϵ_1 of dielectric function of AgGaGeSe₄.

Figure S7. The imaginary part ϵ_2 of dielectric function of AgGaGeSe₄.

Table S1. Crystallographic data and details of structure refinement for AgGaGeSe₄.

Table S2. Selected bond lengths (\AA) and angles (deg) of AgGaGeSe₄.

Table S3. Binding energy values of constituent element core-level electrons of AgGaGeSe₄.

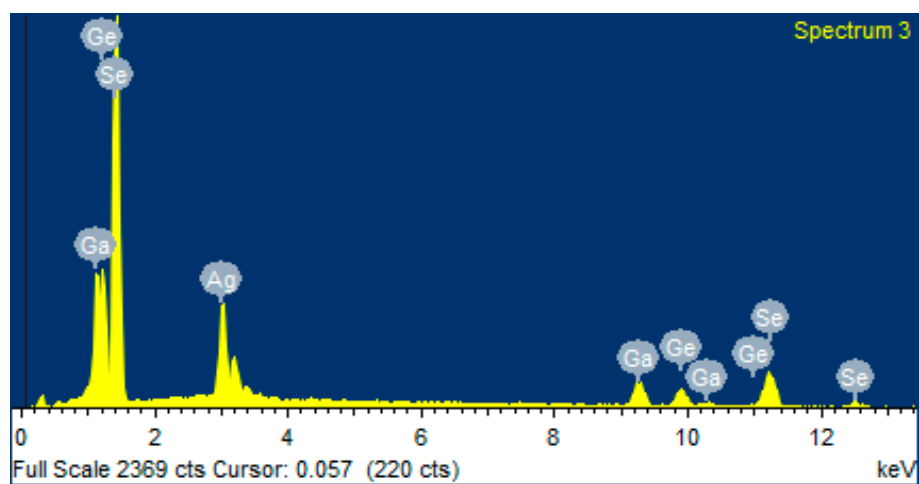


Figure S1. EDS analyses of AgGaGeSe₄.

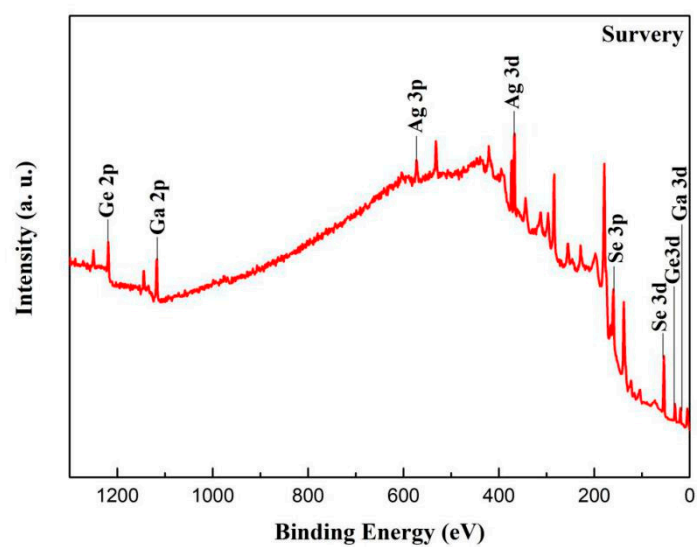


Figure S2. XPS survey scan data of AgGaGeSe₄.

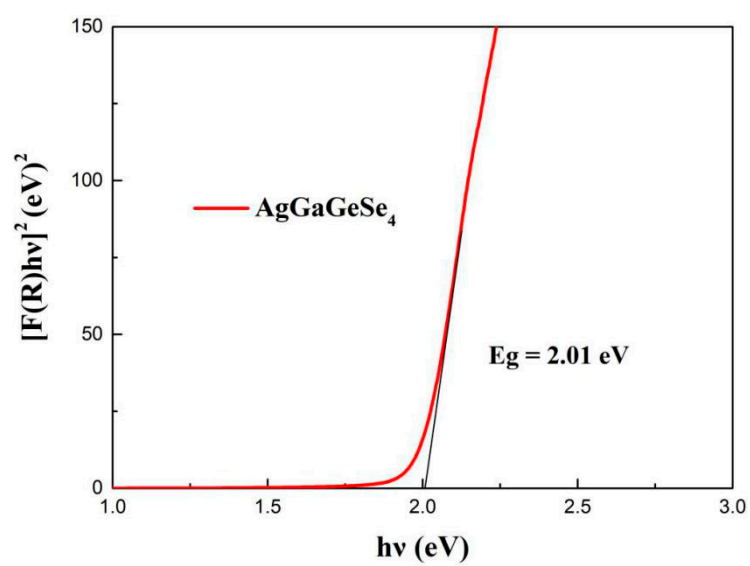


Figure S3. Tauc plot of direct band gap in AgGaGeSe_4 .

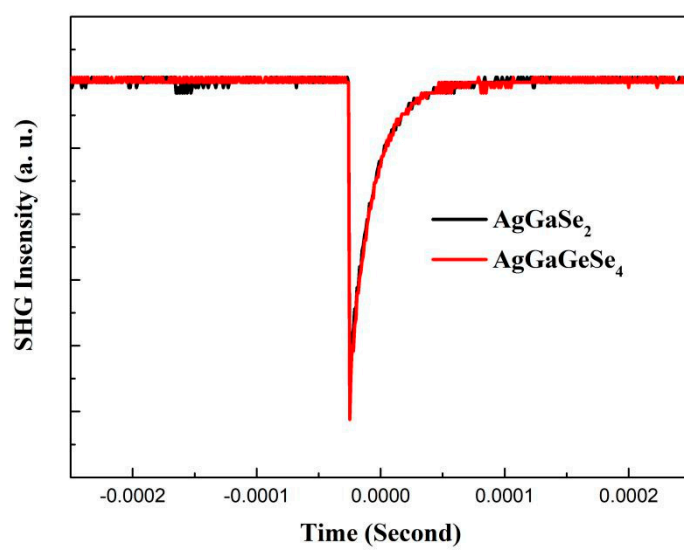


Figure S4. The SHG intensity of a AgGaGeSe_4 sample compared to that of AgGaSe_2 using a $2.0 \mu\text{m}$ laser.

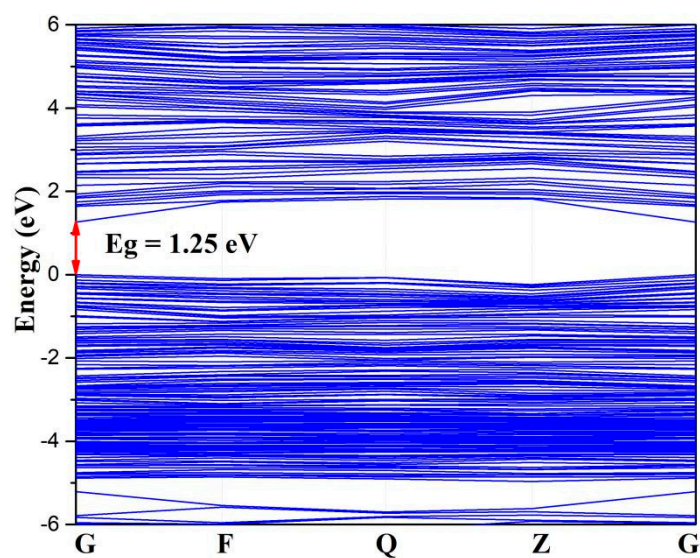


Figure S5. The calculated band structure of AgGaGeSe₄ using the local density approximation (LDA) Ceperley–Alder (CA) approach.

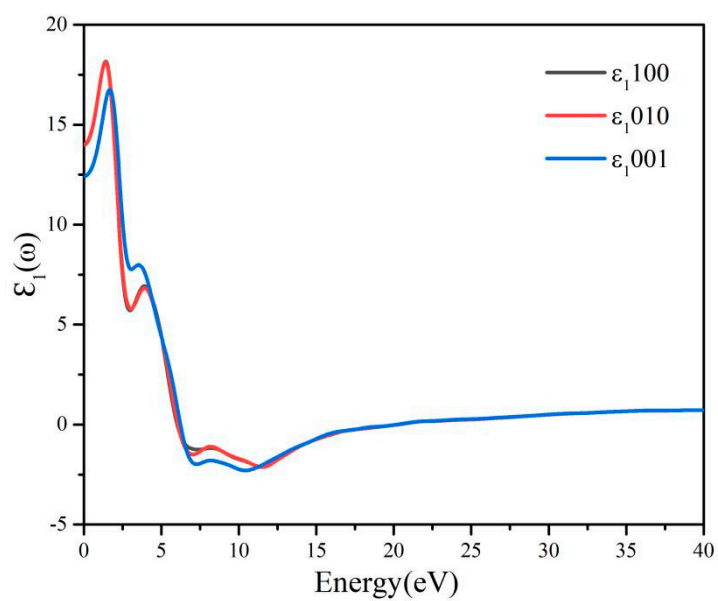


Figure S6. The real part ϵ_1 of dielectric function of AgGaGeSe₄.

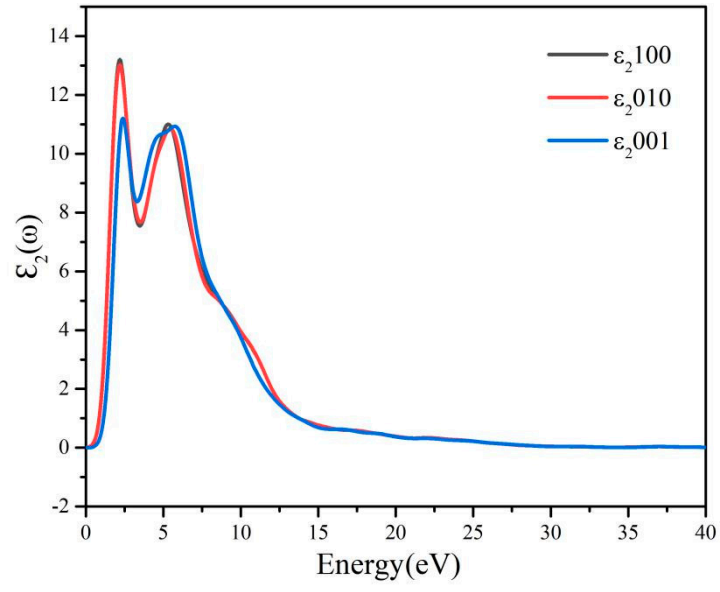


Figure S7. The imaginary part ϵ_2 of dielectric function of AgGaGeSe₄.

Table S1. Crystallographic data and details of structure refinement for AgGaGeSe₄.

Formula	AgGaGeSe ₄
Fw (g/mol)	566.02
Crystal system	Tetragonal
Space-group	$I\bar{4}2d$ (No.122)
a (Å)	5.8056(5)
b (Å)	5.8056(5)
c (Å)	10.3488(10)
α (°)	90
β (°)	90
γ (°)	90
V (Å ³)	348.81(7)
Z	2
Dcal g/cm ³	5.389
	$-6 \leq h \leq 6$
Index ranges	$-6 \leq k \leq 6$
	$-12 \leq l \leq 12$
F(000)	492
R(F) ^a	0.0747
R _w (F _o ²) ^b	0.1327
$\text{Weight} = 1 / [\sigma^2(F_o^2) + (0.0220 * P) ^2 + 84.95 * P]$	
where $P = (\text{Max} (F_o^2, 0) + 2 * F_c^2) / 3$	

Table S2. Selected bond lengths (Å) and angles (deg) of AgGaGeSe₄.

Bond distance	(Å)	Bond distance	(Å)
Ag1–Se	2.375(3)	Ag–Se#3	2.375(3)
Ag–Se#1	2.375(3)	Se–Ga	2.479(4)
Ag–Se#2	2.375(3)	Se–Ga#4	2.479(4)
Bond angle	(deg)	Bond angle	(deg)
Se–Ag–Se#1	114.00(1)	Ag–Se–Ga#4	106.432(2)
Se–Ag–Se#2	107.26(5)	Ag#4–Se–Ga#4	115.467(4)
Se#1–Ag–Se#2	107.26(5)	Ga–Se–Ga#4	103.30(2)
Se–Ag–Se#3	107.26(5)	Se#5–Ga–Se#6	105.80(5)
Se#1–Ag–Se#3	107.26(5)	Se#5–Ga–Se#7	105.80(5)
Se#2–Ag–Se#3	114.00(1)	Se#6–Ga–Se#7	117.10(1)
Ag–Se–Ag#4	109.90(2)	Se#5–Ga–Se	117.10(1)
Ag–Se–Ga	115.468(5)	Se#6–Ga–Se	105.80(5)
Ag#4–Se–Ga	106.432(2)	Se#7–Ga–Se	105.80(5)

Table S3. Binding energy values of constituent element core-level electrons of
AgGaGeSe₄.

Compounds	Element	Peak Energy (eV)	Peak Width FWHM (eV)
AgGaGeSe 4	Ag <i>3d</i>	367.30	1.37
	Ag <i>3p</i>	572.87	1.02
	Ga <i>3d</i>	19.21	2.34
	Ga <i>2p</i>	1117.41	1.44
	Ge <i>3d</i>	30.94	2.33
	Ge <i>2p</i>	1219.01	2.25
	Se <i>3d</i>	54.12	2.55
	Se <i>3p</i>	160.17	2.94