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Designs of SHG materials with mid-infrared transparency based on genetic engineering for Ba_2BiInA_5 (A = Se, Te)

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Electronic Supplementary Information

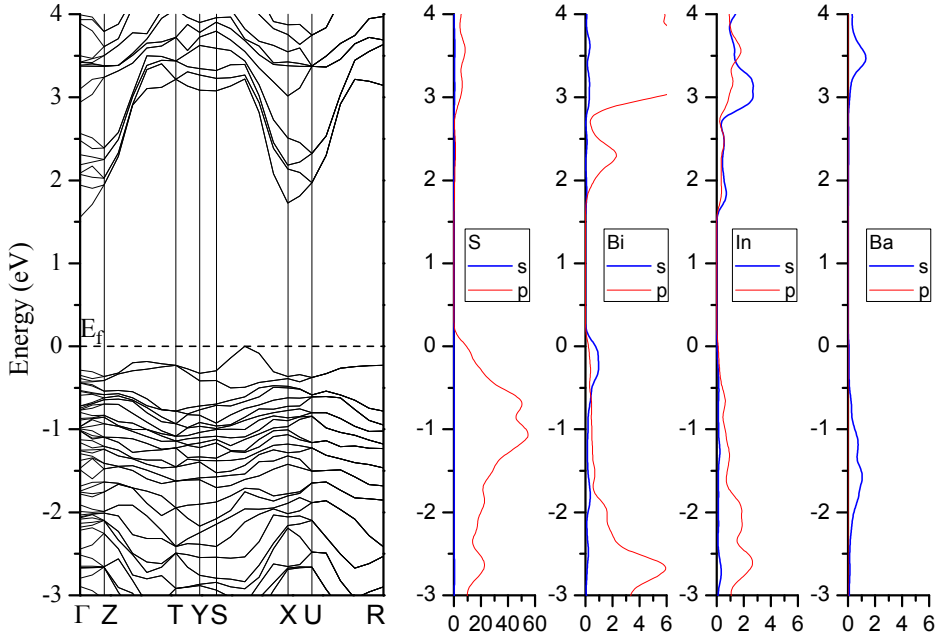

Fig. S1a Energy band structure and projected density of state for Ba_2BiInS_5.

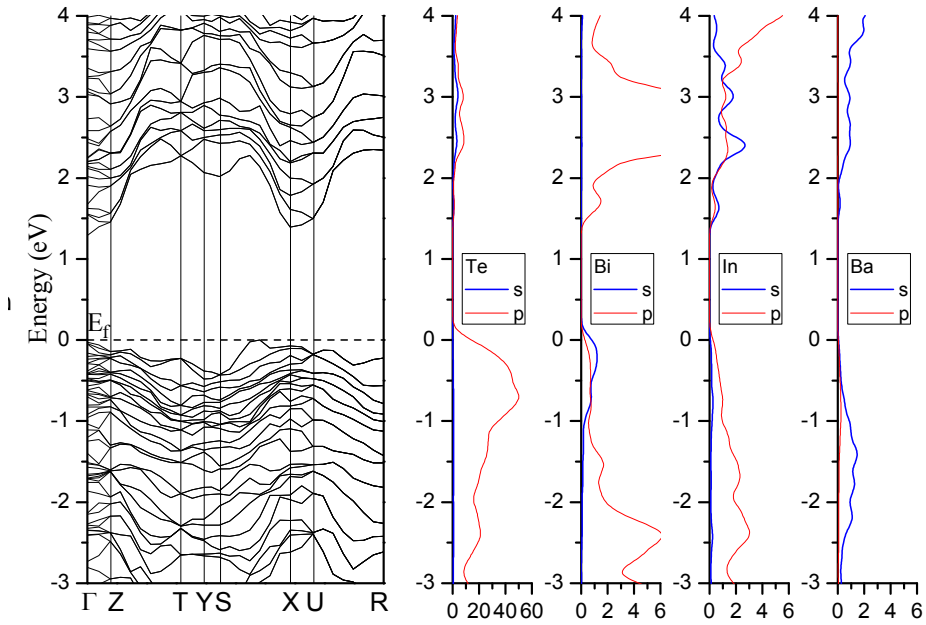

Fig. S1b Energy band structure and projected density of state for $Ba_2BiInTe_5$.

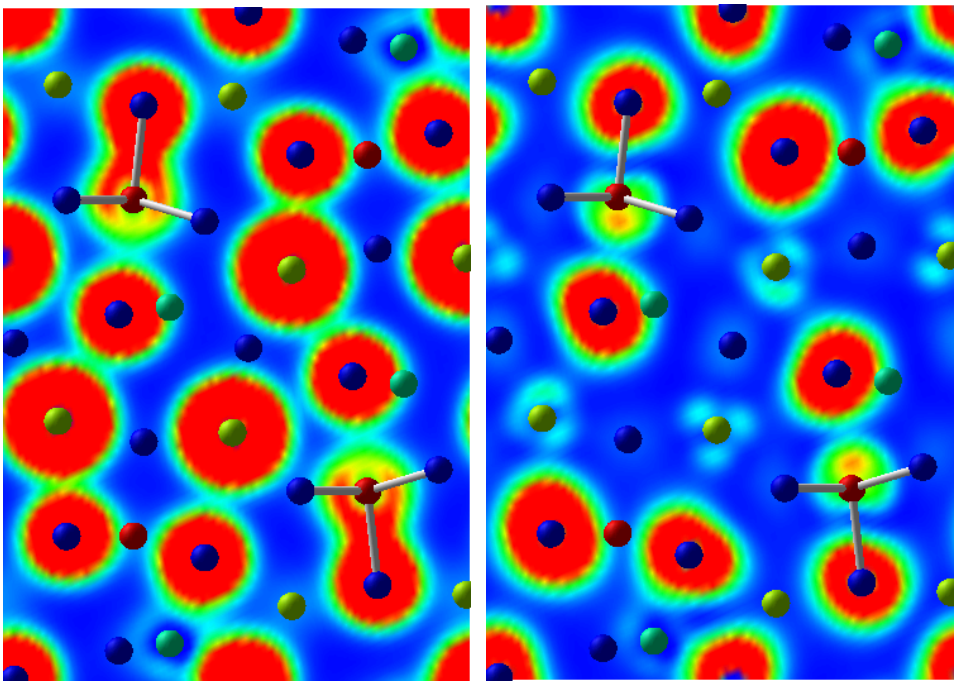

Fig. S2a The PED maps from -1.0 eV to the Fermi level (left), and from -10.0 to -13.0 eV (right); the electron density is represented from blue (0.0 e/Å^3) to red (0.08 e/Å^3) for compound Ba_2BiInS_5.

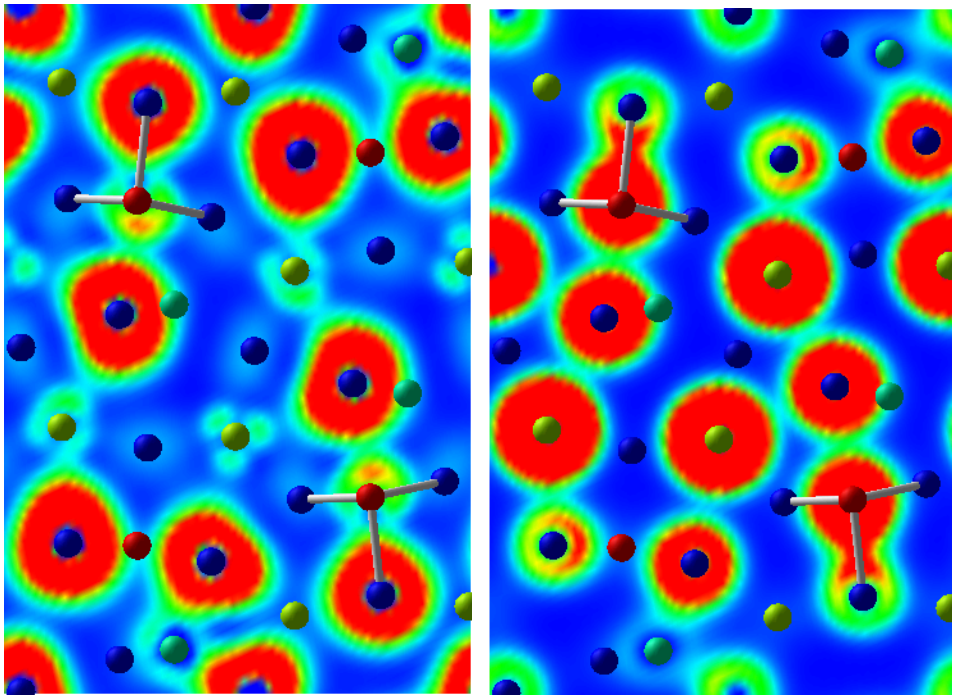

Fig. S2b The PED maps from -1.0 eV to the Fermi level (left), and from -10.0 to -13.0 eV (right); the electron density is represented from blue (0.0 e/Å^3) to red (0.08 e/Å^3) for compound $Ba_2BiInTe_5$.

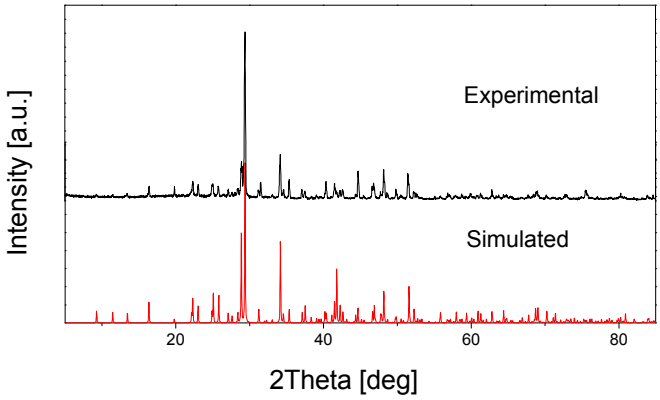

Fig. S3 Experimented and simulated X-ray diffraction patterns for polycrystalline $Ba_2BiInSe_5$ (The radiation wavelength of the X-ray is λ = 1.5418 Å).

Table S1. Atomic coordinates and equivalent isotropic displacement parameters (Å) for compound $Ba_2BiInSe_5$.

Atom	*x*	*y*	*z*	U_{eq}[a]

Ba(1)	-1.0000	0. 6284(1)	0. 5204(1)	0.014(1)
Ba(2)	-1.0000	0. 3872(1)	0. 6447(1)	0.013(1)
Bi(1)	0	0. 2820(1)	0. 3085(1)	0.016(1)
In(1)	-0.5000	0. 4409(1)	0. 3873(1)	0.013(1)
Se(1)	0	0. 1413(1)	0. 3302(1)	0.013(1)
Se(2)	-0.5000	0. 3124(1)	0. 4657(1)	0.015(1)
Se(3)	-0.5000	0. 2837(1)	0. 1632(2)	0.014(1)
Se(4)	-0.5000	0. 5035(1)	0. 5573(2)	0.012(1)
Se(8)	0	0. 4556(1)	0. 2772(1)	0.014(1)

Table S2. Selected bond lengths (Å) for compound $Ba_2BiInSe_5$.

	distance		distance
Ba(1)-Se(1)#9	3.321(2)	Bi(1)-Se(1)	2.706(3)
Ba(1)-Se(3)#6	3.324(2)	Bi(1)-Se(3)#1	2.890(2)
Ba(1)-Se(8)#6	3.746(3)	Bi(1)-Se(2)	3.051(2)
Ba(2)-Se(3)#3	3.276(4)	In(1)-Se(8)#4	2.620(2)
Ba(2)-Se(1)#5	3.310(2)	In(1)-Se(8)	2.620(2)
Ba(2)-Se(2)	3.507(2)	In(1)-Se(2)	2.665(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1/2,-y-1/2,-z; #3 x-1/2,y-1/2,z; #4 x-1/2,y+1/2,z;

#5 -x+1/2,-y+1/2,-z+1; #6 -x+1/2,-y-1/2,-z+1; #9 x,y-1,z