

Supporting Information for

AgIn₅Se₈: a defect diamond-like nonlinear optical selenide

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Table 1. Calculated NLO Properties of AgIn_5Se_8 , LiIn_5Se_8 , AgIn_5S_8 and LiIn_5S_8

	a(Å)	c(Å)	Band gap(eV)	d_{36} (pm/V)	$\Delta n@1 \mu\text{m}$
AgIn_5Se_8	5.698	12.086	1.59	13.1	0.031
LiIn_5Se_8	5.676	11.782	2.08	12.9	0.029
AgIn_5S_8	5.437	11.659	2.01	6.4	0.036
LiIn_5S_8	5.426	11.266	2.64	6.7	0.020

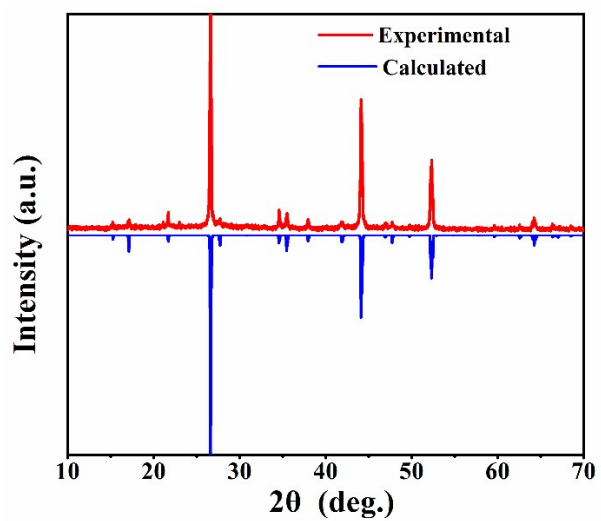


Figure S1 Experiment powder X-ray diffraction pattern and calculated diffraction pattern of AgIn_5Se_8

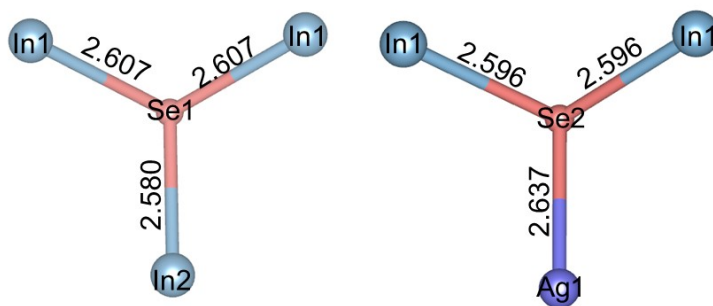


Figure S2 Coordination environment of two sites of Se in AgIn_5Se_8

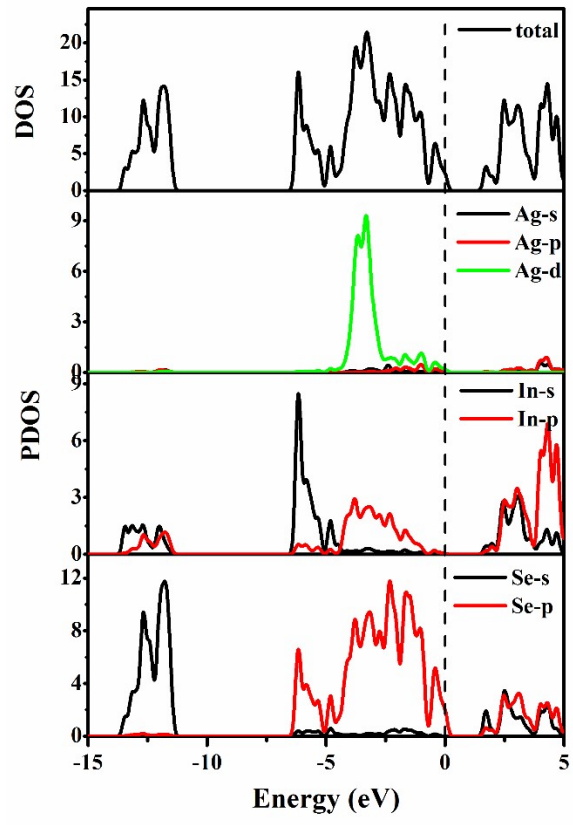


Figure S3 Density of states of AgIn_5Se_8