Electronic Supplementary Material (ESI) for Materials Advances.

Supporting Information

New Crystal Family of GaNGeC Quaternary Compound Including Direct Band Gap Semiconductors and metals

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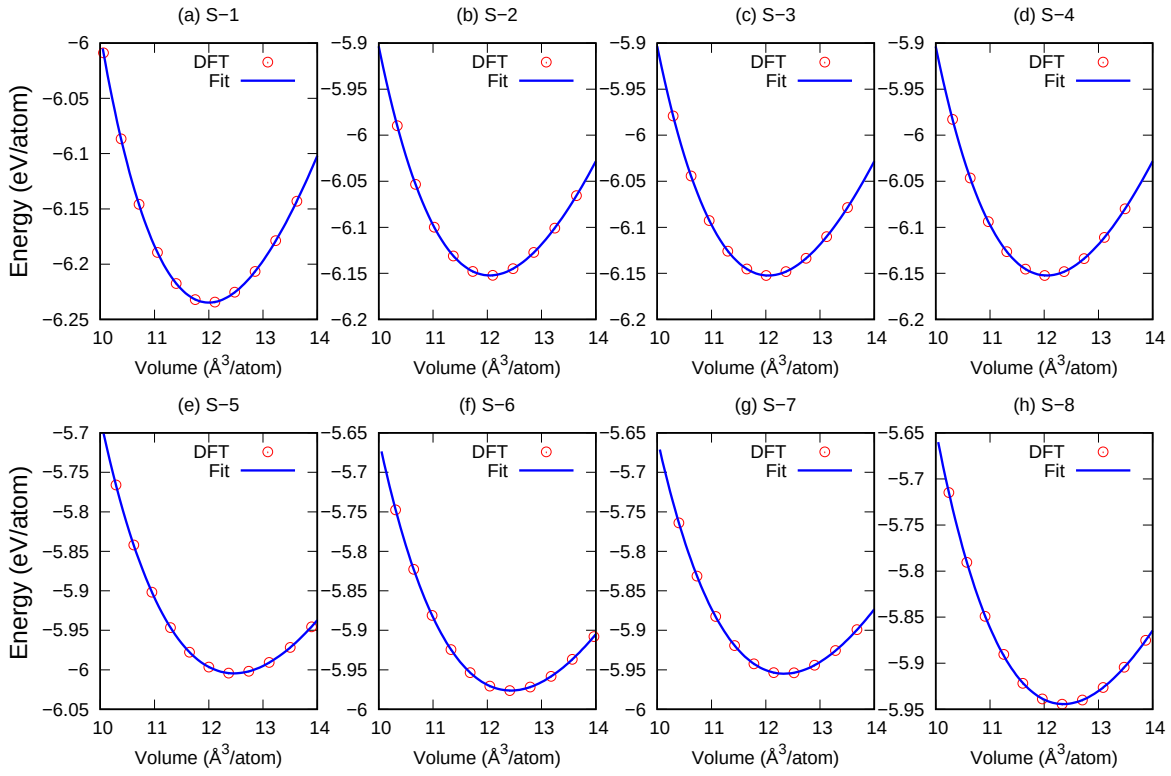

Fig. S1 (Color online) The total energy per atom as a function of volume per atom. The red dot marks the calculated value of the standard density functional theory (DFT), and the blue line marks the fitting result (Fit).

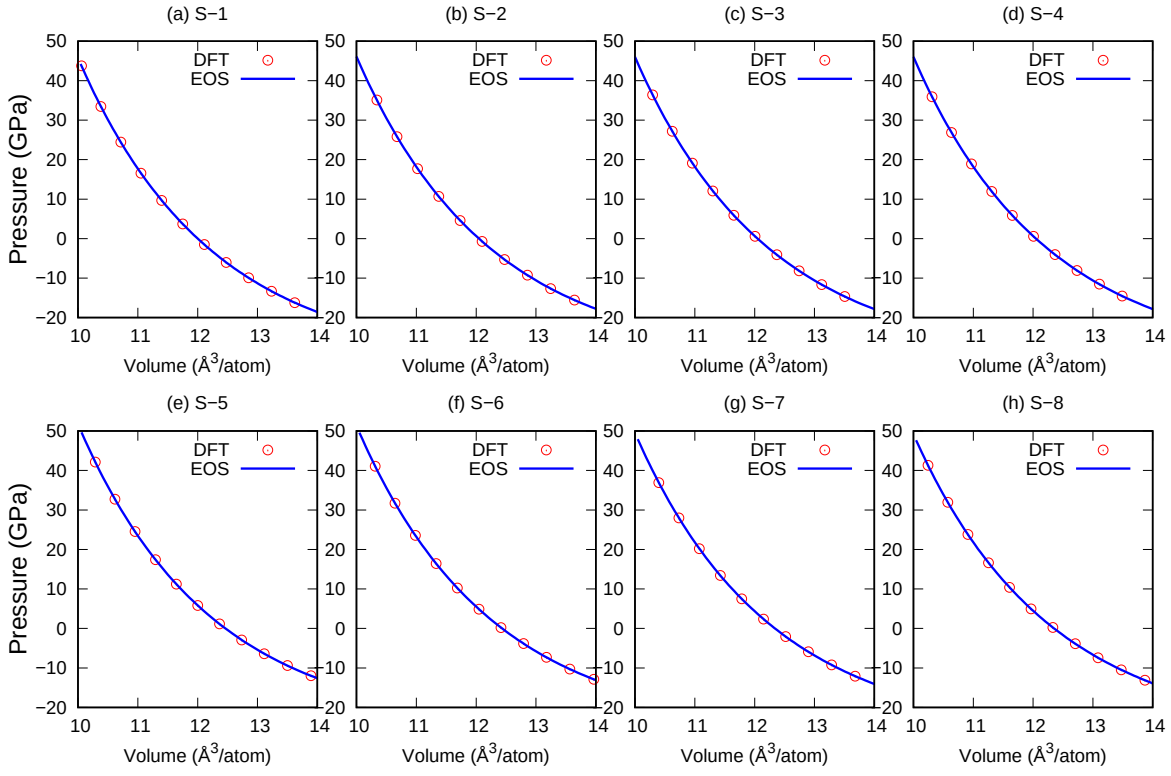

Fig. S2 (Color online) The pressure as a function of volume per atom. The red dot marks the calculated value of the standard density functional theory (DFT), and the blue line is the fitting result of the Vinet equation of state (EOS) (P. Vinet, J. Ferrante, J. H. Rose and J. R. Smith, *J. Geophys. Res.* 1987, **92**, 9319-9325).

Table S1 Fractional Coordinates of the Atom in the Primitive Cell, and Wyckoff Positions of Group.

	S-1	*P*3*m*1 (No.156)
Ge	0.6666666666666714, 0.3333333333333286, 0.3624599819999971	1c
C	0.3333333333333286, 0.6666666666666714, 0.4790199799999968	1b
Ga	0.3333333333333286, 0.6666666666666714, 0.8624199910000031	1b
N	0.6666666666666714, 0.3333333333333286, 0.9960899690000034	1c
	S-2	*Pmm*2 (No. 25)
Ge	0.5000000000000000, 0.0000000000000000, 0.3069426505183119	1c
C	0.0000000000000000, 0.0000000000000000, 0.5409335387865466	1a
Ga	0.0000000000000000, 0.5000000000000000, 0.7934918935126746	1b
N	0.5000000000000000, 0.5000000000000000, 0.0586318951824683	1d
	S-3	*Pmm*2 (No. 25)
Ge	0.0000000000000000, 0.0000000000000000, 0.5877554933025234	1a
C	0.5000000000000000, 0.0000000000000000, 0.8216899701073591	1c
Ga	0.5000000000000000, 0.5000000000000000, 0.0742271464295536	1d
N	0.0000000000000000, 0.5000000000000000, 0.3394273351605525	1a
	S-4	*Pmm*2 (No. 25)
Ge	0.5000000000000000, 0.5000000000000000, 0.8158552834755285	1d
C	0.0000000000000000, 0.5000000000000000, 0.5818794706489309	1b
Ga	0.0000000000000000, 0.0000000000000000, 0.3293138608568018	1a
N	0.5000000000000000, 0.0000000000000000, 0.0641713230187433	1c
	S-5	*R*3*m* (No. 160)
Ge	0.6709841743474934, 0.6709841743474934, 0.6709841743474934	1a
C	0.2911739297909084, 0.2911739297909084, 0.2911739297909084	1a
Ga	0.8190742803260118, 0.8190742803260118, 0.8190742803260118	1a
N	0.1995873262022444, 0.1995873262022444, 0.1995873262022444	1a
	S-6	*P*3*m*1 (No.156)
Ge	0.6666667436180234, 0.3333333243819752, 0.3305940463622838	1c
C	0.3333333069338735, 0.6666667660661290, 0.1905461627035190	1b
Ga	0.6666668219594882, 0.3333332460405103, 0.7739294995641177	1c
N	0.3333332694886195, 0.6666668035113830, 0.9157003673700826	1b
	S-7	*R*3*m* (No. 160)
Ge	0.0456905218556258, 0.0456905218556258, 0.0456905218556258	1a
C	0.1644273372098013, 0.1644273372098013, 0.1644273372098013	1a
Ga	0.5330179664915136, 0.5330179664915136, 0.5330179664915136	1a
N	0.6649541884430761, 0.6649541884430761, 0.6649541884430761	1a
	S-8	*P*3*m*1 (No.156)
Ge	0.0000000000000000, 0.0000000000000000, 0.3022743618233577	1a
C	0.0000000000000000, 0.0000000000000000, 0.6634581556066892	1a
Ga	0.3333333332999970, 0.6666666670000012, 0.7667517986069959	1b
N	0.3333333332999970, 0.6666666670000012, 0.1623056629629663	1b

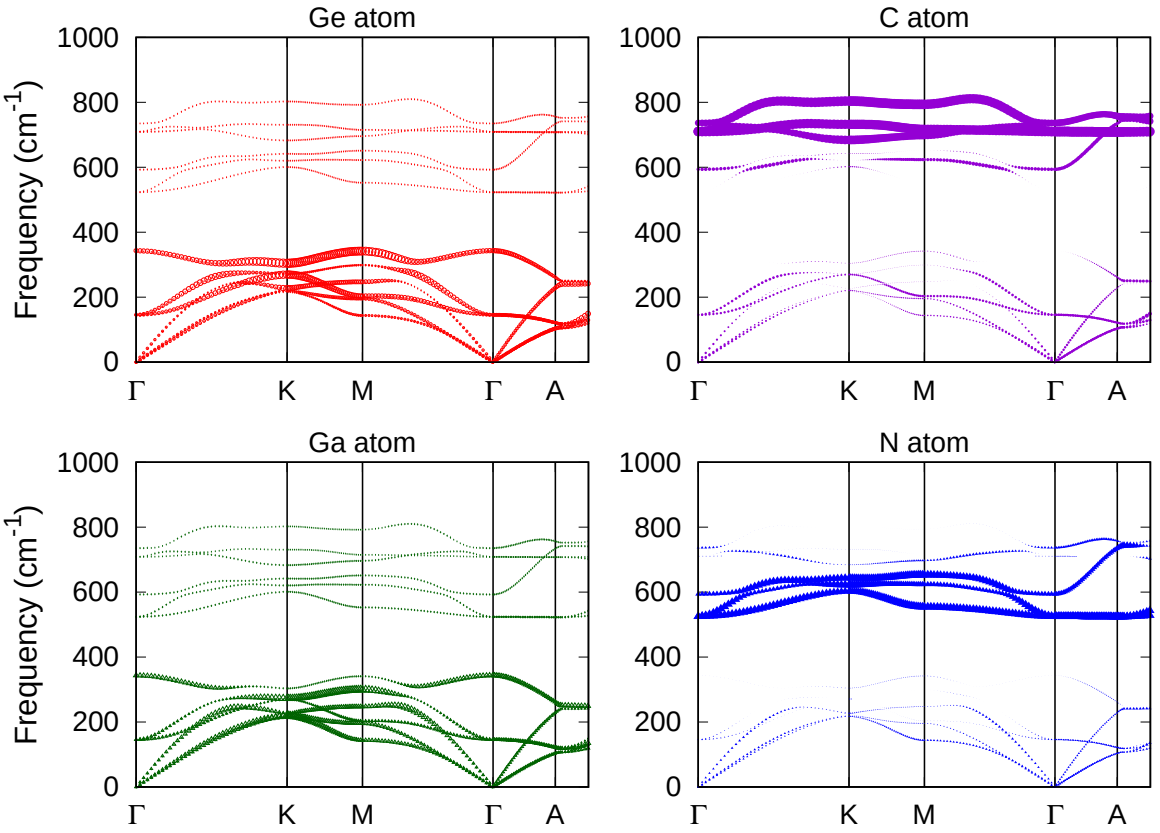

Fig. S3 (Color online) Atom-resolved projected phonon dispersions of S-1 crystal.

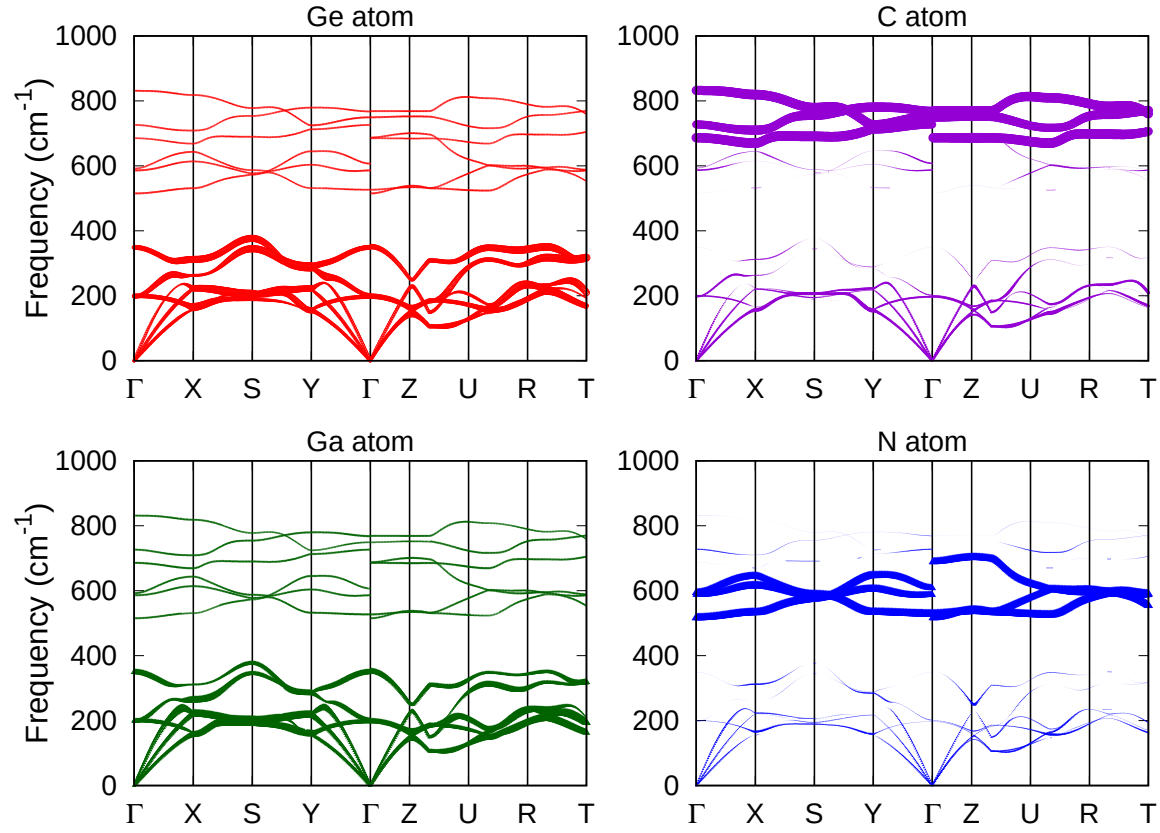

Fig. S4 (Color online) Atom-resolved projected phonon dispersions of S-2 crystal.

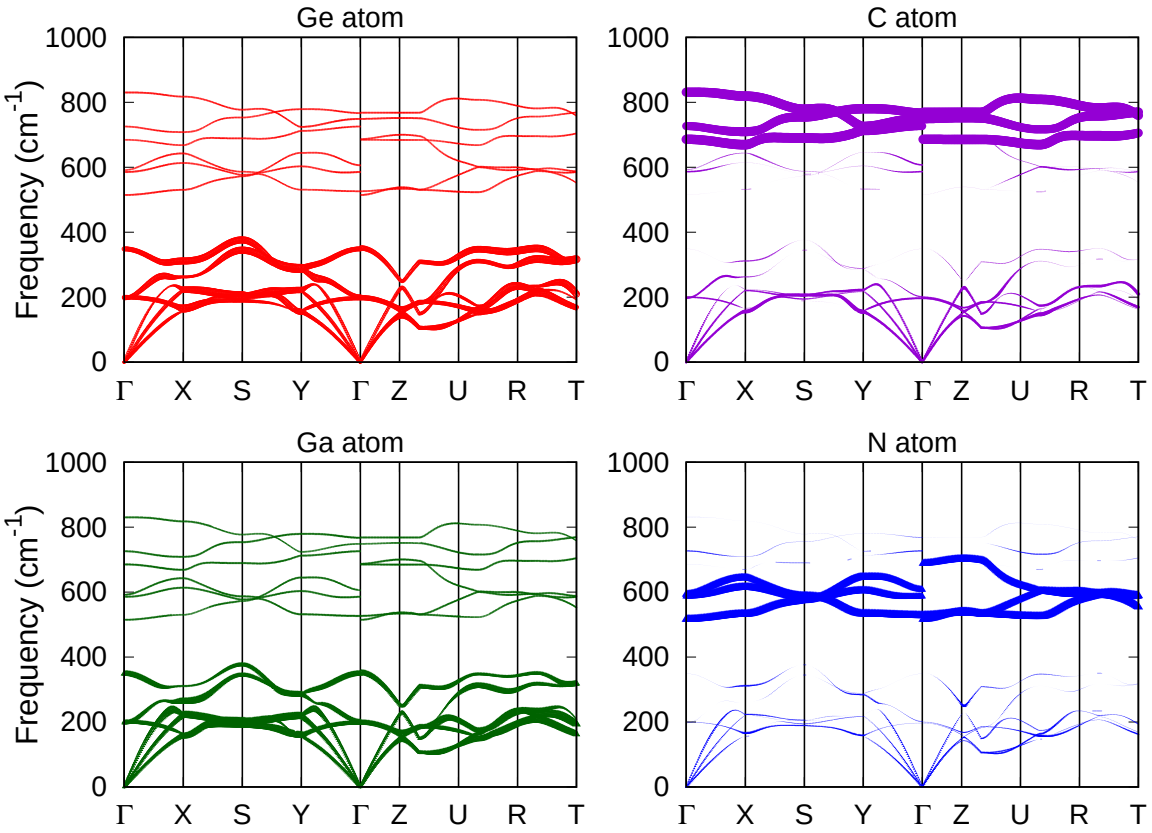

Fig. S5 (Color online) Atom-resolved projected phonon dispersions of S-3 crystal.

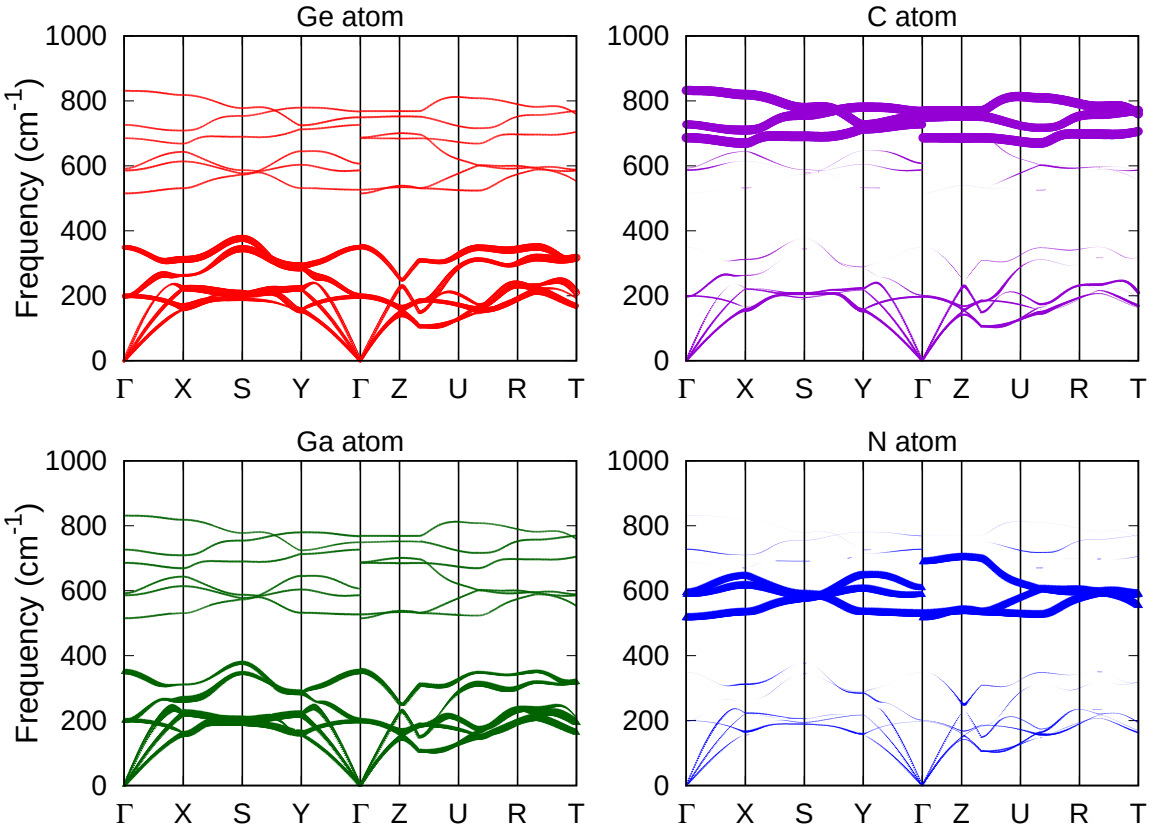

Fig. S6 (Color online) Atom-resolved projected phonon dispersions of S-4 crystal.

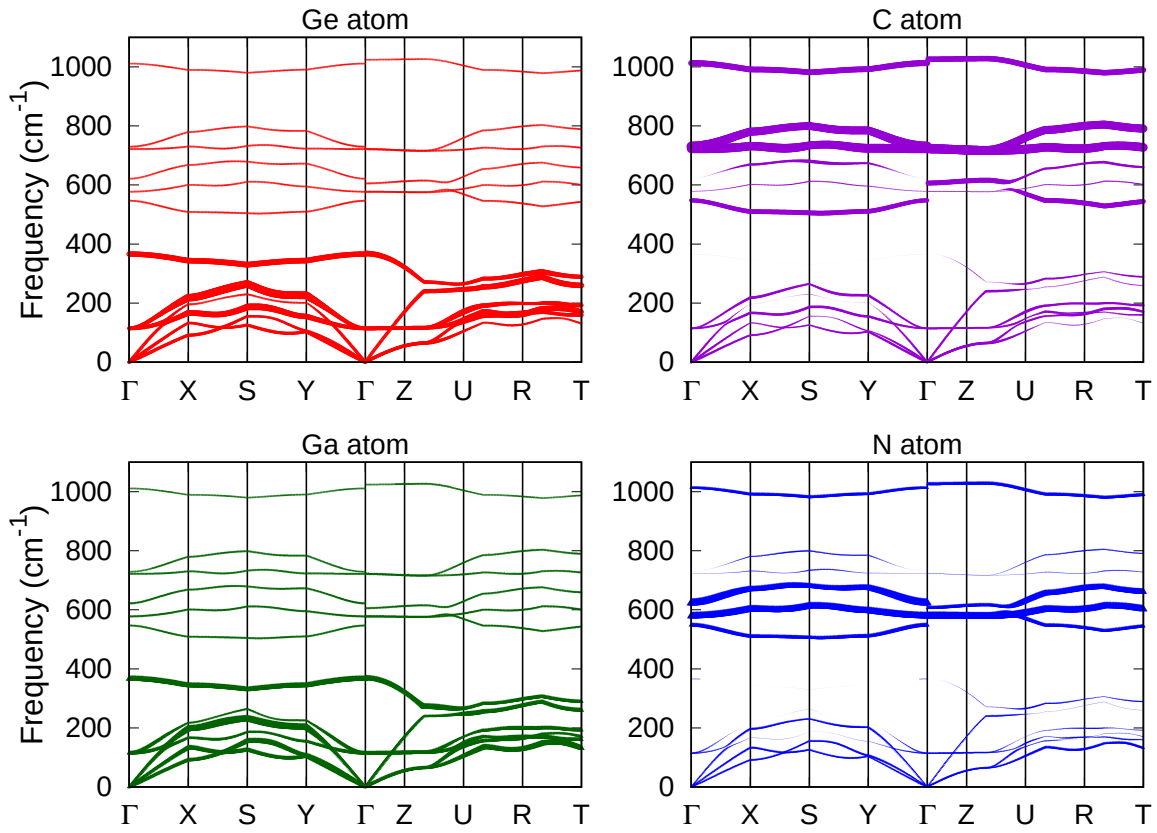

Fig. S7 (Color online) Atom-resolved projected phonon dispersions of S-5 crystal.

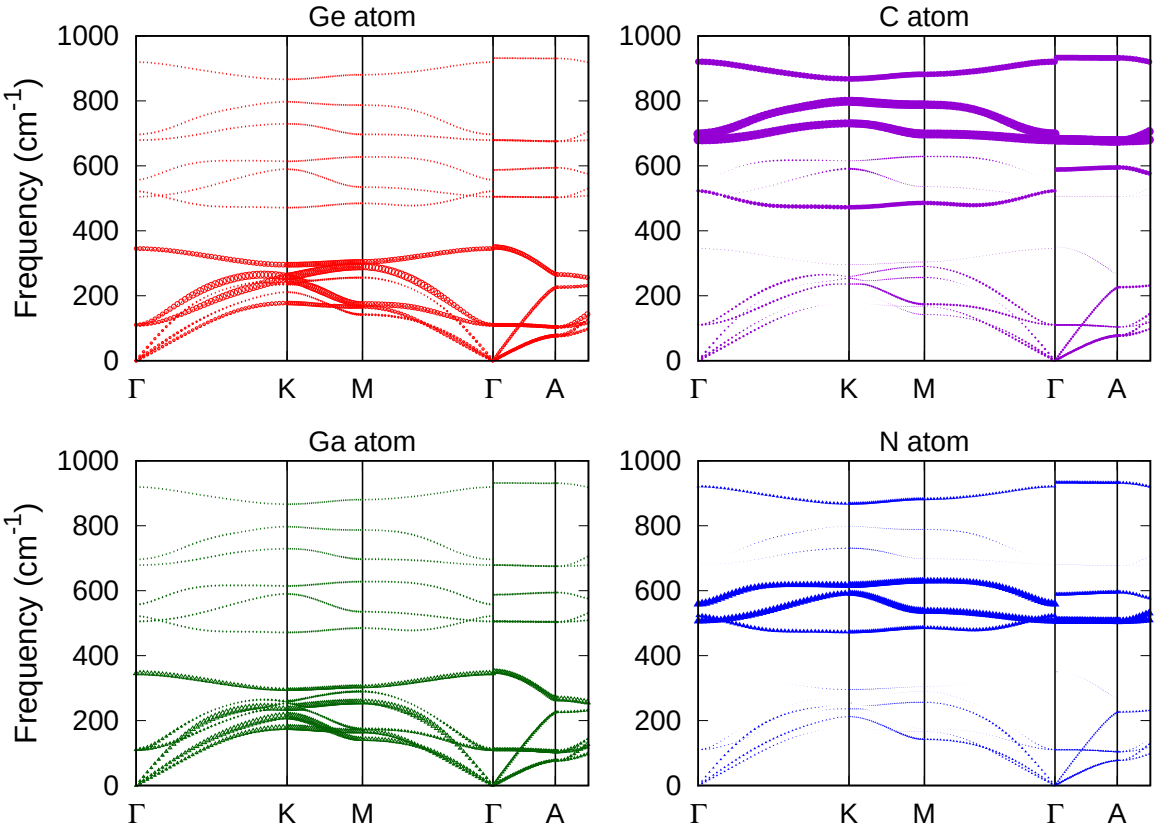

Fig. S8 (Color online) Atom-resolved projected phonon dispersions of S-6 crystal.

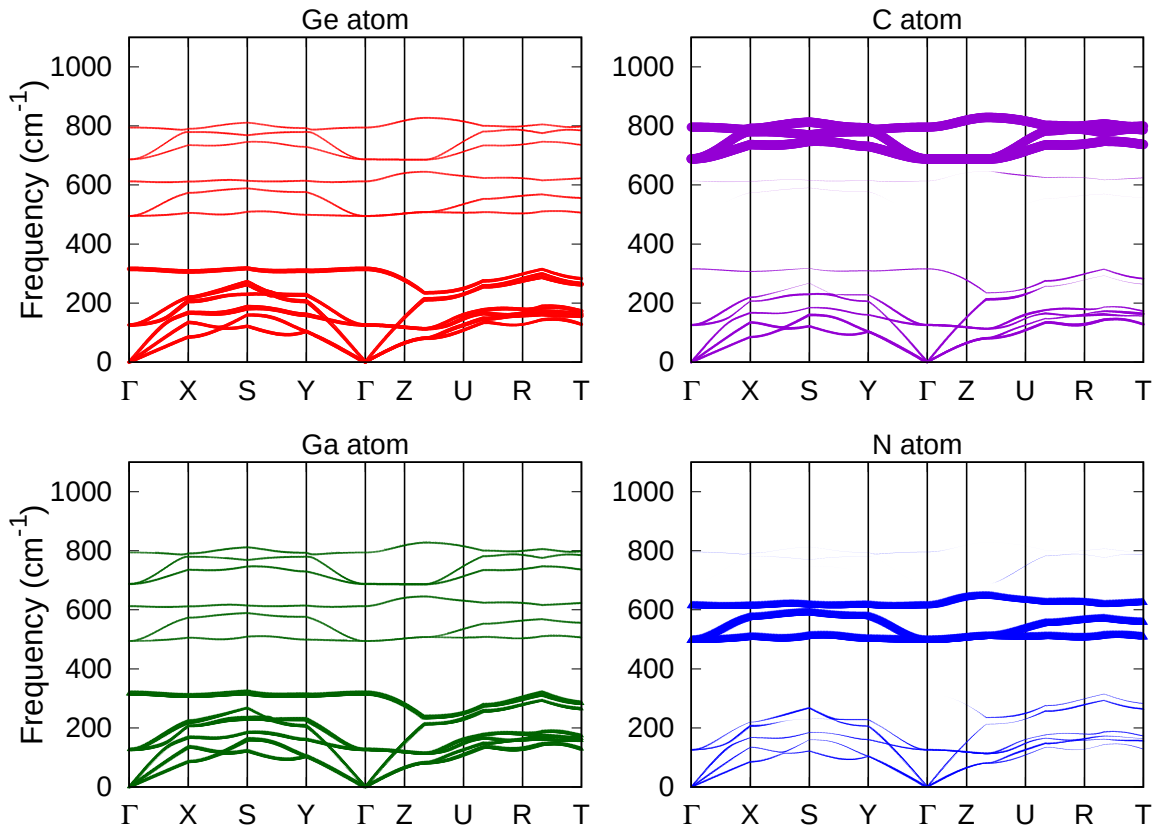

Fig. S9 (Color online) Atom-resolved projected phonon dispersions of S-7 crystal.

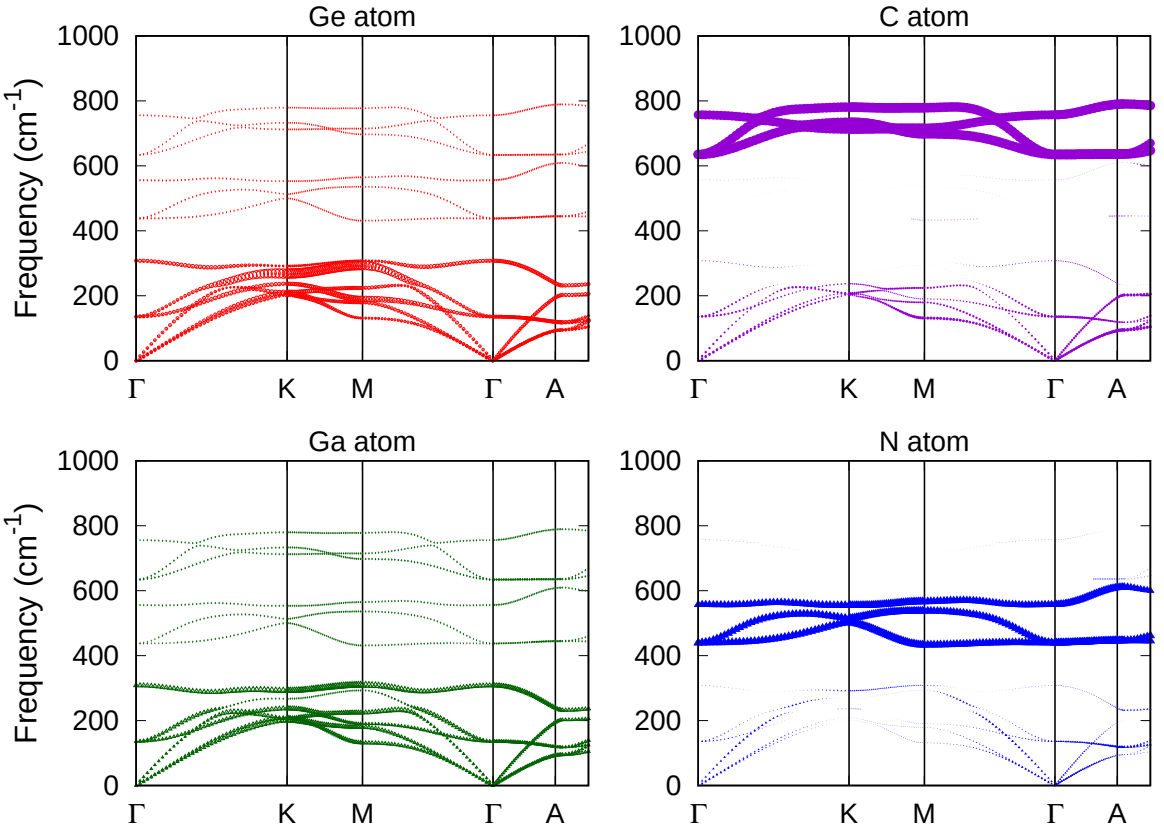

Fig. S10 (Color online) Atom-resolved projected phonon dispersions of S-8 crystal.

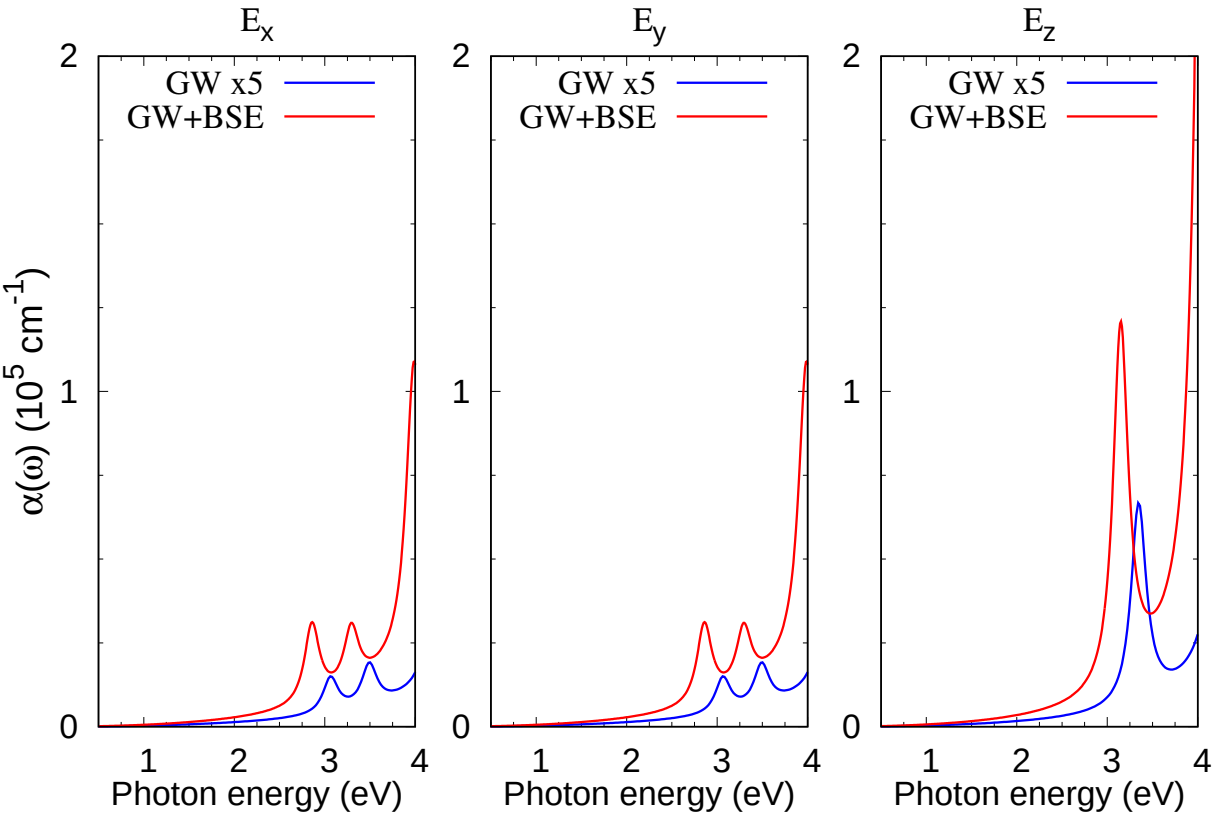

Fig. S11 (Color online) Optical absorption coefficient ($\alpha(\omega)$) of S-1 crystal, where ω is the photon energy and E_x, E_y and E_z indicate the direction of the polarized electric field.

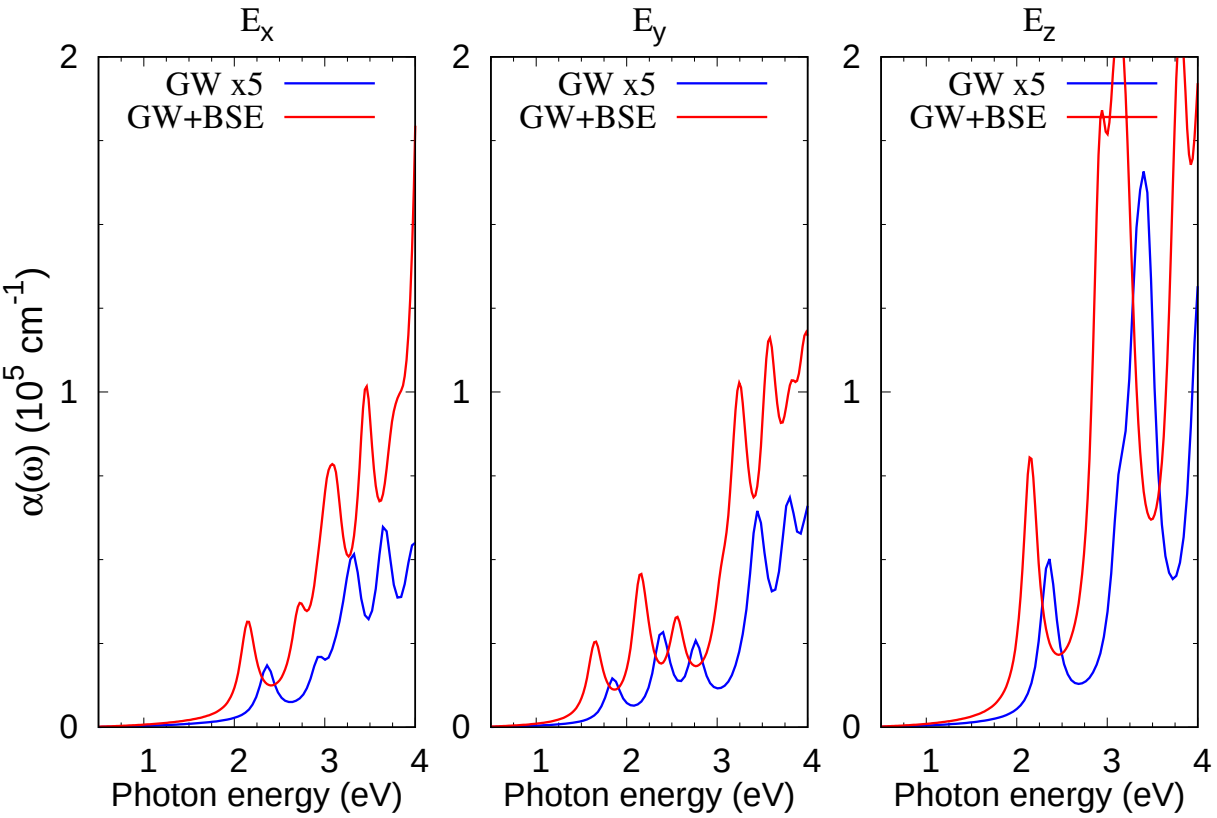

Fig. S12 (Color online) Optical absorption coefficient ($\alpha(\omega)$) of S-2 crystal, where ω is the photon energy and E_x, E_y and E_z indicate the direction of the polarized electric field.

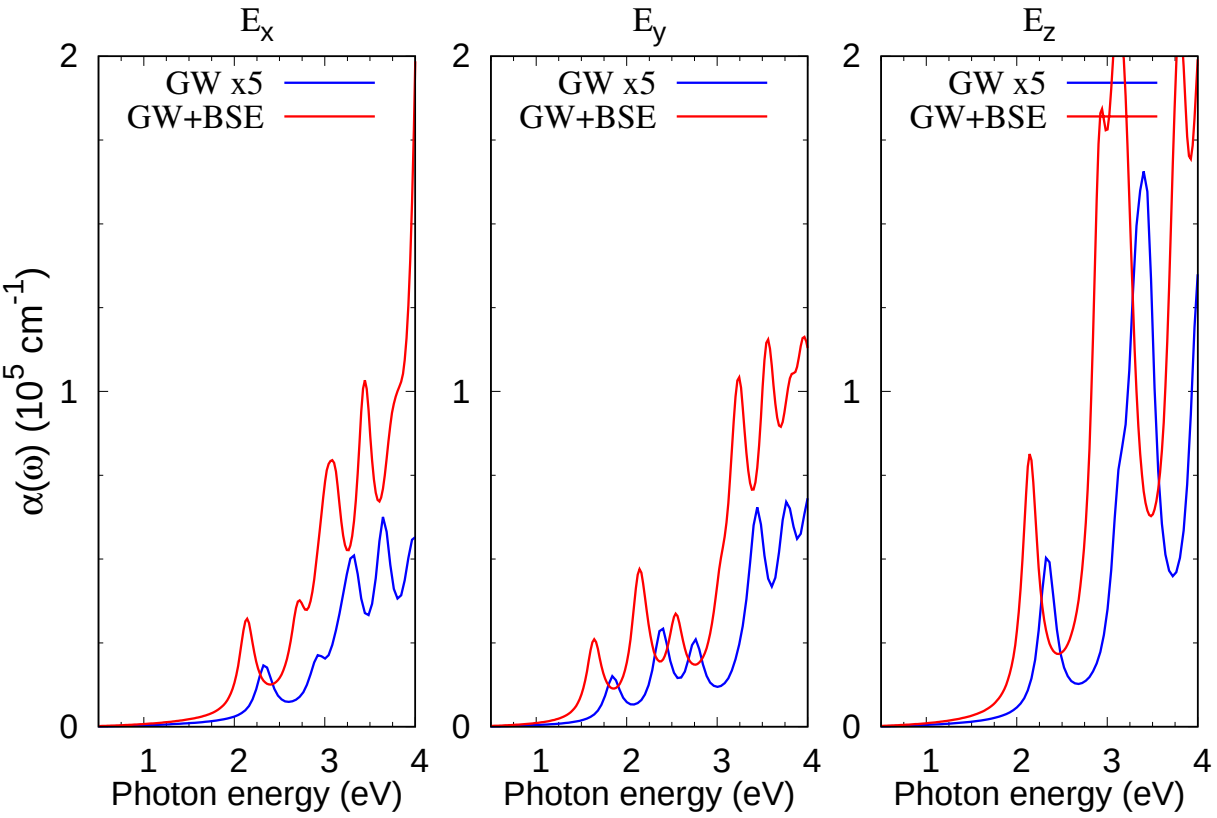

Fig. S13 (Color online) Optical absorption coefficient ($\alpha(\omega)$) of S-3 crystal, where ω is the photon energy and E_x, E_y and E_z indicate the direction of the polarized electric field.

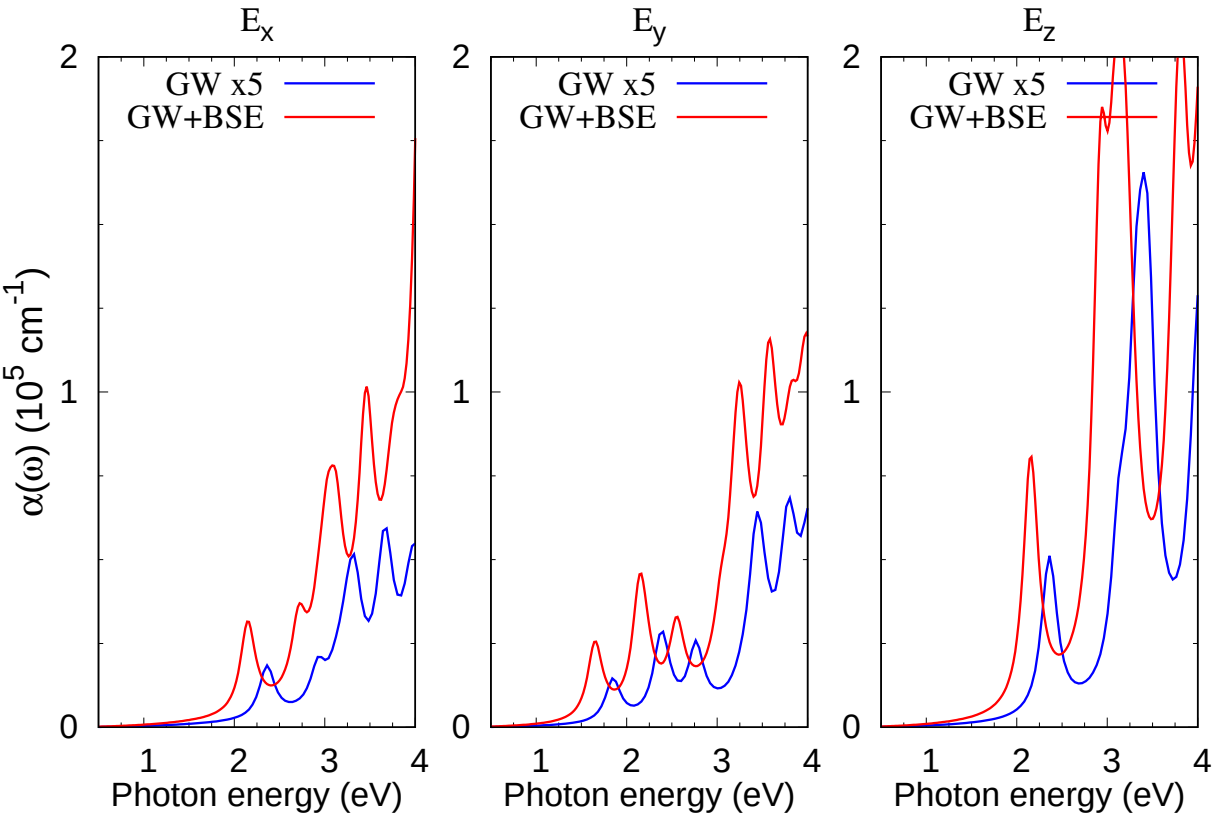

Fig. S14 (Color online) Optical absorption coefficient ($\alpha(\omega)$) of S-4 crystal, where ω is the photon energy and E_x, E_y and E_z indicate the direction of the polarized electric field.

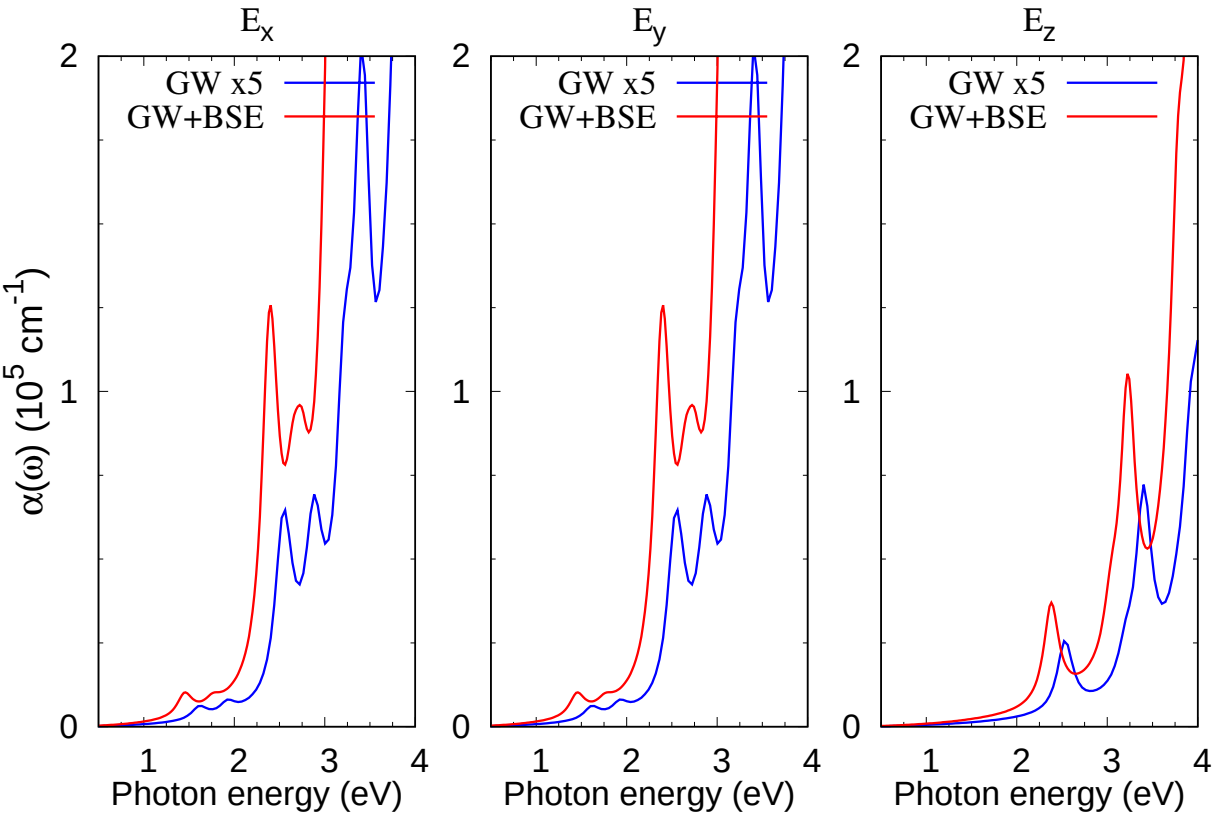

Fig. S15 (Color online) Optical absorption coefficient ($\alpha(\omega)$) of S-5 crystal, where ω is the photon energy and E_x, E_y and E_z indicate the direction of the polarized electric field.

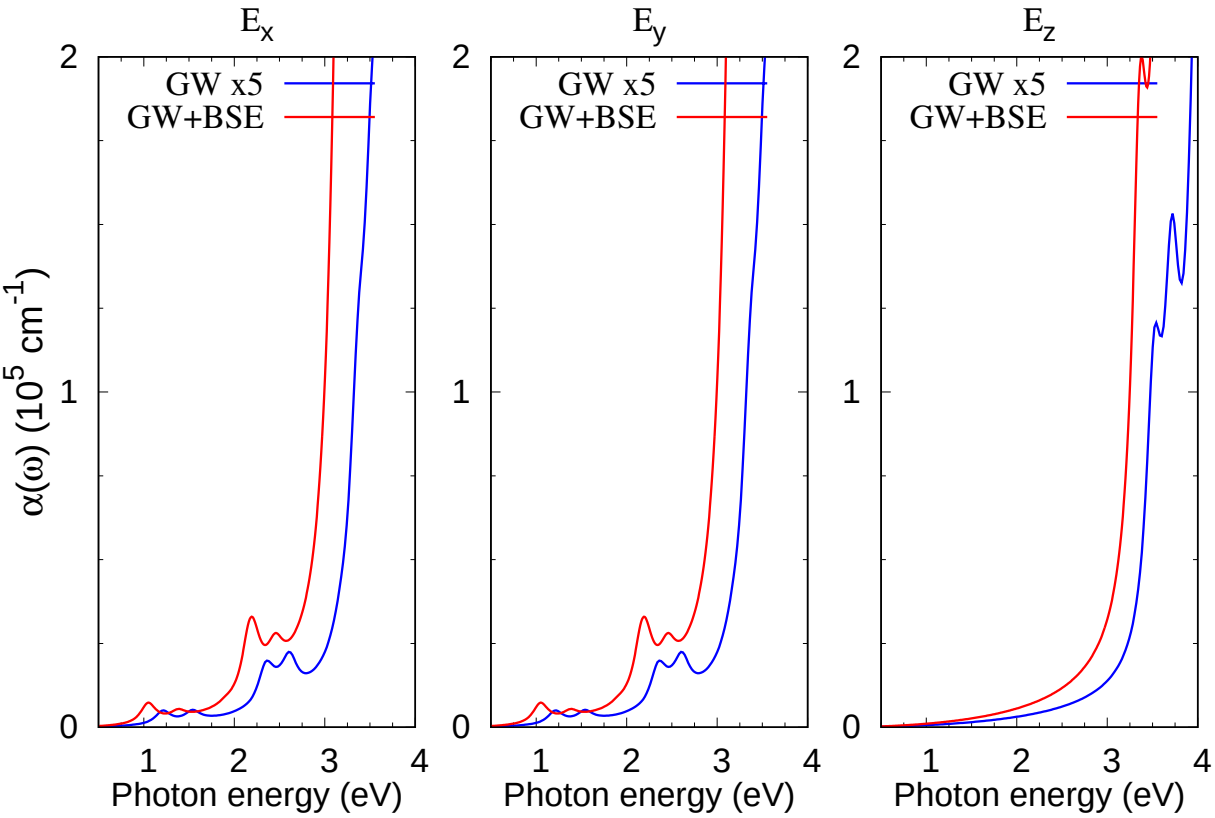

Fig. S16 (Color online) Optical absorption coefficient ($\alpha(\omega)$) of S-6 crystal, where ω is the photon energy and E_x, E_y and E_z indicate the direction of the polarized electric field.

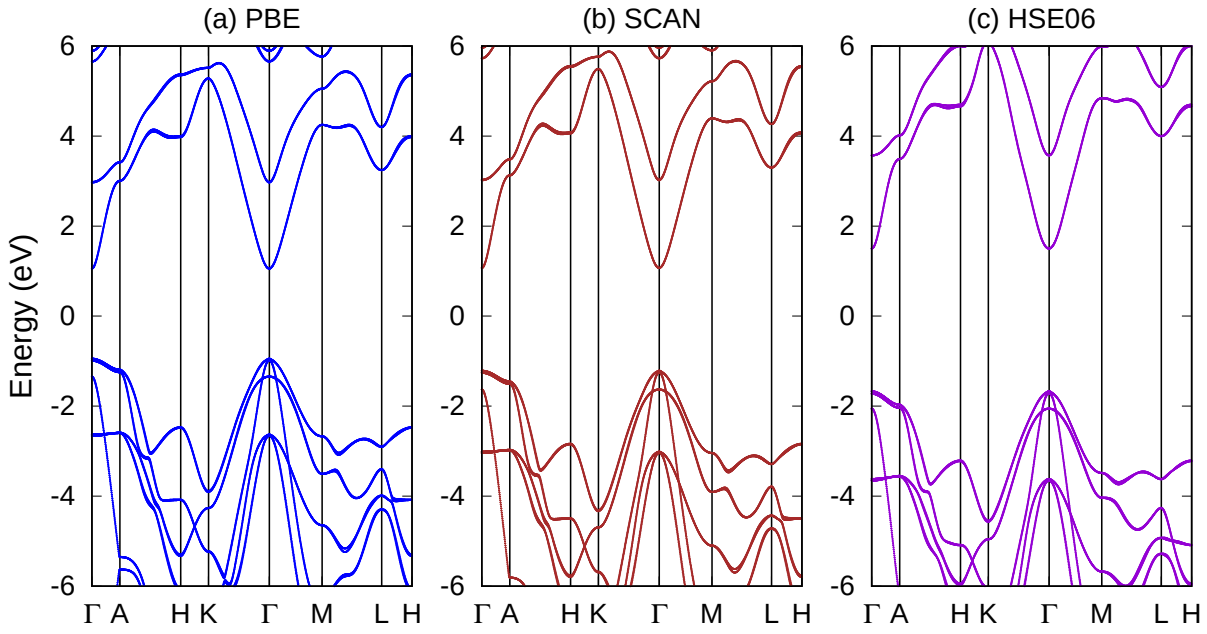

Fig. S17 (Color online) Band structure of the S-1 crystal. (a)-(c) show the results calculated by PBE, SCAN, and HSE06 functionals, respectively.

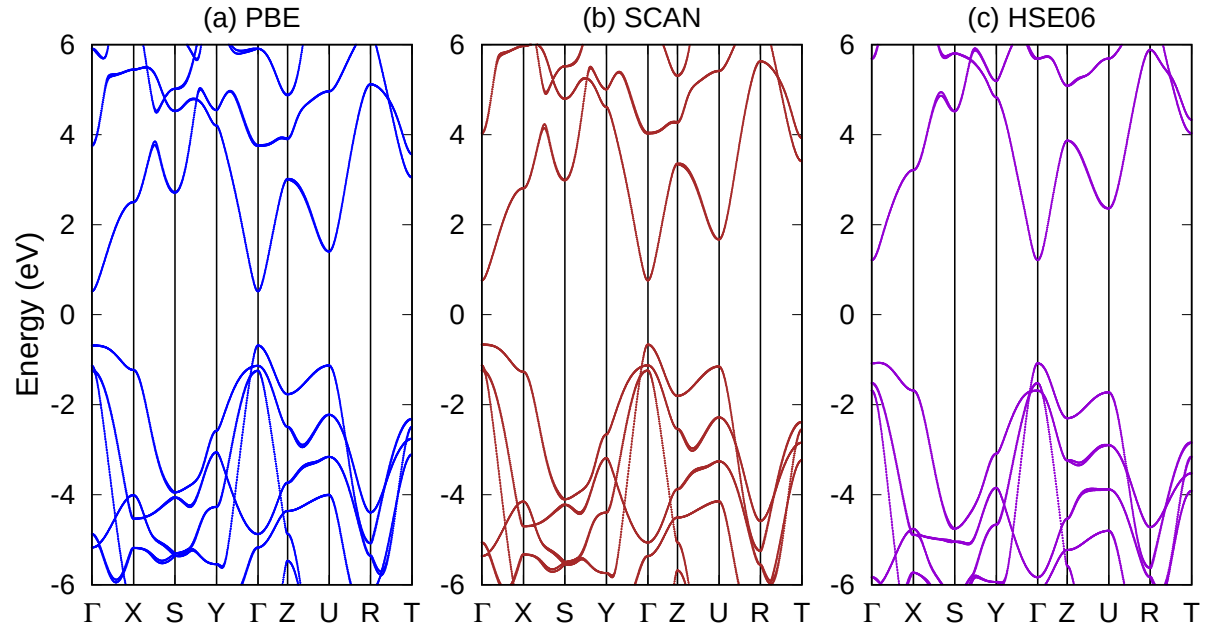

Fig. S18 (Color online) Band structure of the S-2 crystal. (a)-(c) show the results calculated by PBE, SCAN, and HSE06 functionals, respectively.

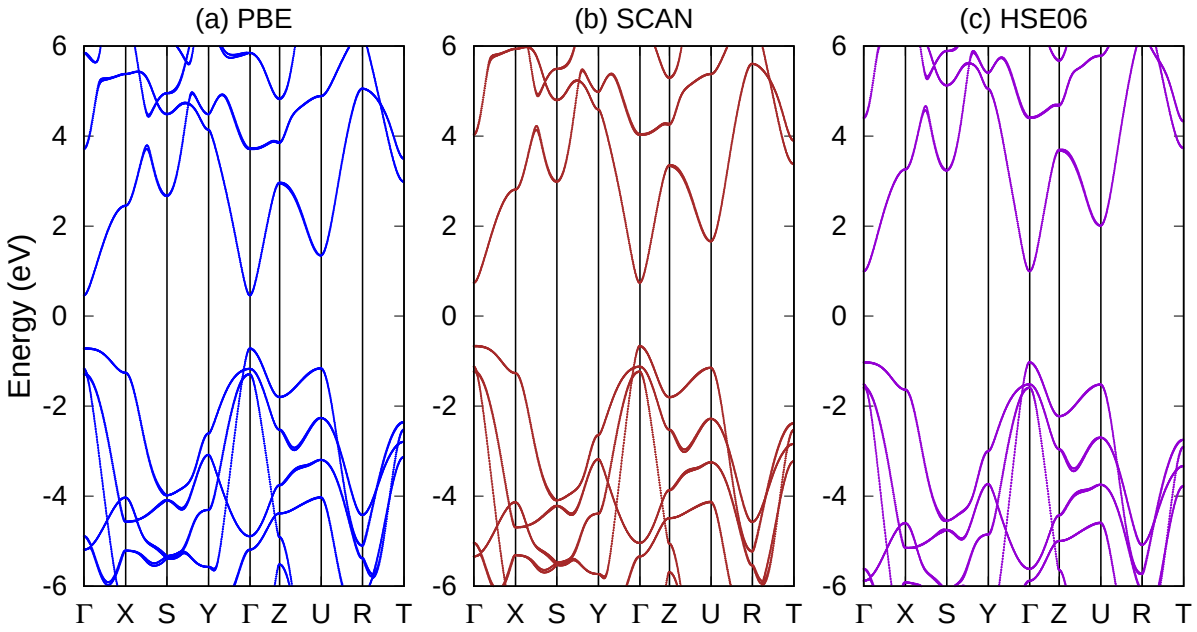

Fig. S19 (Color online) Band structure of the S-3 crystal. (a)-(c) show the results calculated by PBE, SCAN, and HSE06 functionals, respectively.

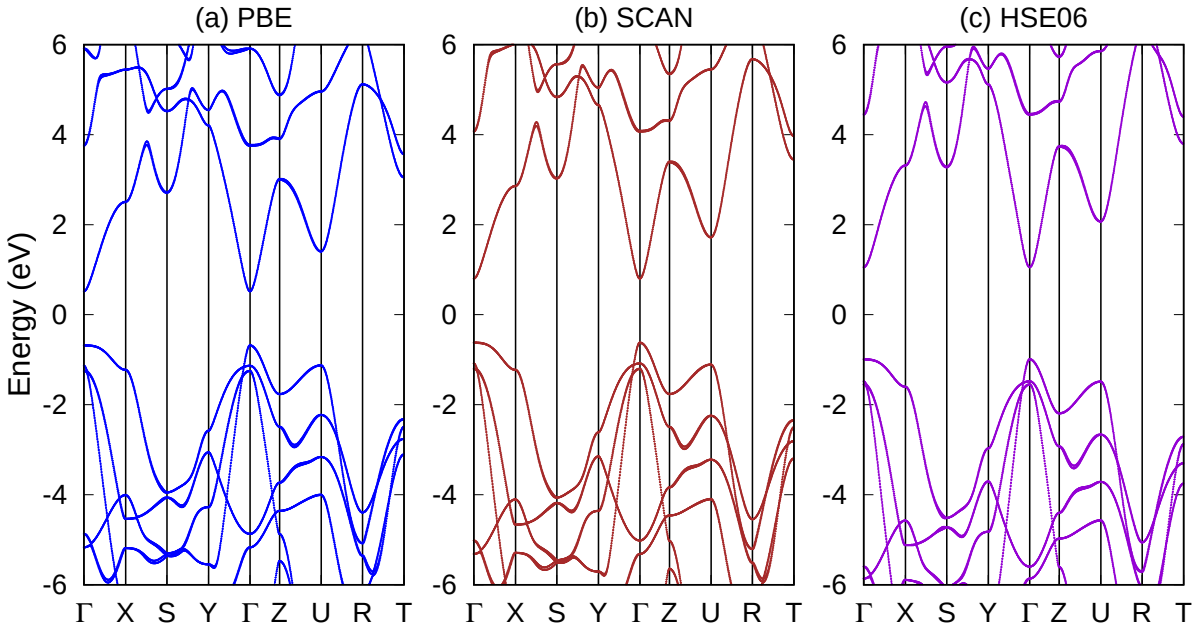

Fig. S20 (Color online) Band structure of the S-8 crystal. (a)-(c) show the results calculated by PBE, SCAN, and HSE06 functionals, respectively.

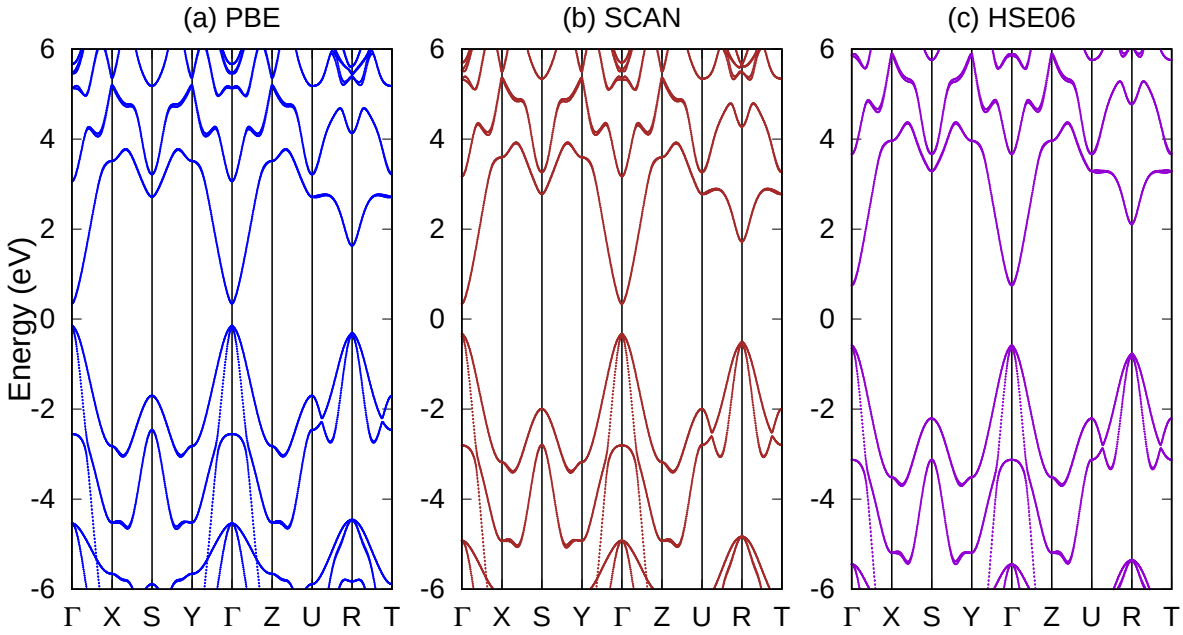

Fig. S21 (Color online) Band structure of the S-5 crystal. (a)-(c) show the results calculated by PBE, SCAN, and HSE06 functionals, respectively.

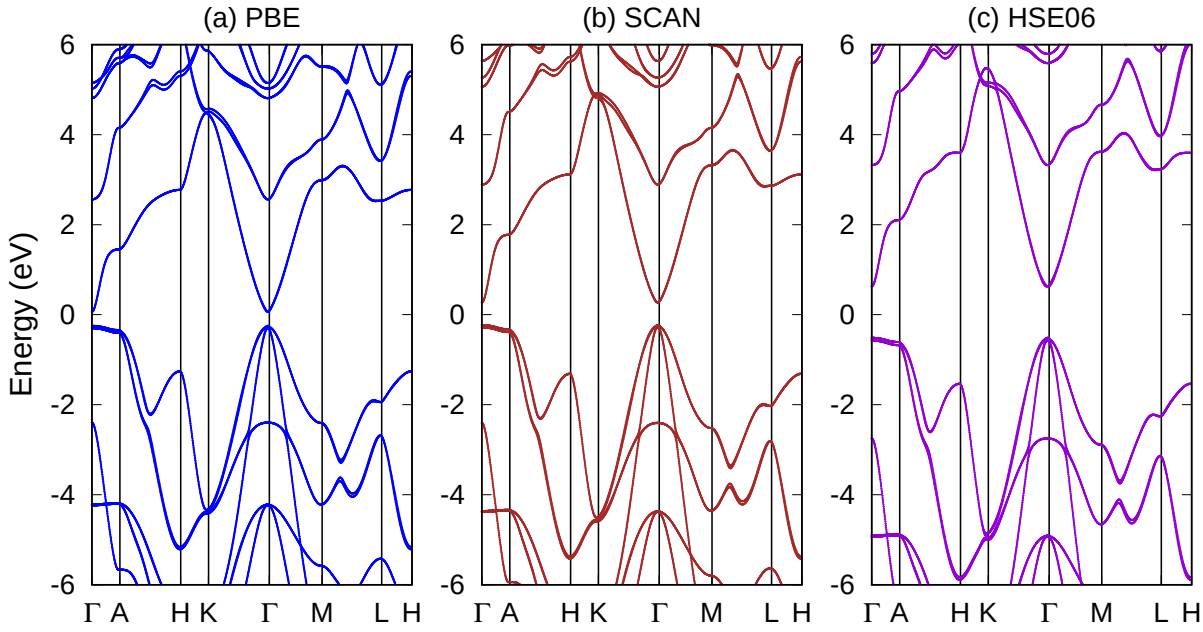

Fig. S22 (Color online) Band structure of the S-8 crystal. (a)-(c) show the results calculated by PBE, SCAN, and HSE06 functionals, respectively.

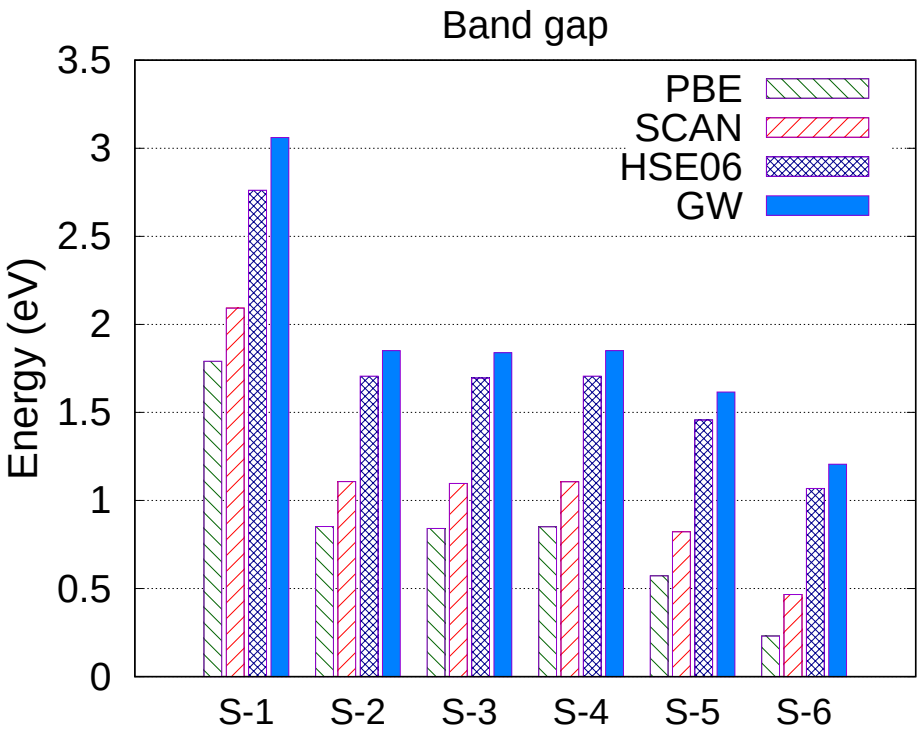

Fig. S23 (Color online) Band gaps calculated by PBE, SCAN, and HSE06 functionals, as well as GW, respectively.

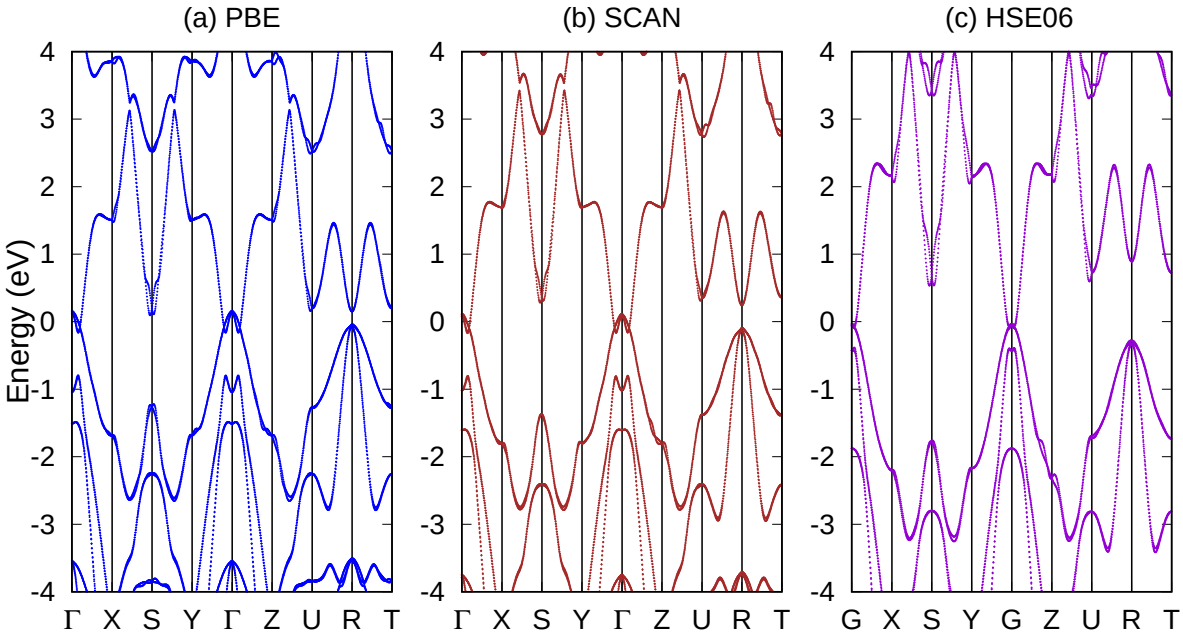

Fig. S24 (Color online) Band structure of the S-7 crystal. (a)-(c) show the results calculated by PBE, SCAN, and HSE06 functionals, respectively.

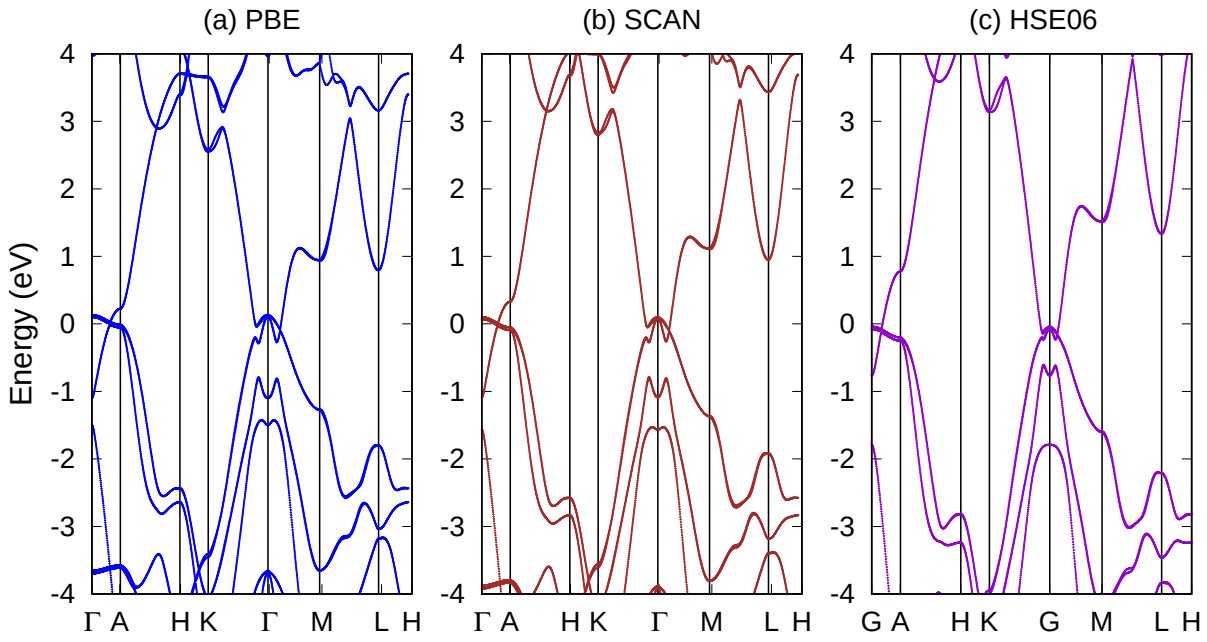

Fig. S25 (Color online) Band structure of the S-8 crystal. (a)-(c) show the results calculated by PBE, SCAN, and HSE06 functionals, respectively.