Supplementary Information

First-principles calculations of nitrogen-doped antimony triselenide: A prospective material for solar cells and infrared optoelectronic devices

Table S1 Optimized structural parameters for Sb_2Se_3 with LDA and GGA (PBE, RPBE, WC PW91 and PBESOL).

Method	a (Å)	Dev (%)	b (Å)	Dev (%)	c (Å)	Dev (%)	V (Å)	Dev (%)
LDA	11.262	-3.1%	11.741	-0.2%	3.875	-2.2%	512.299	5.46%
GGA-PBE	11.688	0.6%	12.612	7.2%	3.968	0.2%	584.947	-7.95%
GGA-RPBE	11.921	2.6%	13.413	14.0%	3.979	0.4%	636.301	-17.43%
GGA-WC	11.451	-1.5%	11.863	0.8%	3.947	-0.4%	536.215	1.04%
GGA-PW91	11.612	-0.1%	12.544	6.6%	3.969	0.2%	578.189	-6.70%
GGA-PBESOL	11.445	-1.5%	11.953	1.6%	3.932	-0.8%	537.859	0.74%
EXP	11.62		11.77		3.962		541.872	

Table S2 Optimized structural parameters for Sb_2Se_3 with GGA-WC.

Sr. No	Cutoff (eV)	Lattice Parameters					
		a	Error (%)	b	Error (%)	c	Error (%)
1	200	11.460	1.4%	12.244	-4.0%	4.028	-1.7%
2	250	11.809	-1.6%	12.688	-7.8%	3.904	1.5%
3	300	11.787	-1.4%	11.935	-1.4%	4.010	-1.2%
4	320	11.451	1.5%	11.862	-0.8%	3.947	0.4%
5	340	11.450	1.5%	11.876	-0.9%	3.988	-0.7%
6	360	11.447	1.5%	11.875	-0.9%	3.988	-0.7%
7	380	11.450	1.5%	11.882	-1.0%	3.989	-0.7%
8	400	11.337	2.4%	11.990	-1.9%	3.943	0.5%

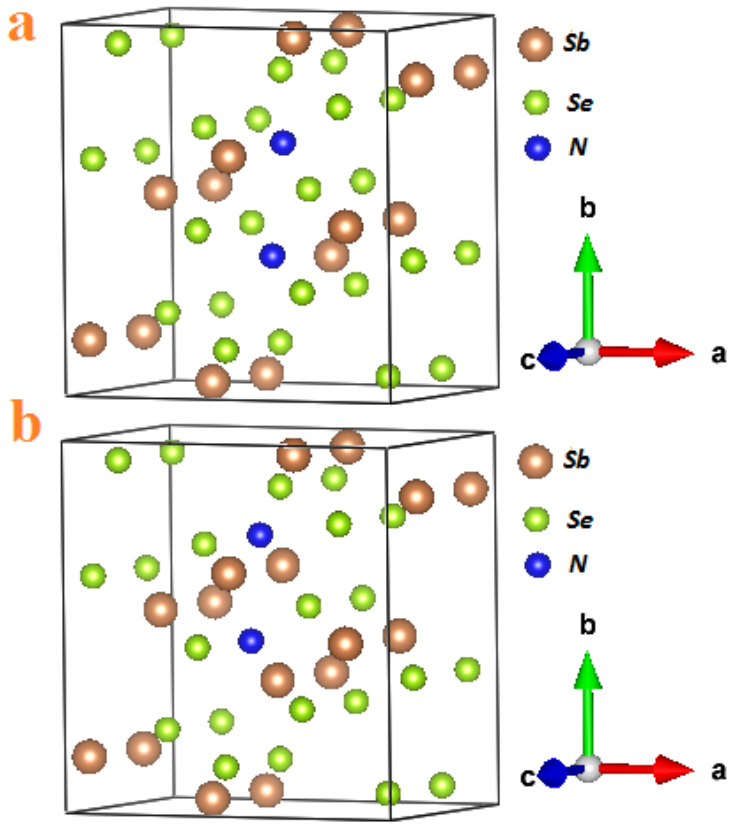

Fig. S1 $Sb_{16}Se_{24}$ supercell models **(a)** 2N atom doped $Sb_{14}N_2Se_{24}$ supercell at Sb site, **(b)** 2N atom doped $Sb_{16}Se_{22}N_2$ supercell at Se site.

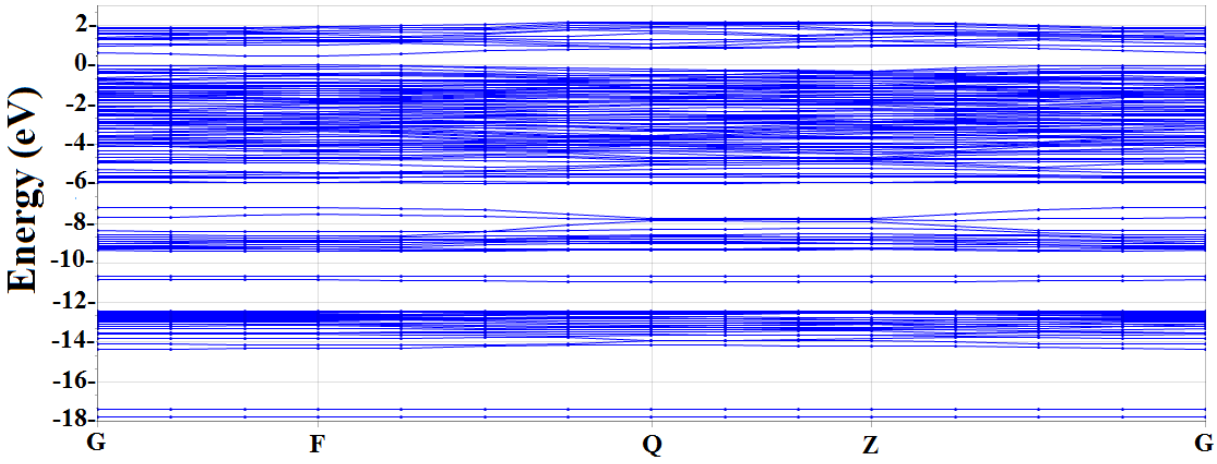

Fig. S2 Energy band structure of 2N atom doped $Sb_{14}N_2Se_{24}$ supercell at Sb site.

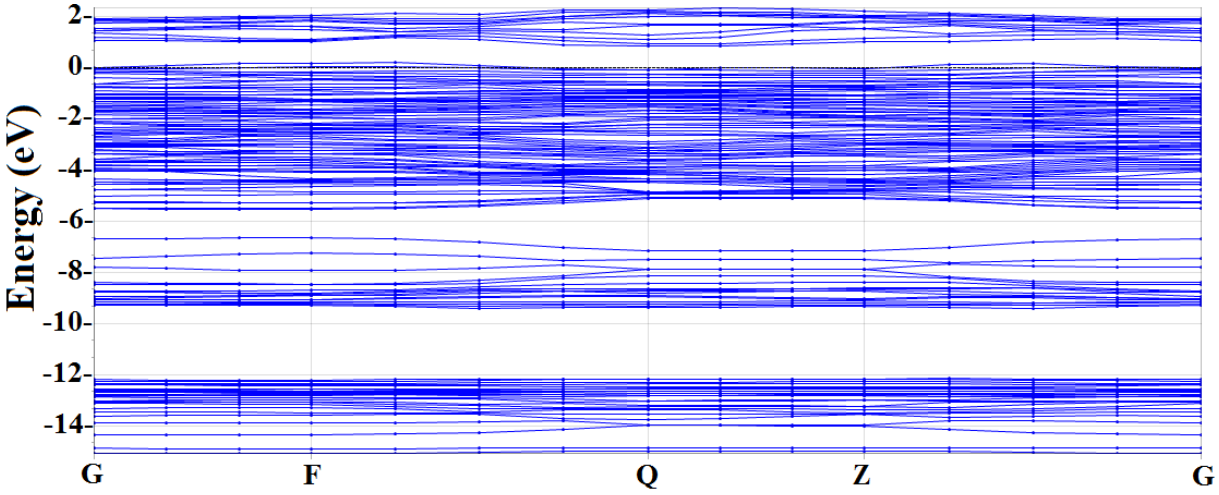

Fig. S3 Energy band structure of 2N atom doped $Sb_{16}Se_{22}N_2$ supercell at Se site.