A comprehensive library of bulk chalcogenides: structural, electronic, optical and elastic properties using first-principles calculations

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1. Optical properties

We can use OLCAO method to calculate the optical properties of crystalline chalcogenides based on the theory of inter-band optical absorptions within the random phase approximation. According to this approach, the optical conductivity is given by:

$$\sigma_1(\hbar w) = \frac{2\Pi e\hbar^2}{3m^2\omega\Omega}\sum_{n,l}|\langle n|\vec{p}|l\rangle^2 f_l[1-f_n]\delta(E_n - E_l - \hbar\omega) \quad (1)$$

f_l is the Fermi-Dirac function of the occupied band state ι and δ function makes sure that the energy is conserved in the transition process between occupied state and unoccupied state with energy Eι and En respectively. Ω is the volume of the unit cell.

There is no intra-band transitions for the materials with an energy gap in their band structure, so that the optical properties can be described by the complex dielectric function which is related to the $\sigma_1(\hbar w)$ by:

$$\varepsilon_2(w) = 4\pi\frac{\sigma_1(w)}{w} \quad (2)$$

By transforming the summation over the unit cell in the equation (3) to an integral over the BZ in **k** space, $\varepsilon_2(w)$ can be given by:

$$\varepsilon_2(\hbar\omega) = \frac{e^2}{\pi m\omega^2}\int dk^3 \sum_{n,l}\left|\langle\Psi_n(\vec{k},\vec{r})\right|-i\hbar\vec{\nabla}\left|\Psi_l(\vec{k},\vec{r})\rangle\right|^2 f_l(\vec{k})[1 - f_n(\vec{k})]\delta(E_n(\vec{k}) - E_l(\vec{k}) - \hbar\omega) \quad (3)$$

The real part of the dielectric function can be derived from ε2 by using Kramers-Kronig relation:

$$\varepsilon_1(\hbar\omega) = 1 + \frac{2}{\pi}P\int_0^\infty \frac{s\varepsilon_2(\hbar\omega)}{s^2-\omega^2}\,ds \quad (4)$$

In OLCAO method, the momentum matrices in the Eqs (2) and (4) for the optical transitions can be easily calculated as sums of two –center integrals between GTOs[1].

2. Mechanical properties

Ab initio calculation method within DFT for the mechanical properties is very powerful method these days. In this section, and to calculate the mechanical properties for the seven crystals, we followed the method of the Hongzhi Yao. et al. work[2]. In this work, a scheme has been applied to calculate the elastic constants of crystals. Starting with the simple Hook's famous law that can relate the stress components σ_i with the strain components ε_j by relation:

$$\sigma_i = \sum_{j=1}^{6} C_{ij}\, \varepsilon_j \tag{5}$$

C_{ij} is the elastic constants of the crystals. From knowing the elastic constants, we could calculate other mechanical properties like compliance tensor S_{ij}, Young's modulus (E), Bulk modulus (K), Shear modulus (G), and Poisson's ratio (η). Here, Voigt – Reuss –Hill (VRH)[3, 4] approximation has been used to derive the above mechanical properties. According to this approximation, the upper and lower bounds for the structural parameters, like bulk and shear modulus are respectively given by:

$$K_V = \frac{(C_{11}+C_{22}+C_{33})}{9} + \frac{2(C_{12}+C_{13}+C_{23})}{9} \tag{6}$$

$$K_R = \frac{1}{(S_{11}+S_{22}+S_{33})+2(S_{12}+S_{13}+S_{23})} \tag{7}$$

$$G_V = \frac{(C_{11}+C_{22}+C_{33}-C_{12}-C_{13}-C_{23})}{15} + \frac{(C_{44}+C_{55}+C_{66})}{5} \tag{8}$$

$$G_R = \frac{15}{4(S_{11}+S_{22}+S_{33})-4(S_{12}+S_{13}+S_{23})+3(S_{44}+S_{55}+S_{66})} \tag{9}$$

So, the average values of the mechanical properties are given by:

$$K = \frac{(K_V+K_R)}{2} \tag{10}$$

$$G = \frac{(G_V+G_R)}{2} \tag{11}$$

$$E = \frac{9KG}{(3K+G)} \tag{12}$$

$$\eta = \frac{(3K-2G)}{2(3K+G)} \tag{13}$$

3. The Supplementary Tables

Table S1 The symmetry, lattice parameters after full VASP relaxation, and the experimental lattice parameters data of the 99 crystals used in our calculations, where GGA has been used as an exchange and correlation potential. (M for monoclinic, T for triclinic, Tr for Trigonal, Tet for tetragonal, O for orthorhombic. The full relaxed crystal structure data are available upon request with a corresponding author. They can also be found on the web site of our research group: **https://info.umkc.edu/ching-esg/?page_id=152**

#	Crystal	Space group	Lattice parameters(our calculations) a, b, c(Å) in 4 decimal points, α, β, γ(deg.) in 2 decimal points	Lattice parameters(experimental) a, b, c(Å) in 4 decimal points, α, β, γ(deg.) in 2 decimal points
1	Cu_2ZnSiS_4	O, $Pmn2_1$(31)	7.3849, 6.4683, 6.1669, 90.00, 90.00, 90.00	7.4374, 6.4001, 6.1394, 90.00, 90.00, 90.00[5]
2	$Cu_2ZnSiSe_4$	O, $Pmn2_1$(31)	7.8439, 6.8452, 6.5190, 90.00, 90.00, 90.00	7.8287, 6.7342, 6.4568, 90.00, 90.00, 90.00[6]
3	$Cu_2ZnSiTe_4$	Tet, I -4 2 m(121)	6.0501, 6.0501, 11.982, 90.00, 90.00, 90.00	5.9612, 5.9612, 11.7887, 90.00, 90.00, 90.00[7]
4	Cu_2ZnGeS_4	O, $Pmn2_1$(31)	7.5152, 6.5574, 6.2375, 90.00, 90.00, 90.00	7.5090, 6.4790, 6.1920, 90.00, 90.00, 90.00[8]
5	$Cu_2ZnGeSe_4$	Tet, I -4(82)	5.6726, 5.6726, 11.2758, 90.00, 90.00, 90.00	5.6112, 5.6112, 11.0473, 90.00, 90.00, 90.00[9]
6	Cu_2ZnSnS_4	Tet, I -4(82)	5.4704, 5.4704, 10.9424, 90.00, 90.00, 90.00	5.4280, 5.4280, 10.8640, 90.00, 90.00, 90.00[10]
7	$Cu_2ZnSnSe_4$	Tet, I -4(82)	5.7674, 5.7674, 11.5315, 90.00, 90.00, 90.00	5.6920, 5.6920, 11.3400, 90.00, 90.00, 90.00[11]
8	$Cu_2ZnSnTe_4$	Tet, I -4(82)	6.1880, 6.1880, 12.3655, 90.00, 90.00, 90.00	6.1300, 6.1300, 12.2071, 90.00, 90.00, 90.00[12]
9	Cu_2CdSiS_4	O, $Pmn2_1$(31)	7.6707, 6.5086, 6.2901, 90.00, 90.00, 90.00	7.5980, 6.4860, 6.2580, 90.00, 90.00, 90.00[13]
10	$Cu_2CdSiSe_4$	O, $Pmn2_1$(31)	8.1096, 6.8922, 6.6344, 90.00, 90.00, 90.00	7.9900, 6.8240, 6.2640, 90.00, 90.00, 90.00[14]
11	Cu_2CdGeS_4	O, $Pmn2_1$(31)	7.7804, 6.6253, 6.3608, 90.00, 90.00, 90.00	7.6920, 6.5550, 6.2990, 90.00, 90.00, 90.00[15]
12	$Cu_2CdGeSe_4$	Tet, I -4 2 m(121)	5.8449, 5.8449, 11.2495, 90.00, 90.00, 90.00	5.7482, 5.7482, 11.0533, 90.00, 90.00, 90.00[16]
13	$Cu_2CdGeTe_4$	Tet, I -4 2 m(121)	6.2531, 6.2531, 12.1218, 90.00, 90.00, 90.00	6.1270, 6.1270, 11.9190, 90.00, 90.00, 90.00[17]
14	Cu_2CdSnS_4	Tet, I -4(82)	5.5763, 5.5763, 11.2449, 90.00, 90.00, 90.00	5.4870, 5.4870, 10.8450, 90.00, 90.00, 90.00[18]
15	$Cu_2CdSnSe_4$	Tet, I -4(82)	5.8715, 5.8715, 11.8107, 90.00, 90.00, 90.00	5.8320, 5.8320, 11.3900, 90.00, 90.00, 90.00[18]
16	$Cu_2CdSnTe_4$	Tet, I -4(82)	6.2917, 6.2917, 12.5987, 90.00, 90.00, 90.00	6.1980, 6.1980, 12.2560, 90.00, 90.00, 90.00[18]
17	Cu_2HgGeS_4	Tet, I -4 2 m(121)	5.5658, 5.5658, 10.6581, 90.00, 90.00, 90.00	5.4930, 5.4930, 10.5510, 90.00, 90.00, 90.00[19]
18	$Cu_2HgGeSe_4$	Tet, I -4 2 m(121)	5.8695, 5.8695, 11.2322, 90.00, 90.00, 90.00	5.7445, 5.7445, 11.0824, 90.00, 90.00, 90.00[20]
19	$Cu_2HgGeTe_4$	Tet, I -4 2 m(121)	6.2629, 6.2629, 12.1144, 90.00, 90.00, 90.00	6.12940, 6.12940, 11.9374, 90.00, 90.00, 90.00[21]
20	Cu_2HgSnS_4	Tet, I -4(82)	5.6439, 5.6439, 11.0670, 90.00, 90.00, 90.00	5.5749, 5.5749, 10.8820, 90.00, 90.00, 90.00[22]
21	$Cu_2HgSnSe_4$	Tet, I -4 2 m(121)	5.9393, 5.9393, 11.6174, 90.00, 90.00, 90.00	5.8288, 5.8288, 11.4179, 90.00, 90.00, 90.00[23]
22	$Cu_2HgSnTe_4$	Tet, I -4 2 m(121)	6.3310, 6.3310, 12.4851, 90.00, 90.00, 90.00	6.1957, 6.1957, 12.2874, 90.00, 90.00, 90.00[24]
23	Cu_2BaGeS_4	Tr, P 3_1(144)	6.5328, 6.5328, 15.2783, 90.00, 90.00, 119.99	6.2150, 6.2150, 15.5340, 90.00, 90.00, 120.00[25]
24	$Cu_2BaGeSe_4$	Tr, P 3_1(144)	6.6141, 6.6141, 16.4332, 90.00, 90.00, 119.99	6.4900, 6.4900, 16.3550, 90.00, 90.00, 120.00[26]
25	Cu_2SrSiS_4	Tr, P 3_1(144)	6.1049, 6.1049, 15.1617, 90.00, 90.00, 120.00	6.0687, 6.0687, 15.1373, 90.00, 90.00, 120.00[27]
26	Cu_2SrGeS_4	Tr, P 3_2(145)	6.2025, 6.2025, 15.3469, 90.00, 90.00, 120.00	6.1430, 6.1430, 15.2820, 90.00, 90.00, 120.00[25]
27	$Cu_2SrGeSe_4$	O, Ama2(40)	10.9140, 10.8817, 6.6361, 90.00, 90.00, 90.00	10.8070, 10.7350, 6.5410, 90.00, 90.00, 90.00[26]
28	Cu_2BaSnS_4	Tr, P 3_1(144)	6.8386, 6.8386, 16.0392, 90.00, 90.00, 120.00	6.3660, 6.3660, 15.8280, 90.00, 90.00, 120.00[25]
29	$Cu_2BaSnSe_4$	O, Ama2(40)	11.2245, 11.4509, 6.8533, 90.00, 90.00, 90.00	11.1110, 11.2270, 6.7440, 90.00, 90.00, 90.00[25]
30	Cu_2SrSnS_4	Tr, P 3_1(144)	6.3616, 6.3616, 15.6245, 90.00, 90.00, 119.99	6.367, 6.367, 15.833, 90.00, 90.00, 120.00[28]
31	$Cu_2SrSnSe_4$	O, Ama2(40)	11.1162, 10.9248, 6.7886, 90.00, 90.00, 90.00	10.9670, 10.7540, 6.6950, 90.00, 90.00, 90.00[25]
32	Cu_2MgSiS_4	O, $Pmn2_1$(31)	7.5952, 6.4612, 6.2147, 90.00, 90.00, 90.00	7.5630, 6.4480, 6.1790, 90.00, 90.00, 90.00[29]
33	$Cu_2MgSiSe_4$	O, $Pmn2_1$(31)	8.0300, 6.8564, 6.5743, 90.00, 90.00, 90.00	7.9530, 6.7970, 6.5070, 90.00, 90.00, 90.00[30]
34	Cu_2MgGeS_4	O, $Pmn2_1$(31)	7.6930, 6.5724, 6.2865, 90.00, 90.00, 90.00	7.6380, 6.5150, 6.2250, 90.00, 90.00, 90.00[29]
35	Cu_2MgSnS_4	Tet, I -4(82)	5.5091, 5.5091, 11.1542, 90.00, 90.00, 90.00	5.4360, 5.4360, 11.0180, 90.00, 90.00, 90.00[31]
36	$Cu_2MgSnSe_4$	Tet, I -4(82)	5.8184, 5.8184, 11.7249, 90.00, 90.00, 90.00	5.7260, 5.7260, 11.5600, 90.00, 90.00, 90.00[32]
37	$Cu_2MgSnTe_4$	Tet, I -4(82)	6.2692, 6.2692, 12.5476, 90.00, 90.00, 90.00	6.1730, 6.1730, 12.3398, 90.00, 90.00, 90.00[32]
38	Ag_2ZnSiS_4	M, Pn(7)	6.6957, 7.7129, 8.1202, 90.00, 90.52, 90.00	6.4052, 6.5484, 7.9340, 90.00, 90.45, 90.00[33]
39	Ag_2ZnSnS_4	Tet, I -4(82)	5.8408, 5.8408, 11.0654, 90.00, 90.00, 90.00	5.8126, 5.8126, 10.7788, 90.00, 90.00, 90.00[34]
40	$Ag_2ZnSnSe_4$	Tet, I -4(82)	6.1106, 6.1106, 11.6683, 90.00, 90.00, 90.00	6.0442, 6.0442, 11.3065, 90.00, 90.00, 90.00[34]
41	Ag_2CdGeS_4	O, $Pna2_1$(33)	13.9844, 8.1157, 6.6928, 90.00, 90.00, 90.00	13.7415, 8.0367, 6.5907, 90.00, 90.00, 90.00[35]
42	Ag_2CdSnS_4	Tet, I -4(82)	5.9150, 5.9150, 11.5511, 90.00, 90.00, 90.00	5.9180, 5.9180, 11.5520, 90.00, 90.00, 90.00[36]
43	$Ag_2CdSnSe_4$	Tet, I -4(82)	6.1844, 6.1844, 12.1072, 90.00, 90.00, 90.00	6.1780, 6.1780, 12.1080, 90.00, 90.00, 90.00[37]
44	$Ag_2CdSnTe_4$	Tet, I -4(82)	6.5545, 6.5545, 12.9953, 90.00, 90.00, 90.00	6.5630, 6.5630, 12.9940, 90.00, 90.00, 90.00[37]
45	Ag_2HgSnS_4	O, $Pmn2_1$(31)	8.1896, 7.2620, 6.8447, 90.00, 90.00, 90.00	8.2074, 7.0330, 6.7180, 90.00, 90.00, 90.00[38]
46	$Ag_2HgSnSe_4$	O, $Pmn2_1$(31)	8.6148, 7.5571, 7.1617, 90.00, 90.00, 90.00	8.4610, 7.3400, 6.9901, 90.00, 90.00, 90.00[39]

47	Ag_2BaGeS_4	Tet, I -4 2 m(121)	6.8499, 6.8499, 8.3308, 90.00, 90.00, 90.00	6.8280, 6.8280, 8.0170, 90.00, 90.00, 90.00[25]
48	$Ag_2BaGeSe_4$	O, I 222(23)	7.0516, 7.5208, 8.4835, 90.00, 90.00, 90.00	7.0580, 7.2630, 8.2630, 90.00, 90.00, 90.00[25]
49	Ag_2BaSnS_4	O, I 222(23)	7.3760, 8.3261, 6.8488, 90.00, 90.00, 90.00	7.1270, 8.1170, 6.8540, 90.00, 90.00, 90.00[25]
50	$Ag_2BaSnSe_4$	O, I 222(23)	7.1503, 7.7114, 8.5929, 90.00, 90.00, 90.00	7.1160, 7.4990, 8.3370, 90.00, 90.00, 90.00[25]
51	Ag_2SrGeS_4	O, I 222(23)	7.0432, 7.7739, 6.8062, 90.00, 90.00, 90.00	6.8200, 6.9730, 7.6900, 90.00, 90.00, 90.00[25]
52	$Ag_2SrGeSe_4$	O, I 222(23)	7.1171, 7.4129, 8.0634, 90.00, 90.00, 90.00	7.1150, 7.3890, 7.9510, 90.00, 90.00, 90.00[25]
53	Ag_2SrSnS_4	O, I 222(23)	7.2909, 7.8802, 6.8971, 90.00, 90.00, 90.00	6.9100, 7.2100, 7.8310, 90.00, 90.00, 90.00[25]
54	$Ag_2SrSnSe_4$	O, I 222(23)	7.1924, 7.6542, 8.1501, 90.00, 90.00, 90.00	7.1930, 7.6570, 8.0340, 90.00, 90.00, 90.00[25]
55	$Ag_2In_2SiS_6$	M, C1c1(9)	12.4013, 7.2787, 12.3814, 90.00, 109.43, 90.00	12.1481, 7.1726, 12.1263, 90.00, 109.25, 90.00[40]
56	$Ag_2In_2GeS_6$	M, C1c1(9)	12.4988, 7.3491, 12.4713, 90.00, 109.50, 90.00	12.2316, 7.2190, 12.2124, 90.00, 109.50, 90.00[40]
57	$Ag_2In_2SiSe_6$	M, C1c1(9)	12.9619, 7.6205, 12.9006, 90.00, 109.39, 90.00	12.6683, 7.4565, 12.6133, 90.00, 109.29, 90.00[41]
58	$Ag_2In_2GeSe_6$	M, C1c1(9)	13.0354, 7.6909, 12.9695, 90.00, 109.47, 90.00	12.6920, 7.4920, 12.6440, 90.00, 109.50, 90.00[41]
59	Ag_2SiS_3	M, $P12_1$ /c1(14)	6.6871, 6.6825, 13.4925, 90.00, 118.21, 90.00	6.6709, 6.6567, 13.1748, 90.00, 118.66, 90.00[42]
60	Ag_2GeS_3	O, Cmc21(36)	11.9886, 7.0452, 6.5496, 90.00, 90.00, 90.00	11.7895, 7.0751, 6.3420, 90.00, 90.00, 90.00[43]
61	Cu_2GeS_3	M, C1c1(9)	6.5056, 11.3409, 6.5456, 90.00, 109.20, 90.00	6.4490, 11.3190, 6.4280, 90.00, 108.37, 90.00[44]
62	Cu_2GeSe_3	O, I mm2(44)	11.8886, 4.0560, 5.5967, 90.00, 90.00, 90.00	11.8540, 3.9540, 5.4890, 90.00, 90.00, 90.00[45]
63	Ag_2SnSe_3	M, P12 /m1(10)	8.3969, 9.2348, 12.9899, 90.00, 105.61, 90.00	7.9770, 7.9120, 13.0230, 90.00, 101.73, 90.00[46]
64	Ag_2SnTe_3	M, C1c1(9)	7.9259, 13.8274, 7.9704, 90.00, 109.03, 90.00	7.4420, 12.8377, 7.4025, 90.00, 109.54, 90.00[47]
65	$Ag_4P_2S_6$	O, $P2_12_12_1$(19)	14.3859, 11.2296, 6.3246, 90.00, 90.00, 90.00	13.9010, 11.0730, 6.3030, 90.00, 90.00, 90.00[48]
66	$Ag_4P_2Se_6$	M, C1c1(9)	14.6566, 11.7643, 6.6156, 90.00, 90.00, 90.00	14.1690, 11.5980, 6.5850, 90.00, 90.00, 90.00[49]
67	$BaZnSiSe_4$	O, Ama2(40)	11.5432, 11.4761, 6.2595, 90.00, 90.00, 90.00	11.3055, 11.2344, 6.1994, 90.00, 90.00, 90.00[50]
68	$BaZnGeSe_4$	O, Ama2(40)	11.5889, 11.5015, 6.3670, 90.00, 90.00, 90.00	11.3255, 11.2527, 6.2917, 90.00, 90.00, 90.00[50]
69	$BaHg_2As_2S_6$	O, Cmca(64)	8.3779, 8.4205, 16.5401, 90.00, 90.00, 90.00	8.1304, 7.9417, 16.3280, 90.00, 90.00, 90.00[51]
70	$BaCd_2As_2S_6$	O, Cmca(64)	8.1111, 8.1509, 17.1184, 90.00, 90.00, 90.00	7.9544, 7.8649, 16.9790, 90.00, 90.00, 90.00[51]
71	Ba_2AlSbS_5	O, Pnma(62)	12.3352, 8.9488, 9.1673, 90.00, 90.00, 90.00	12.1400, 8.8911, 8.9552, 90.00, 90.00, 90.00[52]
72	$Ba_2GaBiSe_5$	O, Pnma(62)	12.9159, 9.2489, 9.5312, 90.00, 90.00, 90.00	12.6910, 9.1900, 9.2450, 90.00, 90.00, 90.00[52]
73	$Ba_2AsGaSe_5$	O, Pnma(62)	12.9076, 9.1005, 9.4202, 90.00, 90.00, 90.00	12.6320, 8.9726, 9.2029, 90.00, 90.00, 90.00[53]
74	$Ba_2LaGaSe_5$	O, Pnma(62)	12.7079, 9.5926, 8.9275, 90.00, 90.00, 90.00	12.5049, 9.6288, 8.7355, 90.00, 90.00, 90.00[54]
75	$Ba_2LuGaSe_5$	T, P-1(2)	7.3981, 8.7027, 9.5441, 103.29, 102.87, 107.25	7.2829, 8.6120, 9.3681, 103.36, 103.05, 107.31[54]
76	$Ba_2LuInSe_5$	O, Cmc21(36)	4.2872, 19.1369, 13.4878, 90.00, 90.00, 90.00	4.2345, 18.7530, 13.2854, 90.00, 90.00, 90.00[54]
77	Ba_4AgInS_6	M, $P12_1$ /c1(14)	8.8287, 9.0183, 18.0285, 90.00, 104.12, 90.00	8.7241, 8.8799, 17.7930, 90.00, 104.14, 90.00[55]
78	$CsCu_5S_3$	O, Pmma(51)	9.6935, 3.9345, 9.1146, 90.00, 90.00, 90.00	9.6365, 3.9547, 8.9490, 90.00, 90.00, 90.00[56]
79	$CsCu_5Se_3$	O, Pmma(51)	10.1783, 4.0949, 9.1844, 90.00, 90.00, 90.00	9.9909, 4.0978, 9.0071, 90.00, 90.00, 90.00[56]
80	$K_2Cu_2GeS_4$	M, P 1 2 / c 1(13)	7.1652, 5.3974, 11.2903, 90.00, 113.07, 90.00	7.0630, 5.4350, 11.0370, 90.00, 112.83, 90.00[57]
81	$Li_2In_2SiS_6$	M, C1c1(9)	12.2913, 7.1458, 12.2786, 90.00, 110.12, 90.00	12.0727, 7.0213, 12.0788, 90.00, 110.06, 90.00[58]
82	$Li_2In_2SiSe_6$	M, C1c1(9)	12.8785, 7.5352, 12.8327, 90.00, 109.86, 90.00	12.6210, 7.3788, 12.5800, 90.00, 109.70, 90.00[58]
83	$Li_2In_2GeS_6$	M, C1c1(9)	12.4239, 7.2505, 12.3802, 90.00, 110.10, 90.00	12.1650, 7.0840, 12.1310, 90.00, 110.26, 90.00[58]
84	$Li_2In_2GeSe_6$	M, C1c1(9)	12.9920, 7.6221, 12.9263, 90.00, 109.92, 90.00	12.7226, 7.4527, 12.6698, 90.00, 109.83, 90.00[58]
85	Lu_5GaS_9	T, P-1(2)	7.7911, 10.1081, 10.2244, 106.30, 100.29, 101.89	7.7350, 10.0330, 10.1200, 106.29, 100.18, 101.95[59]
86	$SrCdGeS_4$	O, Ama2(40)	10.5509, 10.4132, 6.5080, 90.00, 90.00, 90.00	10.3352, 10.2335, 6.4408, 90.00, 90.00, 90.00[60]
87	$SrCdGeSe_4$	O, Ama2(40)	11.0751, 10.9174, 6.7548, 90.00, 90.00, 90.00	10.8245, 10.6912, 6.6792, 90.00, 90.00, 90.00[60]
88	$TlInGe_2S_6$	Tr, P3(143)	10.1605, 10.1605, 9.2651, 90.00, 90.00, 120.00	9.7710, 9.7710, 8.9195, 90.00, 90.00, 120.00[61]
89	$TlInGe_2Se_6$	Tr, P3(143)	10.6304, 10.6304, 9.6646, 90.00, 90.00, 120.00	10.1798, 10.1798, 9.2872, 90.00, 90.00, 120.00[62]
90	$TlGaSn_2Se_6$	Tr, R 3(146)	10.6768, 10.6768, 9.7721, 90.00, 90.00, 119.99	10.3289, 10.3289, 9.4340, 90.00, 90.00, 120.00[63]
91	Tl_2PbZrS_4	M, C12 /c1(15)	15.5773, 8.2886, 6.8722, 90.00, 108.79, 90.00	15.4550, 8.2140, 6.7510, 90.00, 109.09, 90.00[64]
92	$Tl_2PbZrSe_4$	M, C12 /c1(15)	16.0778, 8.5776, 7.1514, 90.00, 108.75, 90.00	15.9060, 8.4720, 7.0160, 90.00, 109.01, 90.00[64]
93	Tl_2PbHfS_4	M, C12 /c1(15)	15.6171, 8.2820, 6.8136, 90.00, 108.90, 90.00	15.4700, 8.2260, 6.7103, 90.00, 109.26, 90.00[64]
94	$Tl_2PbHfSe_4$	M, C12 /c1(15)	16.1215, 8.5728, 7.0959, 90.00, 108.89, 90.00	15.9480, 8.4720, 6.9733, 90.00, 109.12, 90.00[64]
95	$Tl_2CdGeSe_4$	Tet, I -4 2 m(121)	8.1791, 8.1791, 6.8532, 90.00, 90.00, 90.00	8.0145, 8.0145, 6.7234, 90.00, 90.00, 90.00[65]
96	$Tl_2CdSnSe_4$	Tet, I -4 2 m(121)	8.2291, 8.2291, 6.9925, 90.00, 90.00, 90.00	8.0490, 8.0490, 6.8573, 90.00, 90.00, 90.00[65]
97	$Tl_2HgGeSe_4$	Tet, I -4 2 m(121)	8.1699, 8.1699, 6.9259, 90.00, 90.00, 90.00	7.9947, 7.9947, 6.7617, 90.00, 90.00, 90.00[66]
98	$Tl_2HgSiSe_4$	Tet, I -4 2 m(121)	8.1599, 8.1599, 6.8546, 90.00, 90.00, 90.00	8.0032, 8.0032, 6.6879, 90.00, 90.00, 90.00[67]
99	Tl_2HgSnS_4	Tet, I -4 2 m(121)	7.9589, 7.9589, 6.8578, 90.00, 90.00, 90.00	7.8571, 7.85716.6989, 90.00, 90.00, 90.00[68]

Table S2 The results for the energy gap (E_g). The third column is our results, while the fourth column is the other's results. (T) is for calculations and (E) for experimental results. (D) Stands for direct band gap, while (ID) stands for indirect band gap. The reference **74** represents the result from "materials project" website: https://materialsproject.org/ .

#	Crystal	E_g(eV), our calculations	E_g(eV), other experimental and calculated data
1	Cu_2ZnSiS_4	1.380(D)	1.370(D-T)[69]
2	$Cu_2ZnSiSe_4$	0.653(D)	0.560(D-T)[69]
3	$Cu_2ZnSiTe_4$	0.483(ID)	0.150(T)[70]
4	Cu_2ZnGeS_4	0.518(D)	0.500(T)[71]
5	$Cu_2ZnGeSe_4$	0.125(D)	0.060(T)[72], 0.640(T)[73]
6	Cu_2ZnSnS_4	0.390(D)	0.030(T)[74]
7	$Cu_2ZnSnSe_4$	0.136(D)	0.820(T)[75]
8	$Cu_2ZnSnTe_4$	0.324(ID)	0.960(T)[12]
9	Cu_2CdSiS_4	1.233(D)	0.980(T)[76]
10	**$Cu_2CdSiSe_4$**	0.710(D)	**—***
11	Cu_2CdGeS_4	0.541(D)	0.640[77]
12	$Cu_2CdGeSe_4$	0.120(D)	0.020(T)[16]
13	$Cu_2CdGeTe_4$	0.163(ID)	0.000(T)[76]
14	Cu_2CdSnS_4	0.300(D)	0.000(T)[78]
15	$Cu_2CdSnSe_4$	0.120(D)	0.800(T)[79]
16	**$Cu_2CdSnTe_4$**	0.267(ID)	**—***
17	Cu_2HgGeS_4	0.400(D)	0.307(T)[19]
18	$Cu_2HgGeSe_4$	0.005(D)	0.006(T)[20]
19	$Cu_2HgGeTe_4$	0.151(ID)	0.380(T)[80]
20	Cu_2HgSnS_4	0.103(D)	0.191(T)[22]
21	$Cu_2HgSnSe_4$	0.000	0.127(T)[23], 0.0(T)[81]
22	$Cu_2HgSnTe_4$	0.432(D)	0.390(T)[80]
23	Cu_2BaGeS_4	0.778(D)	1.800(D-T)[82]
24	$Cu_2BaGeSe_4$	0.654(D)	1.000(D-T)[82]
25	Cu_2SrSiS_4	2.200(D)	3.30(ID-E)[27], 3.04(E)[83], 2.32(T)[83]
26	Cu_2SrGeS_4	1.184(D)	1.050(T)[76]
27	$Cu_2SrGeSe_4$	0.880(ID)	0.592(T)[76]
28	Cu_2BaSnS_4	0.632(D)	1.460(T)[25]
29	$Cu_2BaSnSe_4$	0.930(D)	1.500(D-T)[25]
30	Cu_2SrSnS_4	1.03(D)	0.46(T)[28], 0.38(T)[84], 1.62(T)[84]
31	$Cu_2SrSnSe_4$	0.785(D)	1.460(D-E)[25]
32	Cu_2MgSiS_4	1.689(D)	2.010(T)[30]
33	$Cu_2MgSiSe_4$	1.047(D)	1.017(T)[30]
34	Cu_2MgGeS_4	0.855(D)	1.249(T)[30]
35	Cu_2MgSnS_4	0.626(D)	0.781(T)[31], 0.35(T)[85]
36	$Cu_2MgSnSe_4$	0.381(D)	0.000-0.580(T)[85]
37	**$Cu_2MgSnTe_4$**	0.389(ID)	**—***
38	Ag_2ZnSiS_4	0.463(D)	1.800(D-T)[33]
39	Ag_2ZnSnS_4	0.750(D)	1.150(D-T)[86]
40	$Ag_2ZnSnSe_4$	0.500(D)	0.940(D-T)[87]
41	Ag_2CdGeS_4	0.998(D)	1.060(T)[88]
42	Ag_2CdSnS_4	0.801(D)	0.974(T)[36]
43	$Ag_2CdSnSe_4$	0.600(D)	0.577(T)[37]
44	$Ag_2CdSnTe_4$	0.680(D)	0.586(T)[37]
45	Ag_2HgSnS_4	0.528(D)	0.170(T)[89]
46	$Ag_2HgSnSe_4$	0.310(D)	0.484(T)[39], 0.23(T)[89]
47	Ag_2BaGeS_4	1.100(D)	1.380(T)[25]
48	$Ag_2BaGeSe_4$	0.700(D)	0.850(T)[25]
49	Ag_2BaSnS_4	1.010(D)	1.260(T)[25]
50	$Ag_2BaSnSe_4$	0.810(D)	0.770(T)[25]

51	Ag_2SrGeS_4	0.630(D)	1.330(T)[25]
52	$Ag_2SrGeSe_4$	0.310(D)	0.680(T)[25]
53	Ag_2SrSnS_4	0.550(D)	1.080(T)[25]
54	$Ag_2SrSnSe_4$	0.410(D)	0.660(T)[25]
55	$Ag_2In_2SiS_6$	1.404(D)	1.570(T)[40]
56	$Ag_2In_2GeS_6$	1.333(D)	1.880(T)[40]
57	$Ag_2In_2SiSe_6$	1.403(D)	0.472(T)[76]
58	$Ag_2In_2GeSe_6$	1.040(D)	0.432 (T)[76]
59	Ag_2SiS_3	1.600(ID)	1.420(T)[42]
60	Ag_2GeS_3	0.663(ID)	0.469(T)[76]
61	Cu_2GeS_3	0.025(ID)	0.110(T)[76]
62	Cu_2GeSe_3	0.000	0.000(T)[90]
63	Ag_2SnSe_3	0.906(ID)	0.059(T)[76]
64	**Ag_2SnTe_3**	0.390(D)	**—***
65	$Ag_4P_2S_6$	1.620(D)	1.437(T)[76]
66	**$Ag_4P_2Se_6$**	1.200(D)	**—***
67	$BaZnSiSe_4$	2.494(D)	2.710(T)[50]
68	$BaZnGeSe_4$	1.708(D)	2.460(T)[50]
69	**$BaHg_2As_2S_6$**	1.541(D)	**—***
70	$BaCd_2As_2S_6$	1.377(D)	1.770(D-T)
71	Ba_2AlSbS_5	2.069(D)	2.400(ID-T)[52]
72	$Ba_2GaBiSe_5$	1.475(D)	1.890(ID-T)[52]
73	$Ba_2AsGaSe_5$	2.031(D)	1.862(T)[76]
74	**$Ba_2LaGaSe_5$**	1.799(ID)	**—***
75	**$Ba_2LuGaSe_5$**	1.375(ID)	**—***
76	**$Ba_2LuInSe_5$**	1.244(D)	**—***
77	Ba_4AgInS_6	1.956(D)	1.686(T)[76]
78	$CsCu_5S_3$	0.390(D)	0.325(T)[76]
79	$CsCu_5Se_3$	0.235(D)	1.010(T)[56]
80	$K_2Cu_2GeS_4$	1.150(ID)	1.457[91]
81	$Li_2In_2SiS_6$	2.062(D)	3.240[58], 2.116(T)[76]
82	$Li_2In_2SiSe_6$	1.600(D)	2.350[58], 1.497(T)[76]
83	$Li_2In_2GeS_6$	1.949(D)	2.990[58], 2.033 (T)[76]
84	$Li_2In_2GeSe_6$	1.146(D)	1.920[58], 1.199 (T)[76]
85	Lu_5GaS_9	1.759(D)	1.890(ID-T)[59]
86	$SrCdGeS_4$	2.423(D)	2.600(E)[60]
87	$SrCdGeSe_4$	1.777(D)	1.900(E)[60]
88	$TlInGe_2S_6$	1.526(D)	2.001(T)[61]
89	$TlInGe_2Se_6$	1.130(D)	1.299(T)[62]
90	$TlGaSn_2Se_6$	1.100(D)	1.143(T)[63]
91	Tl_2PbZrS_4	0.590(D)	0.983(ID-T)[92], 1.240(T)[76]
92	$Tl_2PbZrSe_4$	0.470(D)	0.529(ID-T)[92], 1.0190 (T)[76]
93	Tl_2PbHfS_4	0.580(D)	0.911(ID-T)[92]
94	$Tl_2PbHfSe_4$	0.690(D)	0.659(ID-T)[92], 0.962 (T)[76]
95	**$Tl_2CdGeSe_4$**	0.000	**—***
96	**$Tl_2CdSnSe_4$**	0.000	**—***
97	**$Tl_2HgGeSe_4$**	0.000	**—***
98	$Tl_2HgSiSe_4$	0.000	0.959(T)[76]
99	**Tl_2HgSnS_4**	0.000	**—***

Table S3 Our results for the 99 crystals: the average effective charge on each atoms (Q*), total bond order density (TBOD), and the plasma frequency (ω_p). All numbers here are with three decimal point, except for TBOD, which have four significant figures.

#	Crystal	Q^* (in e^-)	TBOD ($e^-/Å^3$)	ω_p(eV)
1	Cu_2ZnSiS_4	11.017(Cu), 11.611(Zn), 3.098(Si), 6.314(S)	0.0248	19.500
2	$Cu_2ZnSiSe_4$	11.039 (Cu), 11.703 (Zn), 3.368 (Si), 6.212 (Se)	0.0205	18.100
3	$Cu_2ZnSiTe_4$	11.262 (Cu), 11.932 (Zn), 3.788 (Si), 5.938 (Te)	0.0180	17.250
4	Cu_2ZnGeS_4	10.992 (Cu), 11.605 (Zn), 3.372 (Ge), 6.259 (S)	0.0228	19.100
5	$Cu_2ZnGeSe_4$	11.023 (Cu), 11.702 (Zn), 3.573 (Ge), 6.169 (Se)	0.0189	18.100
6	Cu_2ZnSnS_4	11.029 (Cu), 11.631 (Zn), 3.030 (Sn), 6.319 (S)	0.0211	18.900
7	$Cu_2ZnSnSe_4$	11.046 (Cu), 11.714 (Zn), 3.239 (Sn), 6.238 (Se)	0.0180	18.100
8	$Cu_2ZnSnTe_4$	11.258 (Cu), 11.954 (Zn), 3.555(Sn), 5.993 (Te)	0.0163	16.800
9	Cu_2CdSiS_4	11.078 (Cu), 11.138 (Cd), 3.092 (Si), 6.403 (S)	0.0213	19.800
10	$Cu_2CdSiSe_4$	11.077 (Cu), 11.194 (Cd), 3.368 (Si), 6.320 (Se)	0.0177	18.100
11	Cu_2CdGeS_4	11.046(Cu), 11.145 (Cd), 3.371 (Ge), 6.348 (S)	0.0195	19.600
12	$Cu_2CdGeSe_4$	11.061(Cu), 11.188 (Cd), 3.572(Ge), 6.279 (Se)	0.0164	19.100
13	$Cu_2CdGeTe_4$	11.264 (Cu), 11.289 (Cd), 3.925 (Ge), 6.064(Te)	0.0147	17.100
14	Cu_2CdSnS_4	11.065 (Cu), 11.161 (Cd), 3.070 (Sn), 6.409 (S)	0.0181	19.100
15	$Cu_2CdSnSe_4$	11.066 (Cu), 11.201 (Cd), 3.268 (Sn), 6.349 (Se)	0.0155	17.400
16	$Cu_2CdSnTe_4$	11.263 (Cu), 11.296 (Cd), 3.573 (Sn), 6.151(Te)	0.0141	16.300
17	Cu_2HgGeS_4	11.027 (Cu), 11.456(Hg), 3.316 (Ge), 6.293 (S)	0.0132	20.100
18	$Cu_2HgGeSe_4$	11.049(Cu), 11.551(Hg), 3.522(Ge), 6.207 (Se)	0.0112	19.400
19	$Cu_2HgGeTe_4$	11.316 (Cu), 11.816 (Hg), 3.883(Ge), 5.917 (Te)	0.0103	17.100
20	Cu_2HgSnS_4	11.045(Cu), 11.496(Hg), 3.056 (Sn), 6.339 (S)	0.0126	19.100
21	$Cu_2HgSnSe_4$	11.059 (Cu), 11.578 (Hg), 3.264 (Sn), 6.259 (Se)	0.0109	18.500
22	$Cu_2HgSnTe_4$	11.314 (Cu), 11.826 (Hg), 3.622 (Sn), 5.980 (Te)	0.0102	16.500
23	Cu_2BaGeS_4	11.200 (Cu), 8.103 (Ba), 3.367(Ge), 6.532 (S)	0.0133	21.200
24	$Cu_2BaGeSe_4$	11.199(Cu), 8.117(Ba), 3.544(Ge), 6.485 (Se)	0.0123	20.500
25	Cu_2SrSiS_4	11.168(Cu), 6.811(Sr), 3.084(Si), 6.442(S)	0.0193	24.000
26	Cu_2SrGeS_4	11.141 (Cu), 6.854 (Sr), 3.361 (Ge), 6.375 (S)	0.0177	23.900
27	$Cu_2SrGeSe_4$	11.138 (Cu), 6.891 (Sr), 3.541 (Ge), 6.322 (Se)	0.0145	23.500
28	Cu_2BaSnS_4	11.149 (Cu), 8.109(Ba), 3.136 (Sn), 6.614 (S)	0.0110	19.900
29	$Cu_2BaSnSe_4$	11.184 (Cu), 8.125 (Ba), 3.200 (Sn), 6.576 (Se)	0.0111	20.100
30	Cu_2SrSnS_4	11.176(Cu), 6.776(Sr), 3.041(Sn), 6.457(S)	0.0159	23.100
31	$Cu_2SrSnSe_4$	11.147 (Cu), 6.890 (Sr), 3.225 (Sn), 6.397 (Se)	0.0145	23.500
32	Cu_2MgSiS_4	11.069 (Cu), 6.973(Mg), 3.095 (Si), 6.448 (S)	0.0224	19.400
33	$Cu_2MgSiSe_4$	11.079 (Cu), 7.065(Mg), 3.363 (Si), 6.353 (Se)	0.0186	18.200
34	Cu_2MgGeS_4	11.054 (Cu), 6.983(Mg), 3.369 (Ge), 6.385(S)	0.0206	19.400
35	Cu_2MgSnS_4	11.076(Cu), 7.019 (Mg), 3.053 (Sn), 6.444(S)	0.0191	18.100
36	$Cu_2MgSnSe_4$	11.071 (Cu), 7.077 (Mg), 3.256 (Sn), 6.381 (Se)	0.0162	16.900
37	$Cu_2MgSnTe_4$	11.260 (Cu), 7.156 (Mg), 3.569 (Sn), 6.188 (Te)	0.0143	16.100
38	Ag_2ZnSiS_4	10.822 (Ag), 11.506(Zn), 3.133 (Si), 6.429 (S)	0.0145	17.200
39	Ag_2ZnSnS_4	10.939 (Ag), 11.604(Zn), 2.980 (Sn), 6.384 (S)	0.0167	18.200
40	$Ag_2ZnSnSe_4$	10.954 (Ag), 11.684(Zn), 3.192 (Sn), 6.303 (Se)	0.0145	18.100
41	Ag_2CdGeS_4	10.953 (Ag), 11.138 (Cd), 3.314 (Ge), 6.410 (S)	0.0153	18.400
42	Ag_2CdSnS_4	11.065 (Ag), 11.161 (Cd), 3.070 (Sn), 6.409 (S)	0.0144	18.900
43	$Ag_2CdSnSe_4$	10.973(Ag), 11.178 (Cd), 3.206(Sn), 6.417 (Se)	0.0125	17.500
44	$Ag_2CdSnTe_4$	11.100 (Ag), 11.278 (Cd), 3.533 (Sn), 6.247(Te)	0.0115	16.800
45	Ag_2HgSnS_4	10.950 (Ag), 11.470 (Hg), 2.98 (Sn), 6.412(S)	0.0101	18.600
46	$Ag_2HgSnSe_4$	10.965 (Ag), 11.546 (Hg), 3.198 (Sn), 6.331 (Se)	0.0088	16.500
47	Ag_2BaGeS_4	11.071 (Ag), 8.138 (Ba), 3.308 (Ge), 6.603(S)	0.0120	20.900
48	$Ag_2BaGeSe_4$	11.027 (Ag), 8.155(Ba), 3.494 (Ge), 6.574(Se)	0.0100	20.100
49	Ag_2BaSnS_4	11.035(Ag), 8.145 (Ba), 2.998 (Sn), 6.696 (S)	0.0106	20.500
50	$Ag_2BaSnSe_4$	11.018 (Ag), 8.157 (Ba), 3.169 (Sn), 6.659 (Se)	0.0100	19.900
51	Ag_2SrGeS_4	11.018 (Ag), 6.868(Sr), 3.318 (Ge), 6.444 (S)	0.0144	23.500
52	$Ag_2SrGeSe_4$	11.022 (Ag), 6.872(Sr), 3.515 (Ge), 6.392 (Se)	0.0123	23.300
53	Ag_2SrSnS_4	11.015 (Ag), 6.861 (Sr), 3.007 (Sn), 6.525 (S)	0.0133	23.250

54	$Ag_2SrSnSe_4$	11.014(Ag), 6.866(Sr), 3.196 (Sn), 6.477 (Se)	0.0110	23.700
55	$Ag_2In_2SiS_6$	10.921 (Ag), 12.171 (In), 3.141(Si), 6.446(S)	0.0159	17.400
56	$Ag_2In_2GeS_6$	10.911 (Ag), 12.172 (In), 3.377(Ge), 6.409 (S)	0.0149	17.500
57	$Ag_2In_2SiSe_6$	10.951 (Ag), 12.317(In), 3.393(Si), 6.345 (Se)	0.0137	17.100
58	$Ag_2In_2GeSe_6$	10.940 (Ag), 12.314 (In), 3.588 (Ge), 6.317 (Se)	0.0130	16.900
59	Ag_2SiS_3	10.889(Ag), 3.042 (Si), 6.393 (S)	0.0168	19.500
60	Ag_2GeS_3	10.901 (Ag), 3.310 (Ge), 6.295 (S)	0.0159	18.600
61	Cu_2GeS_3	10.981 (Cu), 3.388 (Ge), 6.216 (S)	0.0222	19.500
62	Cu_2GeSe_3	11.017 (Cu), 3.591(Ge), 6.125(Se)	0.0183	19.100
63	Ag_2SnSe_3	10.921 (Ag), 3.496(Sn), 6.221(Se)	0.0062	15.500
64	Ag_2SnTe_3	11.089 (Ag), 3.529 (Sn), 6.097 (Te)	0.0119	15.900
65	$Ag_4P_2S_6$	10.888 (Ag), 4.338(P), S = 6.294 (S)	0.0155	18.900
66	$Ag_4P_2Se_6$	10.939 (Ag), 4.577(P), 6.182(Se)	0.0134	18.700
67	$BaZnSiSe_4$	8.160(Ba), 11.665 (Zn), 3.343(Si), 6.708(Se)	0.0096	20.500
68	$BaZnGeSe_4$	8.158 (Ba), 11.655 (Zn), 3.521 (Ge), 6.666 (Se)	0.0088	20.200
69	$BaHg_2As_2S_6$	8.815(Ba), 11.514 (Hg), 4.540 (As), 6.512 (S)	0.0064	20.100
70	$BaCd_2As_2S_6$	8.181(Ba), 11.164 (Cd), 4.559 (As), 6.729(S)	0.0077	20.500
71	Ba_2AlSbS_5	8.171 (Ba), 2.242 (Al), 4.246 (Sb), 7.033 (S)	0.0063	21.300
72	$Ba_2GaBiSe_5$	8.165 (Ba), 12.733 (Ga), 14.341(Bi), 6.919 (Se)	0.0053	20.600
73	$Ba_2AsGaSe_5$	8.171 (Ba), 4.644(As), 12.675 (Ga), 6.867 (Se)	0.0054	20.900
74	$Ba_2LaGaSe_5$	8.165 (Ba), 9.897(La), 12.683 (Ga), 7.018(Se)	0.0065	22.900
75	$Ba_2LuGaSe_5$	8.951 (Ba), 15.864(Lu), 12.737(Ga), 6.699 (Se)	0.0061	20.500
76	$Ba_2LuInSe_5$	8.989 (Ba), 15.902(Lu), 12.428 (In), 6.738 (Se)	0.0118	20.450
77	Ba_4AgInS_6	8.174 (Ba), 11.365 (Ag), 12.405 (In), 7.255 (S)	0.0050	22.600
78	$CsCu_5S_3$	8.212 (Cs), 11.012 (Cu), 6.242 (S)	0.0181	20.700
79	$CsCu_5Se_3$	8.287(Cs), 11.015 (Cu), 6.212(Se)	0.0162	19.750
80	$K_2Cu_2GeS_4$	6.254 (k), 11.091 (Cu), 3.419 (Ge), 6.472 (S)	0.0136	24.500
81	$Li_2In_2SiS_6$	0.669 (Li), 12.198 (In), 3.147 (Si), 6.519 (S)	0.0167	17.500
82	$Li_2In_2SiSe_6$	0.677 (Li), 12.336(In), 3.400 (Si), 6.428 (Se)	0.0141	16.600
83	$Li_2In_2GeS_6$	0.658 (Li), 12.197 (In), 3.390 (Ge), 6.483 (S)	0.0155	17.400
84	$Li_2In_2GeSe_6$	0.666 (Li), 12.331 (In), 3.604 (Ge), 6.399 (Se)	0.0132	16.700
85	Lu_5GaS_9	15.903 (Lu), 12.322(Ga), 6.684 (S)	0.0102	31.100
86	$SrCdGeS_4$	6.971 (Sr), 11.148(Cd), 3.354 (Ge), 6.631 (S)	0.0121	23.900
87	$SrCdGeSe_4$	6.965 (Sr), 11.203(Cd), 3.555 (Ge), 6.569 (Se)	0.0105	23.500
88	$TlInGe_2S_6$	12.619 (Tl), 12.171(In), 3.326 (Ge), 6.426 (S)	0.0114	18.450
89	$TlInGe_2Se_6$	12.649 (Tl), 12.312 (In), 3.552(Ge), 6.322 (Se)	0.0095	17.900
90	$TlGaSn_2Se_6$	12.711(Tl), 12.603 (Ga), 3.449 (Sn), 6.298(Se)	0.0097	17.890
91	Tl_2PbZrS_4	12.714 (Tl), 13.371 (Pb), 8.941 (Zr), 6.565(S)	0.0075	18.200
92	$Tl_2PbZrSe_4$	12.724(Tl), 13.427 (Pb), 9.027 (Zr), 6.524 (Se)	0.0073	19.500
93	Tl_2PbHfS_4	12.679 (Tl), 13.337 (Pb), 3.296 (Hf), 6.502 (S)	0.0075	18.900
94	$Tl_2PbHfSe_4$	12.681 (Tl), 13.387 (Pb), 3.388(Hf), 6.466(Se)	0.0073	19.400
95	$Tl_2CdGeSe_4$	12.743 (Tl), 11.166 (Cd), 3.545(Ge), 6.450 (Se)	0.0085	18.600
96	$Tl_2CdSnSe_4$	12.751 (Tl), 11.173(Cd), 3.236 (Sn), 6.529 (Se)	0.0080	18.900
97	$Tl_2HgGeSe_4$	12.649 (Tl), 11.535 (Hg), 3.485 (Ge), 6.420 (Se)	0.0062	18.700
98	$Tl_2HgSiSe_4$	12.660 (Tl), 11.544 (Hg), 3.344 (Si), 6.447 (Se)	0.0067	18.450
99	Tl_2HgSnS_4	12.632 (Tl), 11.498 (Hg), 2.993 (Sn), 6.561(S)	0.0066	19.150

Table S4 Our results for the 99 crystals: refractive index (n).

#	Crystal	n
1	Cu_2ZnSiS_4	2.673
2	$Cu_2ZnSiSe_4$	2.894
3	$Cu_2ZnSiTe_4$	3.354
4	Cu_2ZnGeS_4	2.915
5	$Cu_2ZnGeSe_4$	3.741
6	Cu_2ZnSnS_4	3.240
7	$Cu_2ZnSnSe_4$	3.741
8	$Cu_2ZnSnTe_4$	3.605
9	Cu_2CdSiS_4	2.673
10	$Cu_2CdSiSe_4$	2.932
11	Cu_2CdGeS_4	3.016
12	$Cu_2CdGeSe_4$	3.807
13	$Cu_2CdGeTe_4$	3.821
14	Cu_2CdSnS_4	3.391
15	$Cu_2CdSnSe_4$	3.872
16	$Cu_2CdSnTe_4$	3.674
17	Cu_2HgGeS_4	3.162
18	$Cu_2HgGeSe_4$	3.821
19	$Cu_2HgGeTe_4$	3.847
20	Cu_2HgSnS_4	3.566
21	$Cu_2HgSnSe_4$	4.183
22	$Cu_2HgSnTe_4$	3.549
23	Cu_2BaGeS_4	2.915
24	$Cu_2BaGeSe_4$	3.130
25	Cu_2SrSiS_4	2.608
26	Cu_2SrGeS_4	2.828
27	$Cu_2SrGeSe_4$	3.049
28	Cu_2BaSnS_4	2.881
29	$Cu_2BaSnSe_4$	3.025
30	Cu_2SrSnS_4	2.933
31	$Cu_2SrSnSe_4$	3.098
32	Cu_2MgSiS_4	2.588
33	$Cu_2MgSiSe_4$	2.756
34	Cu_2MgGeS_4	2.828
35	Cu_2MgSnS_4	3.001
36	$Cu_2MgSnSe_4$	3.354
37	$Cu_2MgSnTe_4$	3.464
38	Ag_2ZnSiS_4	2.692
39	Ag_2ZnSnS_4	2.765
40	$Ag_2ZnSnSe_4$	3.025
41	Ag_2CdGeS_4	2.664
42	Ag_2CdSnS_4	2.756
43	$Ag_2CdSnSe_4$	2.983
44	$Ag_2CdSnTe_4$	3.130
45	Ag_2HgSnS_4	2.683
46	$Ag_2HgSnSe_4$	2.983
47	Ag_2BaGeS_4	2.262
48	$Ag_2BaGeSe_4$	2.756
49	Ag_2BaSnS_4	2.598
50	$Ag_2BaSnSe_4$	2.738
51	Ag_2SrGeS_4	2.626
52	$Ag_2SrGeSe_4$	2.802
53	Ag_2SrSnS_4	2.645
54	$Ag_2SrSnSe_4$	2.766
55	$Ag_2In_2SiS_6$	2.499
56	$Ag_2In_2GeS_6$	2.549

57	$Ag_2In_2SiSe_6$	2.645
58	$Ag_2In_2GeSe_6$	2.716
59	Ag_2SiS_3	2.479
60	Ag_2GeS_3	2.881
61	Cu_2GeS_3	3.912
62	Cu_2GeSe_3	3.982
63	Ag_2SnSe_3	3.030
64	Ag_2SnTe_3	3.718
65	$Ag_4P_2S_6$	2.677
66	$Ag_4P_2Se_6$	2.924
67	$BaZnSiSe_4$	2.366
68	$BaZnGeSe_4$	2.510
69	$BaHg_2As_2S_6$	2.620
70	$BaCd_2As_2S_6$	2.640
71	Ba_2AlSbS_5	2.533
72	$Ba_2GaBiSe_5$	2.885
73	$Ba_2AsGaSe_5$	2.640
74	$Ba_2LaGaSe_5$	2.706
75	$Ba_2LuGaSe_5$	2.557
76	$Ba_2LuInSe_5$	2.631
77	Ba_4AgInS_6	2.506
78	$CsCu_5S_3$	3.089
79	$CsCu_5Se_3$	3.282
80	$K_2Cu_2GeS_4$	2.549
81	$Li_2In_2SiS_6$	2.330
82	$Li_2In_2SiSe_6$	2.460
83	$Li_2In_2GeS_6$	2.371
84	$Li_2In_2GeSe_6$	2.527
85	Lu_5GaS_9	2.542
86	$SrCdGeS_4$	2.397
87	$SrCdGeSe_4$	2.553
88	$TlInGe_2S_6$	2.635
89	$TlInGe_2Se_6$	2.787
90	$TlGaSn_2Se_6$	2.569
91	Tl_2PbZrS_4	4.375
92	$Tl_2PbZrSe_4$	4.524
93	Tl_2PbHfS_4	4.326
94	$Tl_2PbHfSe_4$	4.424
95	$Tl_2CdGeSe_4$	3.647
96	$Tl_2CdSnSe_4$	3.535
97	$Tl_2HgGeSe_4$	3.715
98	$Tl_2HgSiSe_4$	3.701
99	Tl_2HgSnS_4	3.605

Table S5 The calculated elastic constants C_{ij} (GPa) for the 99 crystals.

#	Crystal	C_{11}	C_{12}	C_{13}	C_{21}	C_{22}	C_{23}	C_{31}	C_{32}	C_{33}	C_{44}	C_{55}	C_{66}
1	Cu_2ZnSiS_4	124.976	57.391	44.792	57.391	122.374	43.791	44.792	43.791	158.825	31.529	30.567	34.298
2	$Cu_2ZnSiSe_4$	96.229	45.824	34.392	45.824	103.007	37.524	34.392	37.524	128.882	25.042	23.982	27.049
3	$Cu_2ZnSiTe_4$	63.565	35.569	37.890	35.569	72.856	42.541	37.890	42.541	73.652	32.672	32.688	30.949
4	Cu_2ZnGeS_4	120.211	52.512	40.167	52.512	116.010	37.896	40.166	37.896	149.271	29.284	28.284	32.728
5	$Cu_2ZnGeSe_4$	77.649	47.234	44.566	47.234	86.378	48.803	44.566	48.803	75.521	35.650	35.570	33.268
6	Cu_2ZnSnS_4	72.691	43.560	55.953	43.560	85.985	62.501	55.953	62.501	110.213	41.257	41.460	40.641
7	$Cu_2ZnSnSe_4$	58.336	32.462	43.225	32.462	64.581	46.351	43.225	46.351	86.307	32.969	33.471	32.705
8	$Cu_2ZnSnTe_4$	58.309	35.196	35.468	35.196	63.549	38.069	35.468	38.069	64.511	27.304	27.251	27.084
9	Cu_2CdSiS_4	115.978	57.955	44.042	57.955	113.375	42.610	44.042	42.610	134.174	25.553	26.324	28.012
10	$Cu_2CdSiSe_4$	92.815	45.688	34.498	45.688	87.940	31.211	34.498	31.211	106.086	20.252	21.125	22.874
11	Cu_2CdGeS_4	107.377	53.835	45.122	53.835	107.520	45.241	45.122	45.241	137.512	23.802	23.980	26.313
12	$Cu_2CdGeSe_4$	79.622	49.112	48.528	49.112	78.109	47.718	48.528	47.718	72.839	32.070	31.906	33.251
13	$Cu_2CdGeTe_4$	61.859	33.689	37.224	33.689	56.851	34.725	37.224	34.725	61.191	25.808	26.211	26.277
14	Cu_2CdSnS_4	81.601	49.905	56.101	49.905	78.827	54.768	56.101	54.768	89.189	35.515	35.381	34.104
15	$Cu_2CdSnSe_4$	53.107	28.512	29.042	28.512	53.405	29.165	29.042	29.165	53.578	28.665	28.535	28.883
16	$Cu_2CdSnTe_4$	53.240	31.697	41.200	31.697	55.045	42.130	41.200	42.130	74.027	24.182	24.100	23.996
17	Cu_2HgGeS_4	91.607	41.997	34.980	41.997	62.280	20.251	34.980	20.251	44.574	38.184	38.072	41.502
18	$Cu_2HgGeSe_4$	76.607	42.868	46.248	42.868	66.328	41.050	46.248	41.050	67.276	31.611	31.175	30.375
19	$Cu_2HgGeTe_4$	59.697	35.159	33.704	35.159	61.822	34.719	33.704	34.719	54.490	26.612	26.509	27.334
20	Cu_2HgSnS_4	92.442	65.655	64.542	65.655	95.905	66.146	64.542	66.146	94.226	33.419	33.155	35.502
21	$Cu_2HgSnSe_4$	69.685	46.054	46.316	46.054	72.405	47.754	46.316	47.754	70.463	28.198	28.222	28.303
22	$Cu_2HgSnTe_4$	56.820	34.403	34.799	34.403	56.934	34.881	34.799	34.881	56.881	25.068	24.708	24.928
23	Cu_2BaGeS_4	91.526	57.293	35.981	57.293	85.189	33.136	35.981	33.136	45.259	14.519	14.432	16.261
24	$Cu_2BaGeSe_4$	74.751	27.232	29.783	27.232	74.851	29.275	29.783	29.275	76.172	23.457	23.792	23.722
25	Cu_2SrSiS_4	106.158	36.917	44.395	36.917	100.984	41.916	44.395	41.916	117.708	31.362	31.478	33.361
26	Cu_2SrGeS_4	121.086	52.218	52.595	52.218	102.803	43.683	52.595	43.683	102.665	28.609	29.105	30.070
27	$Cu_2SrGeSe_4$	86.694	28.535	29.741	28.535	57.957	13.409	29.741	13.409	83.557	17.348	23.242	19.489
28	Cu_2BaSnS_4	54.238	27.629	24.297	27.629	33.311	13.575	24.297	13.575	27.860	10.552	9.874	3.574
29	$Cu_2BaSnSe_4$	68.021	23.982	27.424	23.982	54.231	15.902	27.424	15.902	71.806	15.819	21.226	18.588
30	Cu_2SrSnS_4	81.661	37.439	34.976	37.439	83.164	36.293	34.976	36.293	79.998	23.533	23.361	22.766
31	$Cu_2SrSnSe_4$	69.817	26.140	19.786	26.140	55.530	10.355	19.786	10.355	72.686	15.669	20.656	17.804
32	Cu_2MgSiS_4	118.587	53.850	50.725	53.850	102.415	40.535	50.725	40.535	135.986	25.646	26.055	28.408
33	$Cu_2MgSiSe_4$	89.5117	40.327	37.097	40.327	83.675	33.952	37.097	33.9518	111.539	20.349	20.702	22.255
34	Cu_2MgGeS_4	126.815	66.822	46.391	66.822	118.181	43.109	46.391	43.109	118.821	24.575	23.829	26.440
35	Cu_2MgSnS_4	96.3197	62.230	55.544	62.230	88.115	51.446	55.544	51.446	75.628	36.222	36.388	35.120
36	$Cu_2MgSnSe_4$	70.736	44.451	43.001	44.451	68.456	41.848	43.001	41.848	64.961	29.271	29.221	28.145
37	$Cu_2MgSnTe_4$	60.0377	37.087	34.139	37.087	57.992	33.112	34.139	33.1118	51.7118	23.712	23.550	21.842
38	Ag_2ZnSiS_4	53.457	-22.437	42.503	-22.437	-2.748	-10.656	42.503	-10.656	76.139	-2.695	25.667	-2.784
39	Ag_2ZnSnS_4	71.801	48.005	47.971	48.005	71.685	47.955	47.971	47.955	67.4917	27.074	26.925	28.778
40	$Ag_2ZnSnSe_4$	61.230	40.581	40.641	40.581	61.196	40.623	40.641	40.623	57.131	22.924	23.187	23.730
41	Ag_2CdGeS_4	76.828	42.406	38.791	42.406	71.311	36.552	38.791	36.552	92.942	16.185	14.349	16.290
42	Ag_2CdSnS_4	63.466	44.086	45.333	44.086	63.341	45.326	45.333	45.326	62.837	22.994	23.163	23.059
43	$Ag_2CdSnSe_4$	55.160	37.990	39.102	37.990	55.158	39.100	39.102	39.100	53.765	19.968	19.834	19.925
44	$Ag_2CdSnTe_4$	47.132	31.145	32.097	31.145	47.116	32.107	32.097	32.107	45.540	17.551	17.517	16.093
45	Ag_2HgSnS_4	68.560	40.264	34.727	40.264	69.749	36.083	34.727	36.083	85.812	13.058	12.766	14.130
46	$Ag_2HgSnSe_4$	59.111	35.892	31.231	35.892	58.706	29.974	31.231	29.974	73.069	11.029	10.617	11.716
47	Ag_2BaGeS_4	77.374	52.474	35.288	52.474	76.402	35.335	35.288	35.335	45.096	18.817	18.758	24.899
48	$Ag_2BaGeSe_4$	76.896	31.395	24.057	31.395	34.235	19.477	24.057	19.477	39.674	12.256	13.807	16.255
49	Ag_2BaSnS_4	36.370	19.794	28.966	19.794	43.647	23.611	28.966	23.611	79.775	15.707	15.190	12.780
50	$Ag_2BaSnSe_4$	68.014	26.482	20.622	26.482	30.774	17.588	20.622	17.588	36.255	11.128	12.724	13.802
51	Ag_2SrGeS_4	43.133	28.024	38.966	28.024	49.684	32.831	38.966	32.831	97.287	18.336	14.875	16.842
52	$Ag_2SrGeSe_4$	80.985	33.469	26.381	33.469	34.559	23.170	26.381	23.170	42.890	12.774	14.141	13.827
53	Ag_2SrSnS_4	31.386	36.637	28.514	36.637	120.002	40.945	28.514	40.945	85.624	13.888	11.926	10.520
54	$Ag_2SrSnSe_4$	73.253	26.703	22.009	26.703	27.094	20.446	22.009	20.446	40.819	9.307	11.774	11.225
55	$Ag_2In_2SiS_6$	62.397	24.651	18.747	24.651	48.765	21.433	18.747	21.433	54.904	16.189	18.491	15.286
56	$Ag_2In_2GeS_6$	59.840	22.764	16.832	22.764	46.533	20.049	16.832	20.049	51.170	16.026	17.930	15.674
57	$Ag_2In_2SiSe_6$	51.461	20.407	14.099	20.407	42.726	17.660	14.099	17.660	47.593	14.958	15.841	13.838
58	$Ag_2In_2GeSe_6$	48.802	19.024	12.829	19.024	40.715	16.820	12.829	16.820	45.953	14.302	15.031	14.160
59	Ag_2SiS_3	56.251	34.466	27.971	34.466	58.916	28.570	27.971	28.570	46.196	15.302	14.926	15.758
60	Ag_2GeS_3	71.166	41.876	35.486	41.876	77.900	38.918	35.486	38.918	86.252	14.643	15.354	16.457

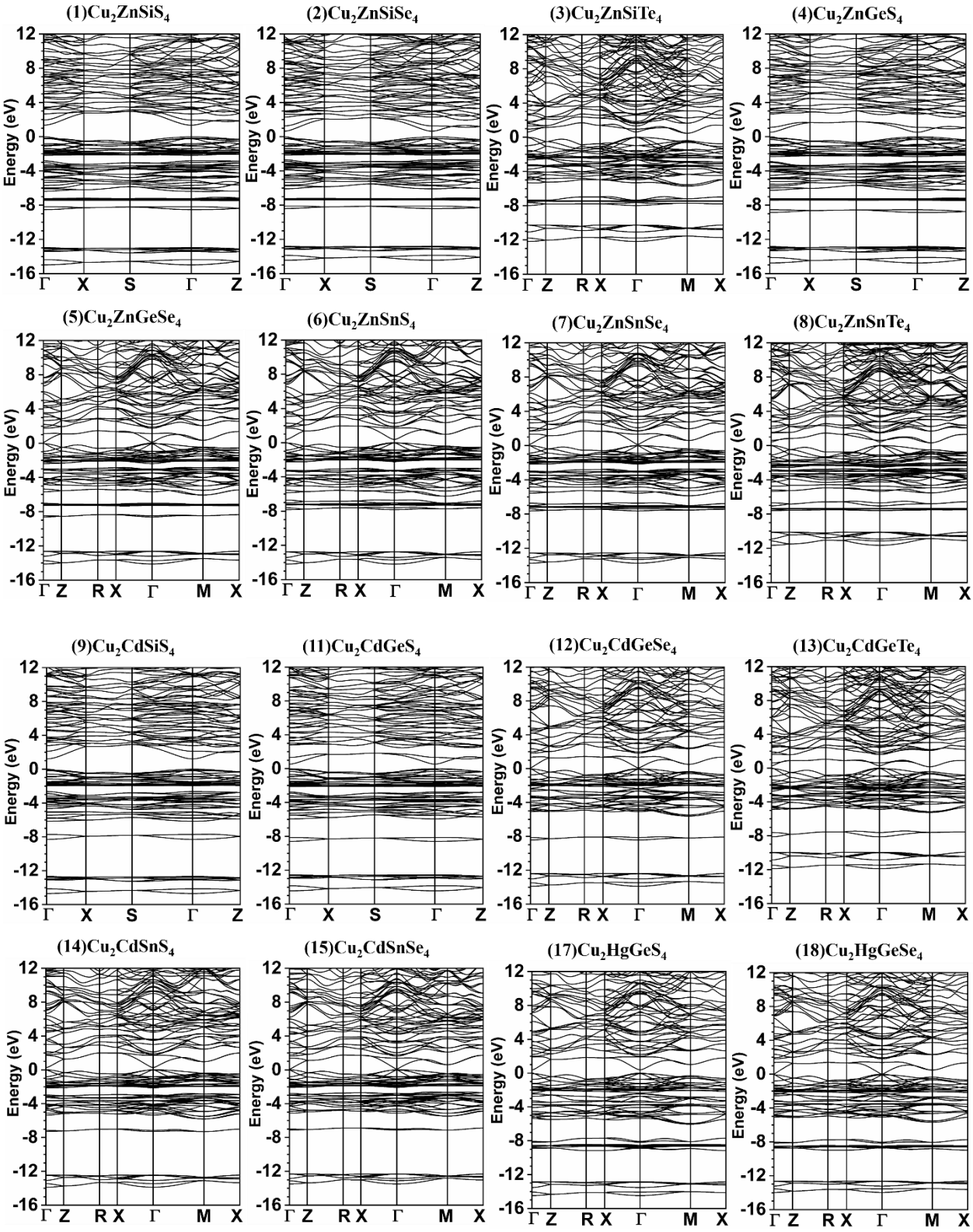
61	Cu_2GeS_3	134.693	56.017	49.563	56.017	138.913	53.530	49.563	53.530	137.221	27.360	27.744	38.041
62	Cu_2GeSe_3	90.258	22.124	33.831	22.124	91.791	45.794	33.831	45.794	70.491	35.640	36.984	17.619
63	Ag_2SnSe_3	46.999	12.497	-1.610	12.497	44.1259	0.256	-1.610	0.256	-1.121	-0.159	-0.120	4.707
64	Ag_2SnTe_3	56.492	26.361	25.011	26.361	58.182	26.233	25.011	26.233	59.115	10.149	10.030	14.159
65	$Ag_4P_2S_6$	37.452	23.542	13.658	23.542	51.270	23.162	13.658	23.162	48.369	11.005	8.009	13.303
66	$Ag_4P_2Se_6$	31.154	18.140	15.169	18.140	46.173	20.972	15.169	20.972	62.375	11.283	8.404	13.372
67	$BaZnSiSe_4$	40.965	16.652	14.171	16.652	40.530	14.486	14.171	14.486	64.844	15.783	11.062	11.318
68	$BaZnGeSe_4$	39.497	16.506	13.042	16.506	39.480	13.947	13.042	13.947	61.662	14.608	9.338	10.987
69	$BaHg_2As_2S_6$	46.118	17.648	25.198	17.648	32.077	19.779	25.198	19.779	47.645	8.514	10.991	15.820
70	$BaCd_2As_2S_6$	46.680	16.588	28.578	16.588	34.653	20.911	28.578	20.911	54.494	11.812	13.559	13.439
71	Ba_2AlSbS_5	56.807	13.313	12.537	13.313	57.296	21.717	12.537	21.717	41.783	23.407	15.138	12.243
72	$Ba_2GaBiSe_5$	54.028	13.957	12.762	13.957	50.574	23.053	12.762	23.053	34.942	21.601	13.082	12.918
73	$Ba_2AsGaSe_5$	47.541	9.792	12.274	9.792	44.902	17.968	12.274	17.968	38.743	20.964	12.079	10.432
74	$Ba_2LaGaSe_5$	56.987	25.786	17.675	25.786	82.040	37.402	17.675	37.402	53.490	28.969	12.802	21.871
75	$Ba_2LuGaSe_5$	56.099	21.670	20.891	21.670	67.588	17.551	20.891	17.551	38.863	19.413	16.909	23.118
76	$Ba_2LuInSe_5$	79.547	20.711	25.759	20.711	46.703	26.135	25.759	26.135	54.520	17.584	25.982	21.249
77	Ba_4AgInS_6	70.360	26.779	20.979	26.779	59.713	28.105	20.979	28.105	62.069	22.670	19.739	25.820
78	$CsCu_5S_3$	89.317	30.515	30.104	30.515	93.144	22.175	30.104	22.175	44.843	9.642	10.110	20.477
79	$CsCu_5Se_3$	50.747	23.266	18.869	23.266	76.543	13.073	18.869	13.073	44.015	5.641	9.501	12.384
80	$K_2Cu_2GeS_4$	46.915	18.919	16.287	18.919	45.211	22.245	16.287	22.245	41.702	25.412	14.767	18.222
81	$Li_2In_2SiS_6$	54.789	18.628	15.121	18.628	38.523	12.765	15.121	12.765	56.461	15.127	18.488	17.284
82	$Li_2In_2SiSe_6$	44.302	16.361	11.831	16.361	31.895	10.733	11.831	10.733	47.676	13.175	15.257	14.784
83	$Li_2In_2GeS_6$	51.774	17.779	14.309	17.779	37.755	12.434	14.309	12.434	54.835	14.871	17.995	16.915
84	$Li_2In_2GeSe_6$	41.449	15.851	11.212	15.851	31.826	10.783	11.212	10.783	46.087	12.523	14.725	14.161
85	Lu_5GaS_9	94.631	38.181	28.394	38.181	87.606	29.276	28.394	29.276	88.562	29.456	27.999	39.844
86	$SrCdGeS_4$	50.802	18.578	22.073	18.579	59.205	19.702	22.073	19.702	83.01	22.488	15.569	12.785
87	$SrCdGeSe_4$	44.558	15.534	19.281	15.534	48.720	17.101	19.281	17.101	67.284	20.065	12.742	9.143
88	$TlInGe_2S_6$	26.336	9.936	7.368	9.936	27.018	7.252	7.368	7.252	24.577	10.493	10.558	8.967
89	$TlInGe_2Se_6$	20.923	7.654	6.508	7.654	20.517	6.521	6.508	6.521	20.370	6.840	6.476	7.142
90	$TlGaSn_2Se_6$	21.987	5.729	6.283	5.729	22.677	6.326	6.283	6.326	21.722	7.413	6.075	8.384
91	Tl_2PbZrS_4	71.592	20.608	30.530	20.608	77.784	30.792	30.530	30.792	65.220	31.490	28.886	20.175
92	$Tl_2PbZrSe_4$	62.568	18.418	26.385	18.418	69.103	25.800	26.385	25.800	54.044	29.239	28.127	18.590
93	Tl_2PbHfS_4	73.009	21.428	30.886	21.428	79.663	31.599	30.886	31.599	66.162	31.080	30.297	19.067
94	$Tl_2PbHfSe_4$	62.910	18.813	27.567	18.813	69.648	26.378	27.567	26.378	56.452	29.631	27.679	18.247
95	$Tl_2CdGeSe_4$	35.066	16.506	13.086	16.506	35.053	13.110	13.086	13.110	65.206	7.475	7.586	7.795
96	$Tl_2CdSnSe_4$	34.887	15.674	12.567	15.674	34.889	12.598	12.567	12.598	62.725	8.659	8.659	9.516
97	$Tl_2HgGeSe_4$	33.585	17.241	12.772	17.241	33.632	12.799	12.772	12.799	61.386	6.186	6.156	8.609
98	$Tl_2HgSiSe_4$	34.860	17.898	13.350	17.898	34.888	13.357	13.350	13.357	65.017	6.202	6.498	8.021
99	Tl_2HgSnS_4	39.745	15.593	12.873	15.593	39.185	12.504	12.873	12.504	73.254	6.998	6.857	8.873

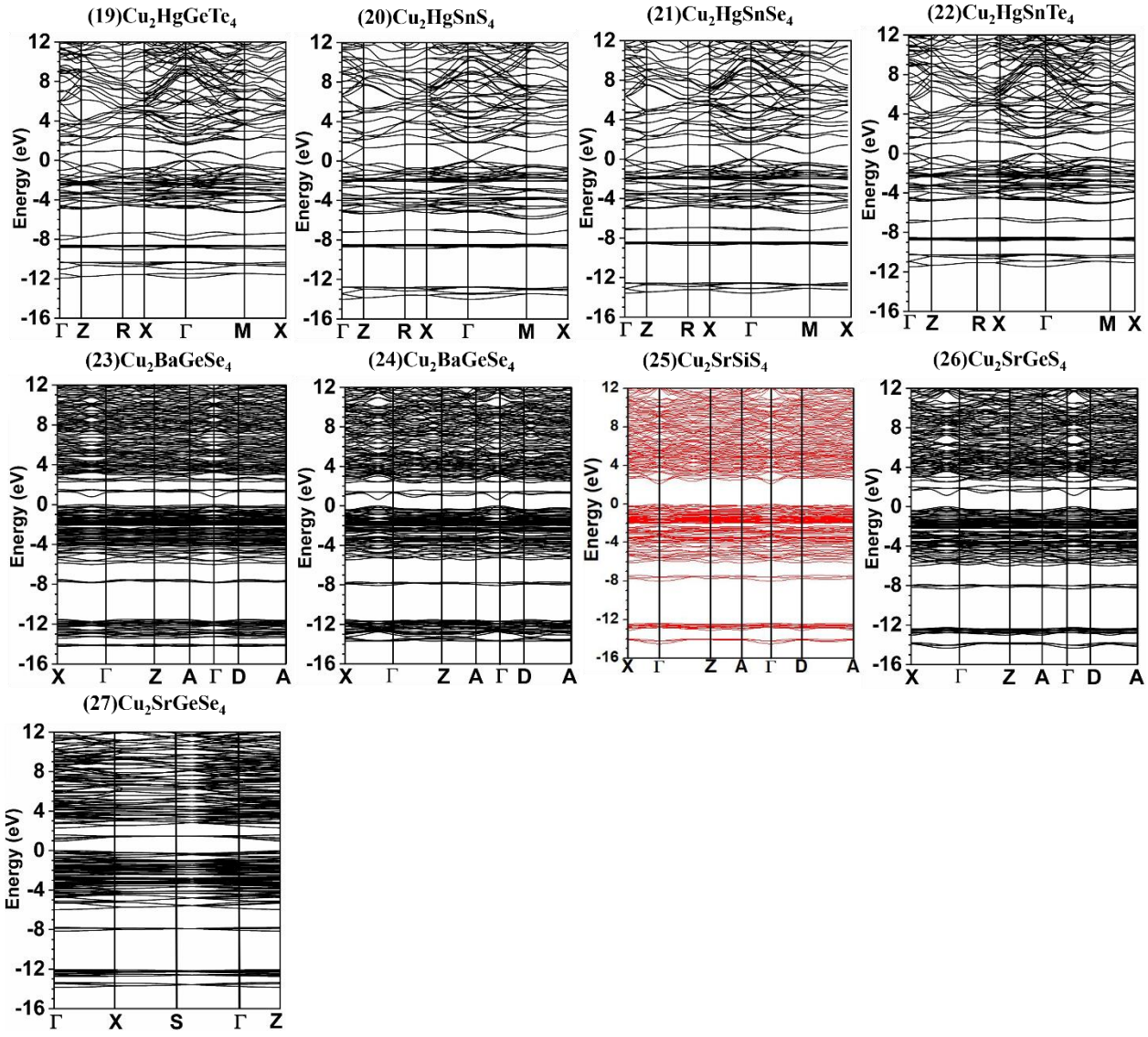
Table S6 Calculated Young modulus (E), Bulk modulus (K), Shear modulus (G), Poisson's ratio (η), and Pugh's modulus ratio (G/K) for the 99 crystals.

#	Crystal	E (GPa)	K (GPa)	G (GPa)	η	G/K
1	Cu_2ZnSiS_4	93.126	77.250	35.843	0.299	0.464
2	$Cu_2ZnSiSe_4$	74.351	62.316	28.571	0.301	0.458
3	$Cu_2ZnSiTe_4$	61.878	48.641	24.022	0.288	0.494
4	Cu_2ZnGeS_4	88.466	71.463	34.191	0.293	0.478
5	$Cu_2ZnGeSe_4$	66.938	56.607	25.688	0.302	0.454
6	Cu_2ZnSnS_4	74.818	60.896	28.882	0.295	0.474
7	$Cu_2ZnSnSe_4$	60.584	48.061	23.484	0.290	0.488
8	$Cu_2ZnSnTe_4$	52.559	44.463	20.169	0.303	0.454
9	Cu_2CdSiS_4	75.925	64.650	29.106	0.304	0.450
10	$Cu_2CdSiSe_4$	63.029	56.323	23.993	0.314	0.426
11	Cu_2CdGeS_4	74.031	70.103	27.957	0.324	0.399
12	$Cu_2CdGeSe_4$	61.468	57.525	23.250	0.322	0.404
13	$Cu_2CdGeTe_4$	50.368	42.912	19.307	0.304	0.449
14	Cu_2CdSnS_4	65.538	62.530	24.725	0.325	0.395
15	$Cu_2CdSnSe_4$	50.871	34.987	20.225	0.258	0.578
16	$Cu_2CdSnTe_4$	46.157	42.952	17.472	0.321	0.407
17	Cu_2HgGeS_4	64.026	36.019	26.595	0.204	0.738
18	$Cu_2HgGeSe_4$	57.736	50.952	22.018	0.311	0.432
19	$Cu_2HgGeTe_4$	50.546	42.245	19.432	0.301	0.459
20	Cu_2HgSnS_4	64.868	72.857	23.996	0.351	0.329
21	$Cu_2HgSnSe_4$	53.615	54.369	20.071	0.335	0.369
22	$Cu_2HgSnTe_4$	47.229	41.868	17.999	0.312	0.429
23	Cu_2BaGeS_4	40.178	46.784	14.805	0.357	0.316
24	$Cu_2BaGeSe_4$	59.645	43.776	23.428	0.273	0.535
25	Cu_2SrSiS_4	83.363	63.148	32.564	0.280	0.516
26	Cu_2SrGeS_4	76.908	68.357	29.299	0.313	0.429
27	$Cu_2SrGeSe_4$	55.519	39.820	21.899	0.268	0.549
28	Cu_2BaSnS_4	12.787	17.056	4.650	0.375	0.273
29	$Cu_2BaSnSe_4$	49.115	35.858	19.311	0.272	0.538
30	Cu_2SrSnS_4	60.025	51.313	22.997	0.305	0.448
31	$Cu_2SrSnSe_4$	49.689	33.991	19.775	0.256	0.582
32	Cu_2MgSiS_4	78.047	71.424	29.611	0.317	0.414
33	$Cu_2MgSiSe_4$	62.347	55.851	23.725	0.314	0.425
34	Cu_2MgGeS_4	74.524	72.668	28.036	0.329	0.386
35	Cu_2MgSnS_4	67.158	65.208	25.278	0.328	0.387
36	$Cu_2MgSnSe_4$	54.339	50.579	20.568	0.320	0.406
37	$Cu_2MgSnTe_4$	44.901	41.570	17.008	0.320	0.409
38	Ag_2ZnSiS_4	34.698	21.450	14.100	0.230	0.657
39	Ag_2ZnSnS_4	51.529	54.941	19.175	0.352	0.349
40	$Ag_2ZnSnSe_4$	43.804	46.639	16.303	0.343	0.349
41	Ag_2CdGeS_4	46.640	52.740	17.241	0.353	0.327
42	Ag_2CdSnS_4	43.192	50.553	15.908	0.358	0.315
43	$Ag_2CdSnSe_4$	37.396	43.665	13.776	0.357	0.315
44	$Ag_2CdSnTe_4$	32.876	36.491	32.876	0.350	0.901
45	Ag_2HgSnS_4	41.254	49.446	15.156	0.360	0.306
46	$Ag_2HgSnSe_4$	34.389	42.686	12.590	0.365	0.295
47	Ag_2BaGeS_4	44.575	46.035	16.650	0.339	0.362
48	$Ag_2BaGeSe_4$	33.695	30.678	12.793	0.317	0.417
49	Ag_2BaSnS_4	36.533	31.614	13.972	0.307	0.442
50	$Ag_2BaSnSe_4$	30.550	27.316	11.628	0.314	0.426
51	Ag_2SrGeS_4	40.220	40.102	15.088	0.333	0.376
52	$Ag_2SrGeSe_4$	32.853	33.213	12.303	0.335	0.370
53	Ag_2SrSnS_4	37.847	39.987	14.098	0.342	0.352
54	$Ag_2SrSnSe_4$	27.609	28.254	10.324	0.337	0.365

55	$Ag_2In_2SiS_6$	42.267	32.698	16.452	0.284	0.503
56	$Ag_2In_2GeS_6$	41.125	30.522	16.122	0.275	0.528
57	$Ag_2In_2SiSe_6$	37.318	27.264	14.670	0.272	0.538
58	$Ag_2In_2GeSe_6$	36.026	25.737	14.220	0.266	0.552
59	Ag_2SiS_3	36.151	37.137	13.512	0.338	0.364
60	Ag_2GeS_3	45.946	51.853	16.988	0.352	0.327
61	Cu_2GeS_3	86.215	78.050	32.759	0.316	0.419
62	Cu_2GeSe_3	66.695	49.809	26.117	0.277	0.524
63	Ag_2SnSe_3	7.983	6.334	3.094	0.290	0.488
64	Ag_2SnTe_3	32.831	36.275	12.167	0.349	0.335
65	$Ag_4P_2S_6$	28.793	26.883	10.894	0.321	0.405
66	$Ag_4P_2Se_6$	30.814	26.386	11.803	0.305	0.447
67	$BaZnSiSe_4$	35.352	25.914	13.889	0.272	0.536
68	$BaZnGeSe_4$	33.095	24.950	12.939	0.279	0.518
69	$BaHg_2As_2S_6$	29.009	27.051	10.978	0.312	0.406
70	$BaCd_2As_2S_6$	32.183	28.554	12.263	0.312	0.429
71	Ba_2AlSbS_5	41.785	27.607	16.744	0.247	0.606
72	$Ba_2GaBiSe_5$	37.221	26.119	14.741	0.262	0.564
73	$Ba_2AsGaSe_5$	35.469	23.427	14.214	0.247	0.607
74	$Ba_2LaGaSe_5$	49.132	37.689	19.151	0.282	0.508
75	$Ba_2LuGaSe_5$	44.828	30.228	17.890	0.252	0.592
76	$Ba_2LuInSe_5$	49.157	35.308	19.384	0.268	0.549
77	Ba_4AgInS_6	53.439	38.170	21.094	0.266	0.553
78	$CsCu_5S_3$	42.324	40.648	15.954	0.326	0.392
79	$CsCu_5Se_3$	33.026	30.929	12.490	0.322	0.404
80	$K_2Cu_2GeS_4$	37.130	25.715	14.741	0.259	0.573
81	$Li_2In_2SiS_6$	41.436	26.432	16.725	0.238	0.633
82	$Li_2In_2SiSe_6$	34.625	22.032	13.983	0.238	0.635
83	$Li_2In_2GeS_6$	40.268	25.409	16.291	0.235	0.641
84	$Li_2In_2GeSe_6$	33.268	21.337	13.413	0.240	0.629
85	Lu_5GaS_9	75.751	49.729	30.394	0.246	0.611
86	$SrCdGeS_4$	46.681	34.140	18.347	0.272	0.537
87	$SrCdGeSe_4$	38.147	28.854	14.905	0.279	0.517
88	$TlInGe_2S_6$	21.375	13.930	8.589	0.244	0.617
89	$TlInGe_2Se_6$	14.097	10.891	5.488	0.284	0.504
90	$TlGaSn_2Se_6$	16.406	11.207	6.531	0.256	0.583
91	Tl_2PbZrS_4	59.137	41.681	23.401	0.263	0.561
92	$Tl_2PbZrSe_4$	52.858	35.969	21.057	0.255	0.585
93	Tl_2PbHfS_4	59.568	42.615	23.507	0.267	0.552
94	$Tl_2PbHfSe_4$	53.300	36.853	21.168	0.259	0.574
95	$Tl_2CdGeSe_4$	26.123	23.841	9.915	0.317	0.416
96	$Tl_2CdSnSe_4$	28.141	23.231	10.839	0.298	0.466
97	$Tl_2HgGeSe_4$	23.976	23.190	9.0294	0.328	0.389
98	$Tl_2HgSiSe_4$	24.498	24.184	9.202	0.331	0.380
99	Tl_2HgSnS_4	28.160	25.140	10.721	0.313	0.426

4. The Supplementary Figures

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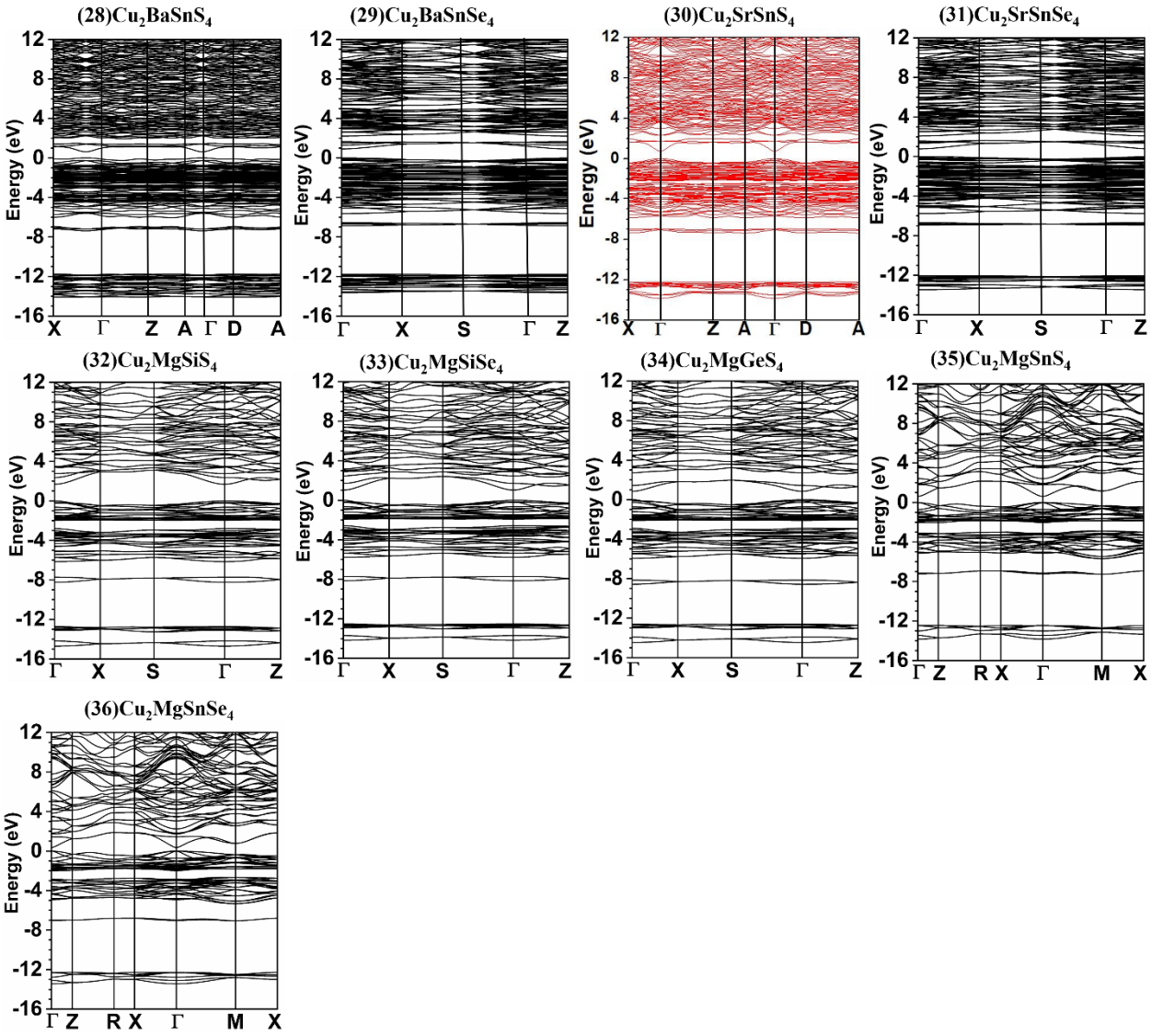
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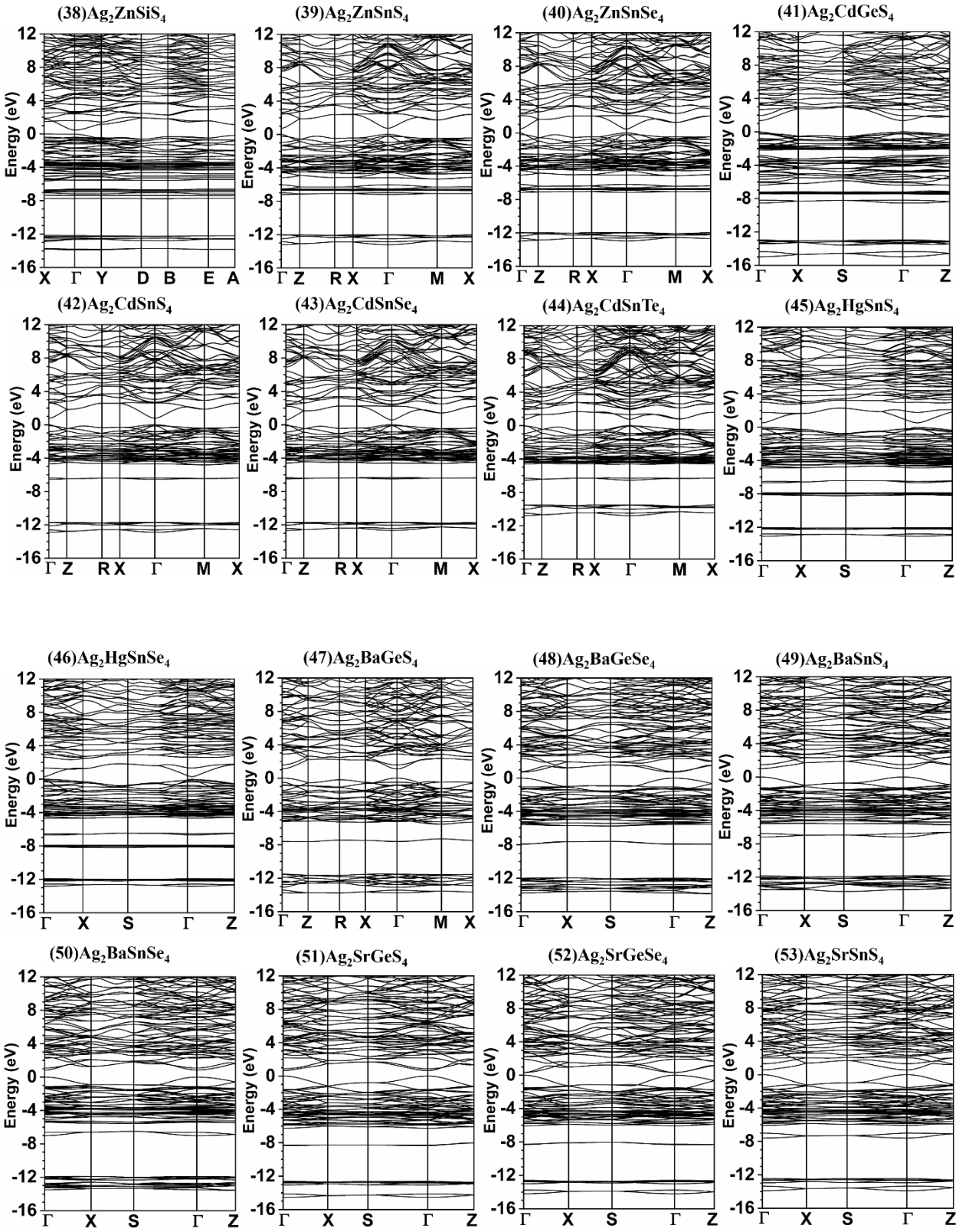
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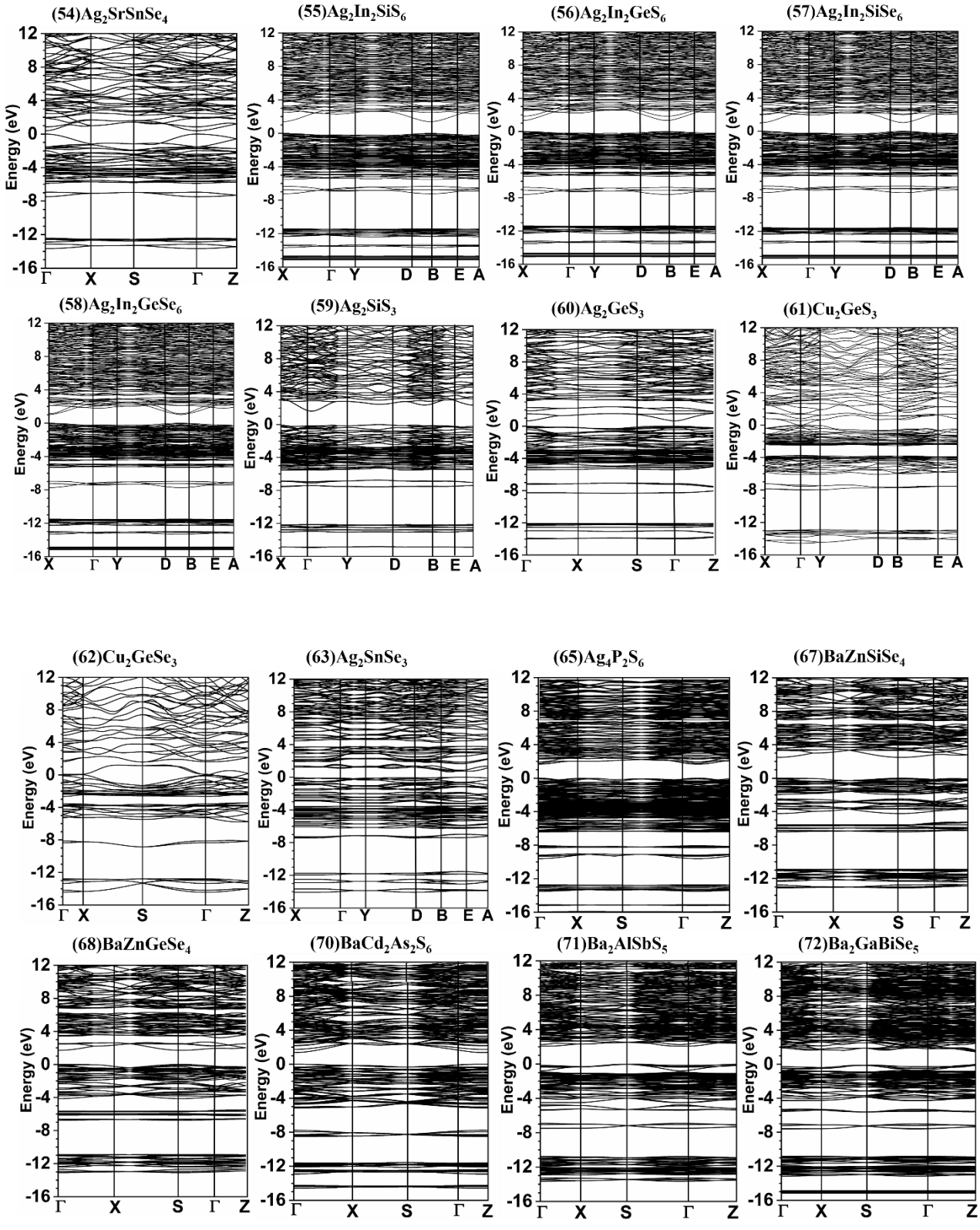
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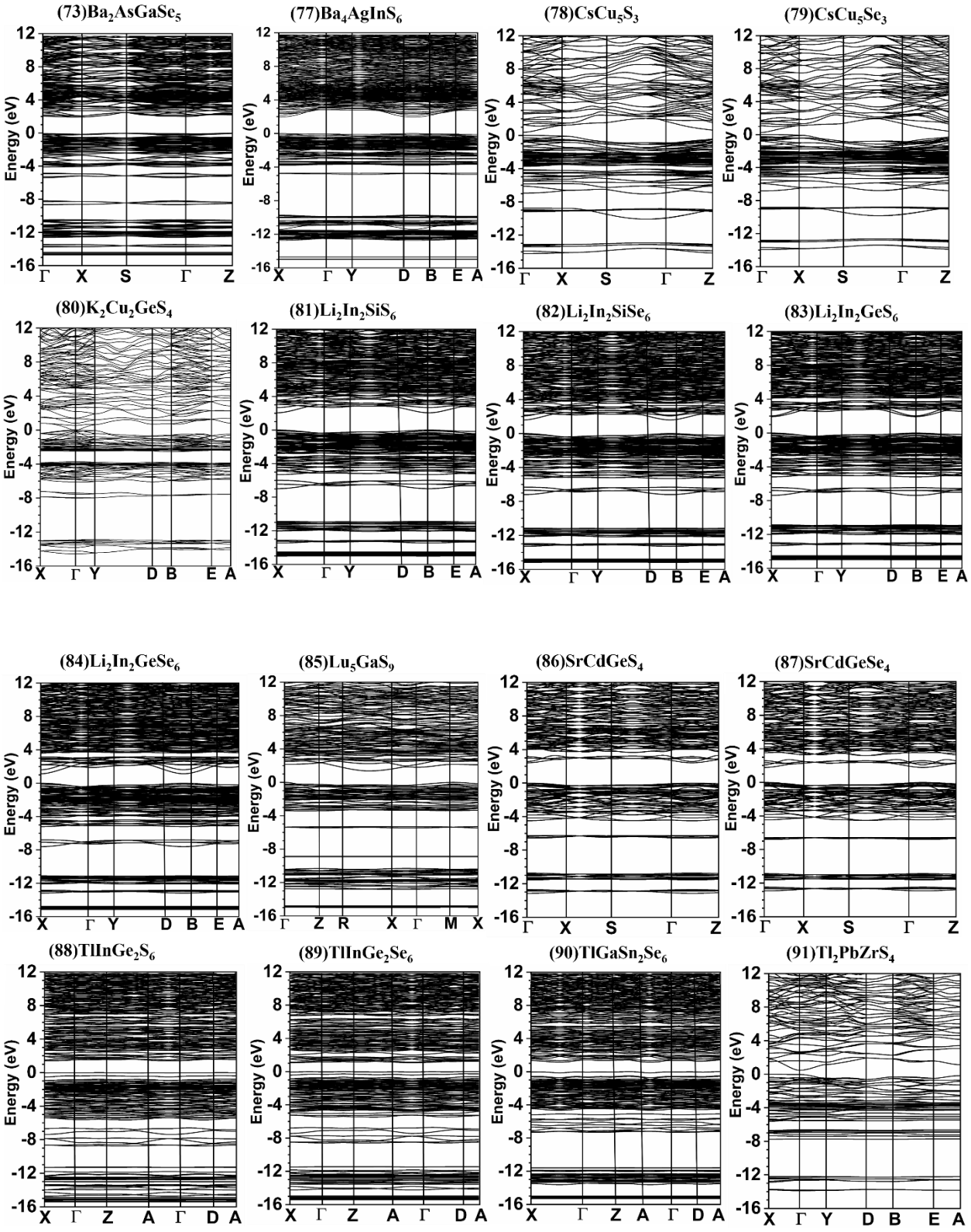
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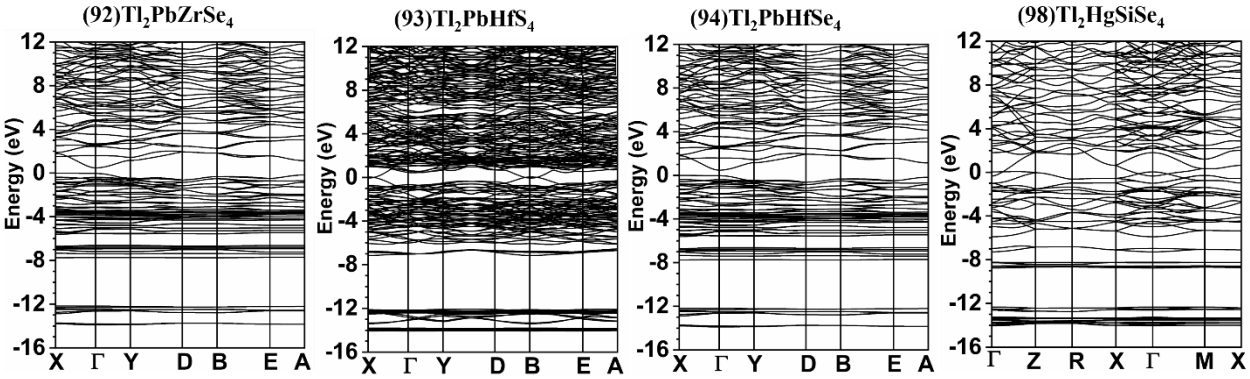
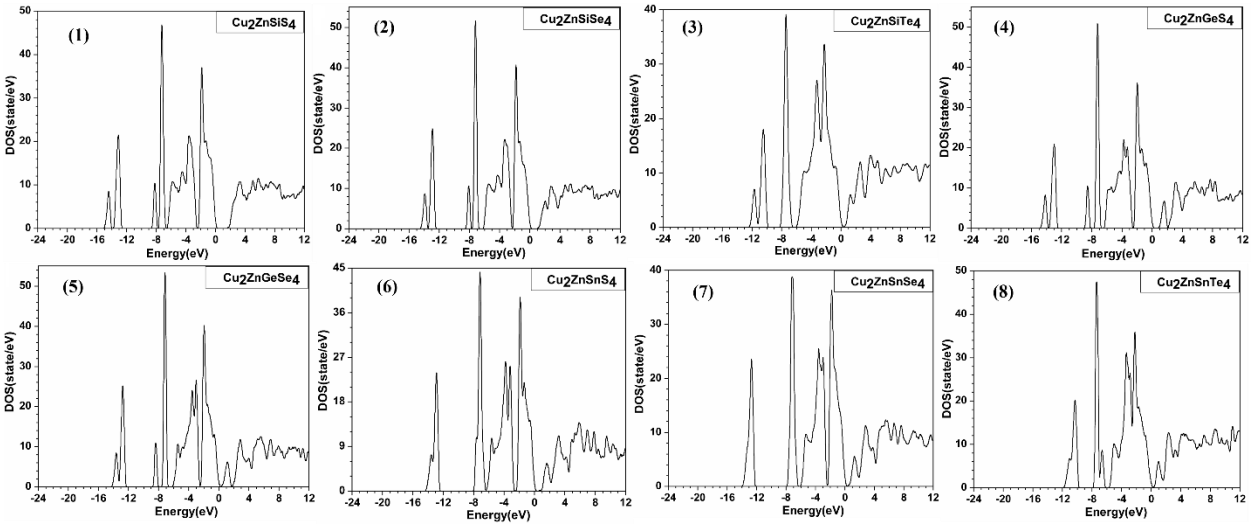
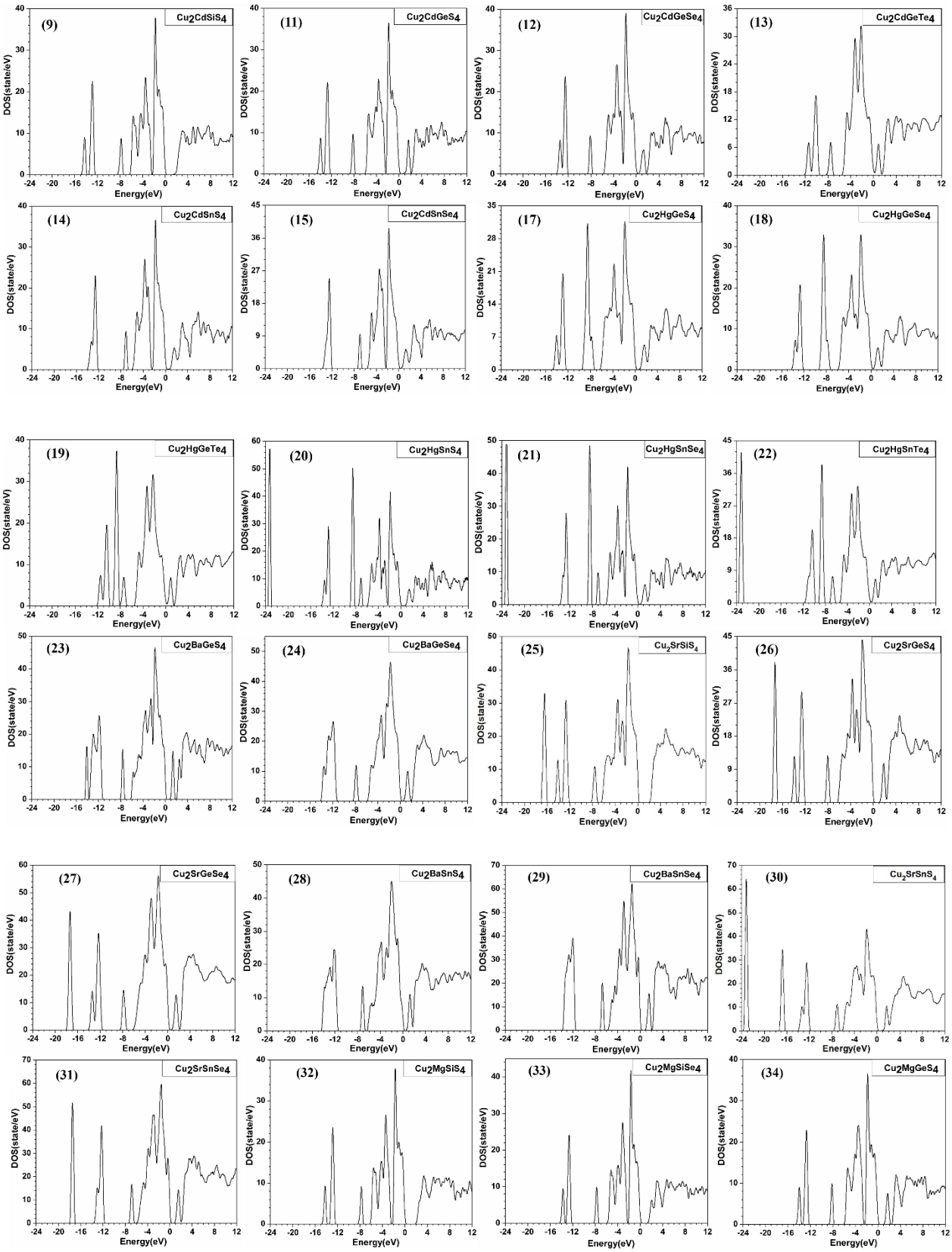


Fig.S1. Band structure for chalcogenide crystals.

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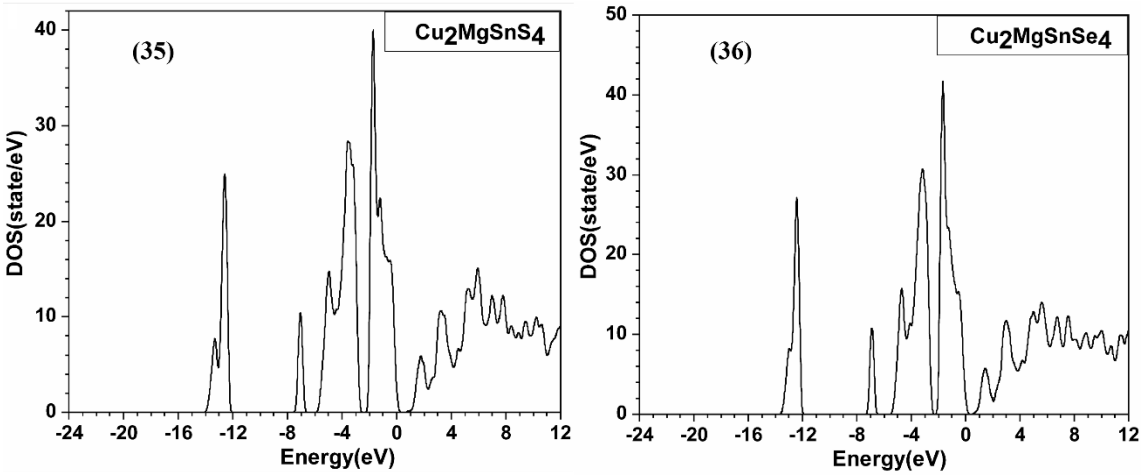
Energy(eV)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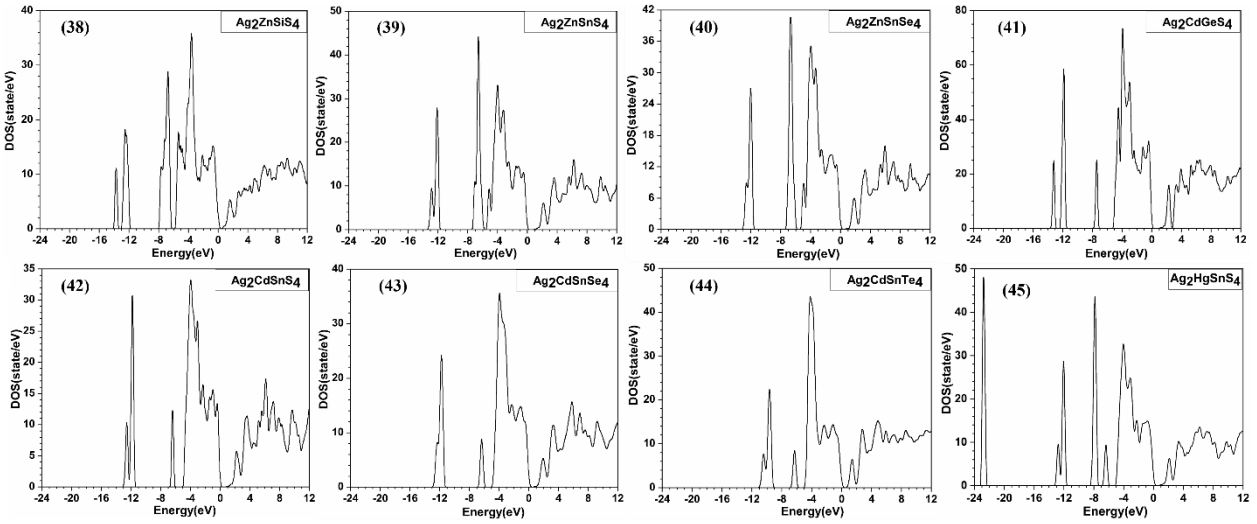
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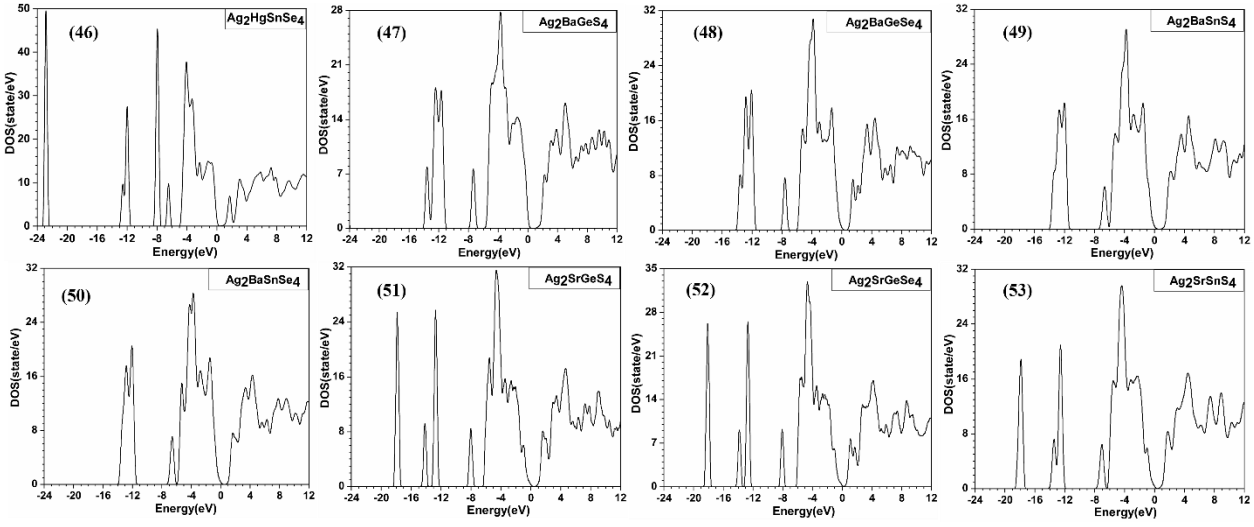
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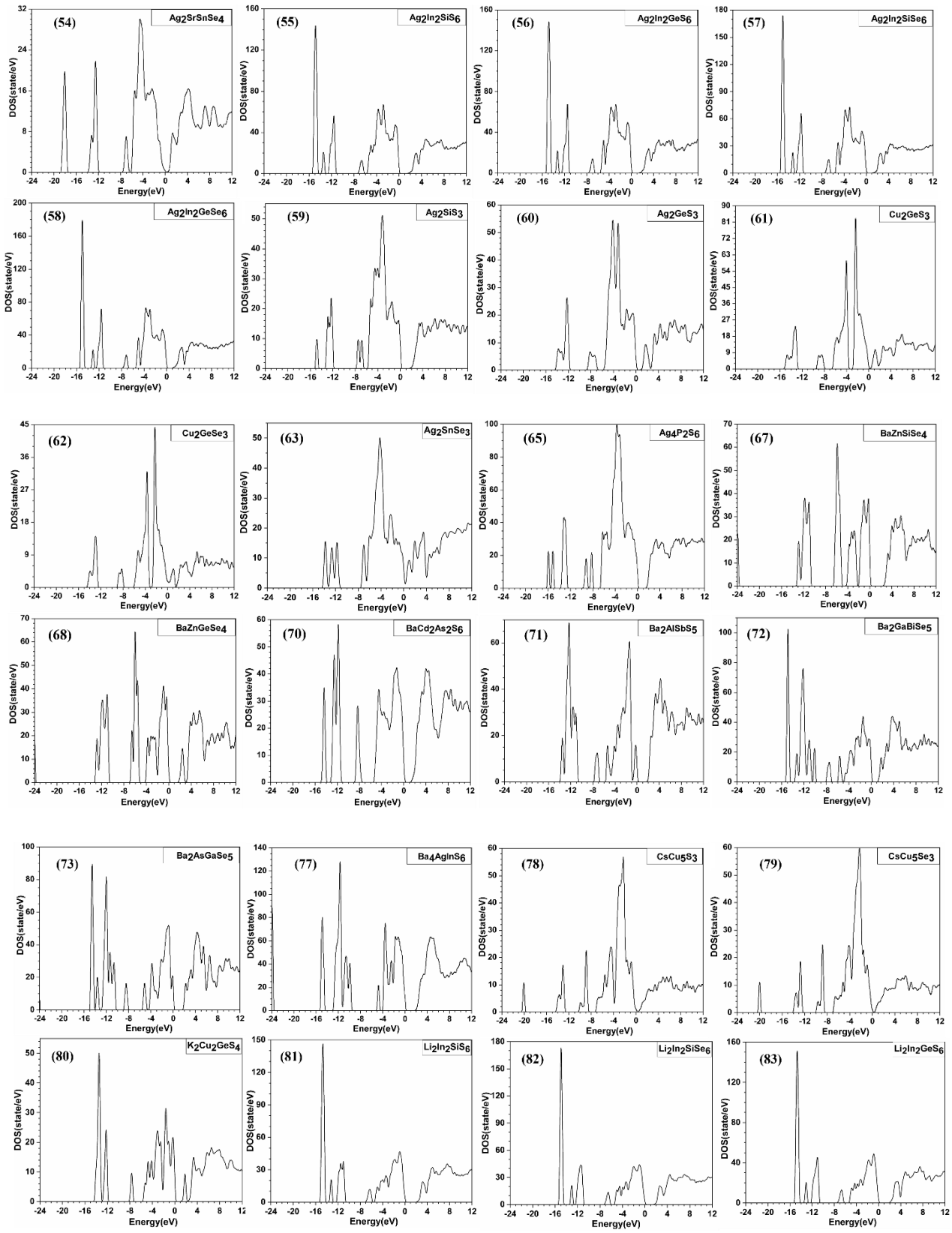
DOS(state/eV)
Energy(eV)


(54) Ag2SrSnSe4
(55) Ag2In2SiS6
(56) Ag2In2GeS6
(57) Ag2In2SiSe6
(58) Ag2In2GeSe6
(59) Ag2SiS3
(60) Ag2GeS3
(61) Cu2GeS3
(62) Cu2GeSe3
(63) Ag2SnSe3
(65) Ag4P2S6
(67) BaZnSiSe4
(68) BaZnGeSe4
(70) BaCd2As2S6
(71) Ba2AlSbS5
(72) Ba2GaBiSe5
(73) Ba2AsGaSe5
(77) Ba4AgInS6
(78) CsCu5S3
(79) CsCu5Se3
(80) K2Cu2GeS4
(81) Li2In2SiS6
(82) Li2In2SiSe6
(83) Li2In2GeS6
DOS(state/eV)
Energy(eV)

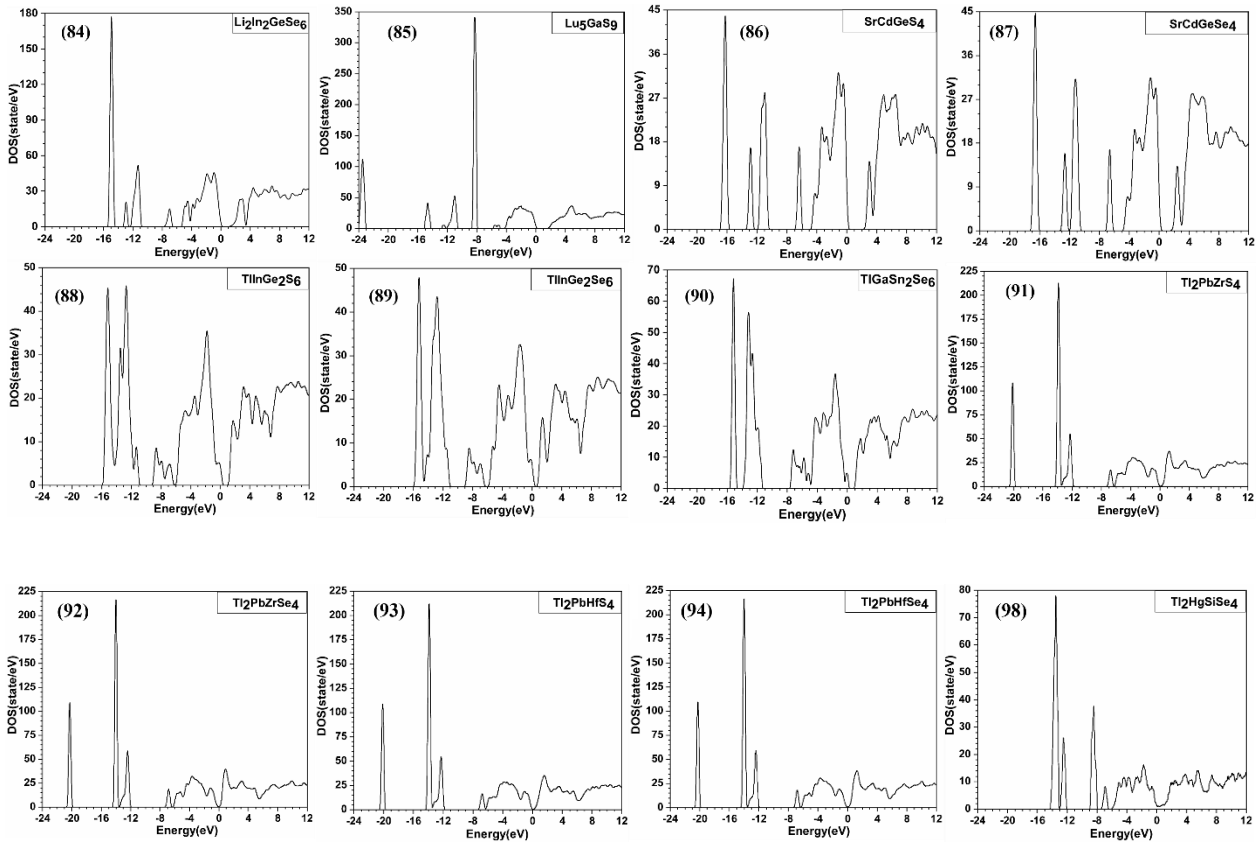


Fig. S2. TDOS for the chalcogenide crystals.

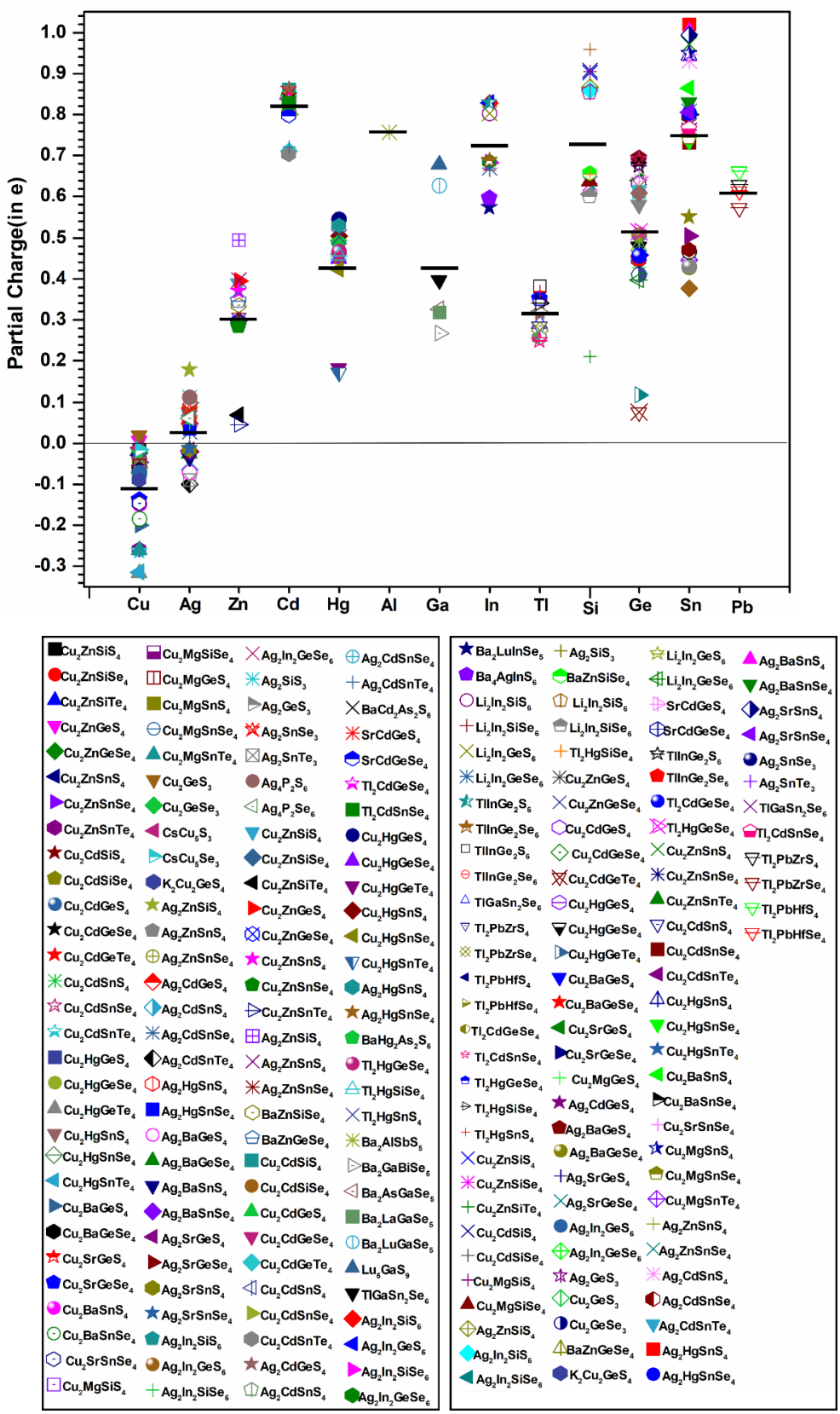


Fig. S3. Distribution of partial charge of the elements from Cu to Pb.

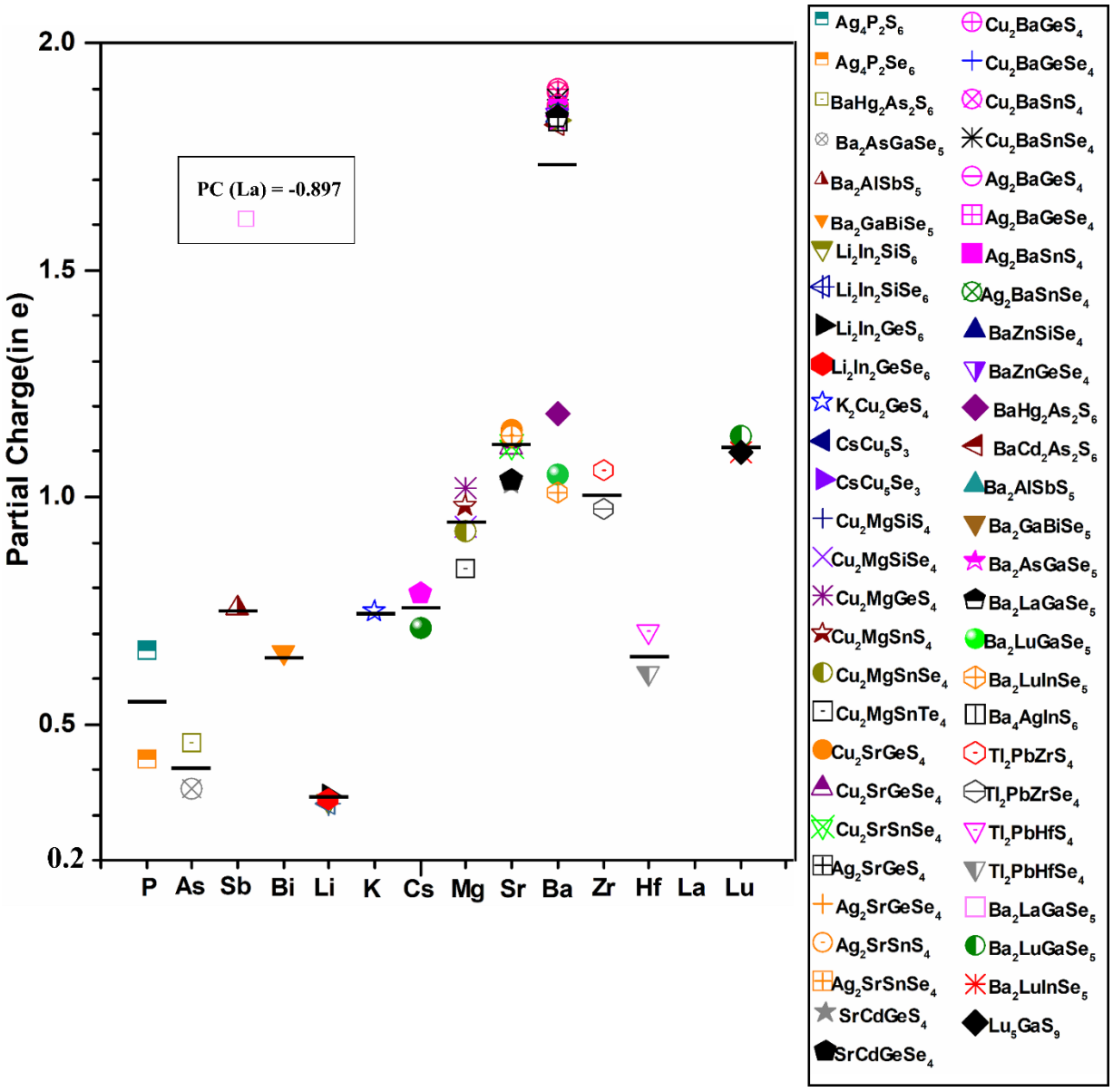


Fig. S4. Distribution of partial charge of the elements from P to Lu.

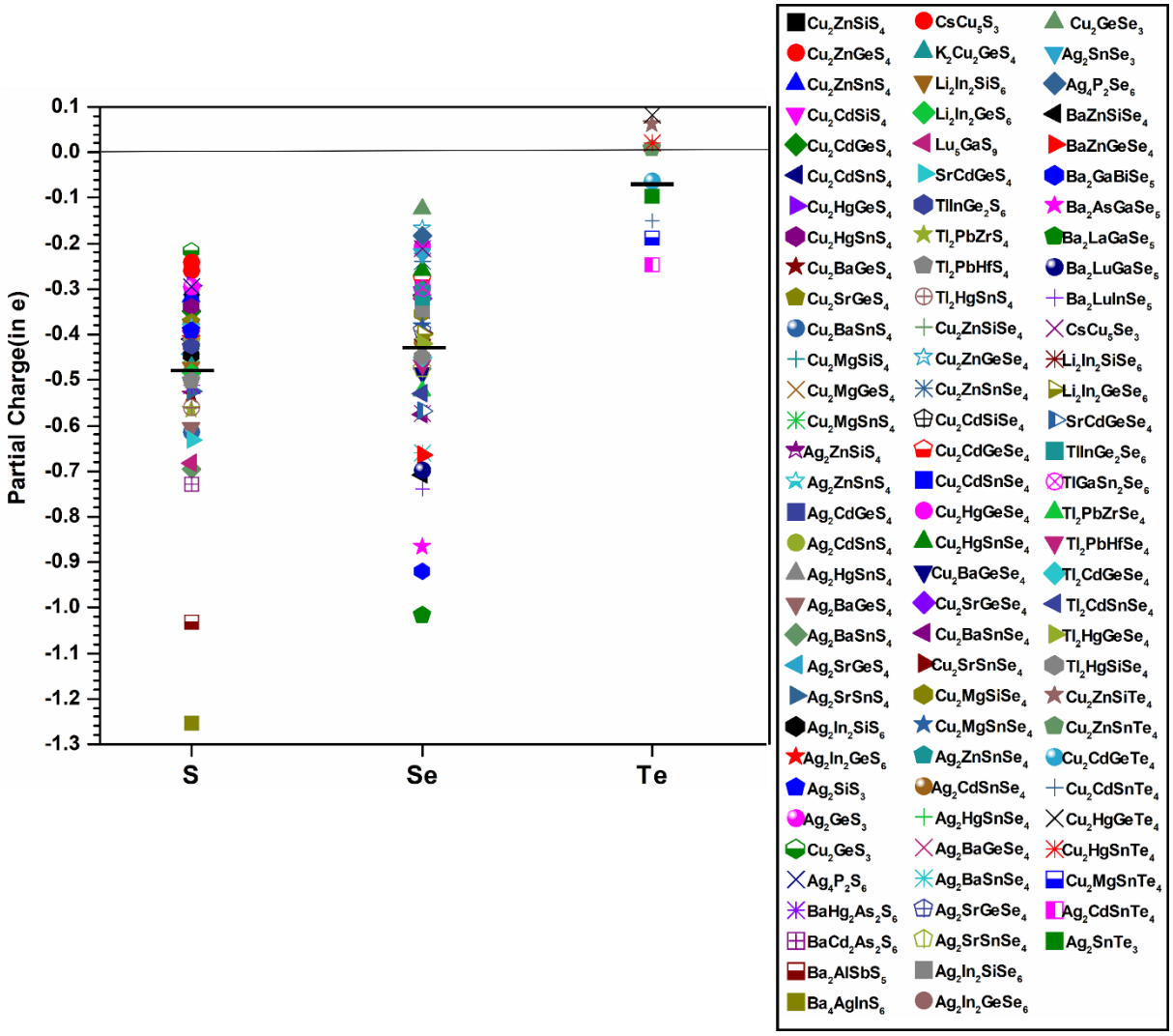
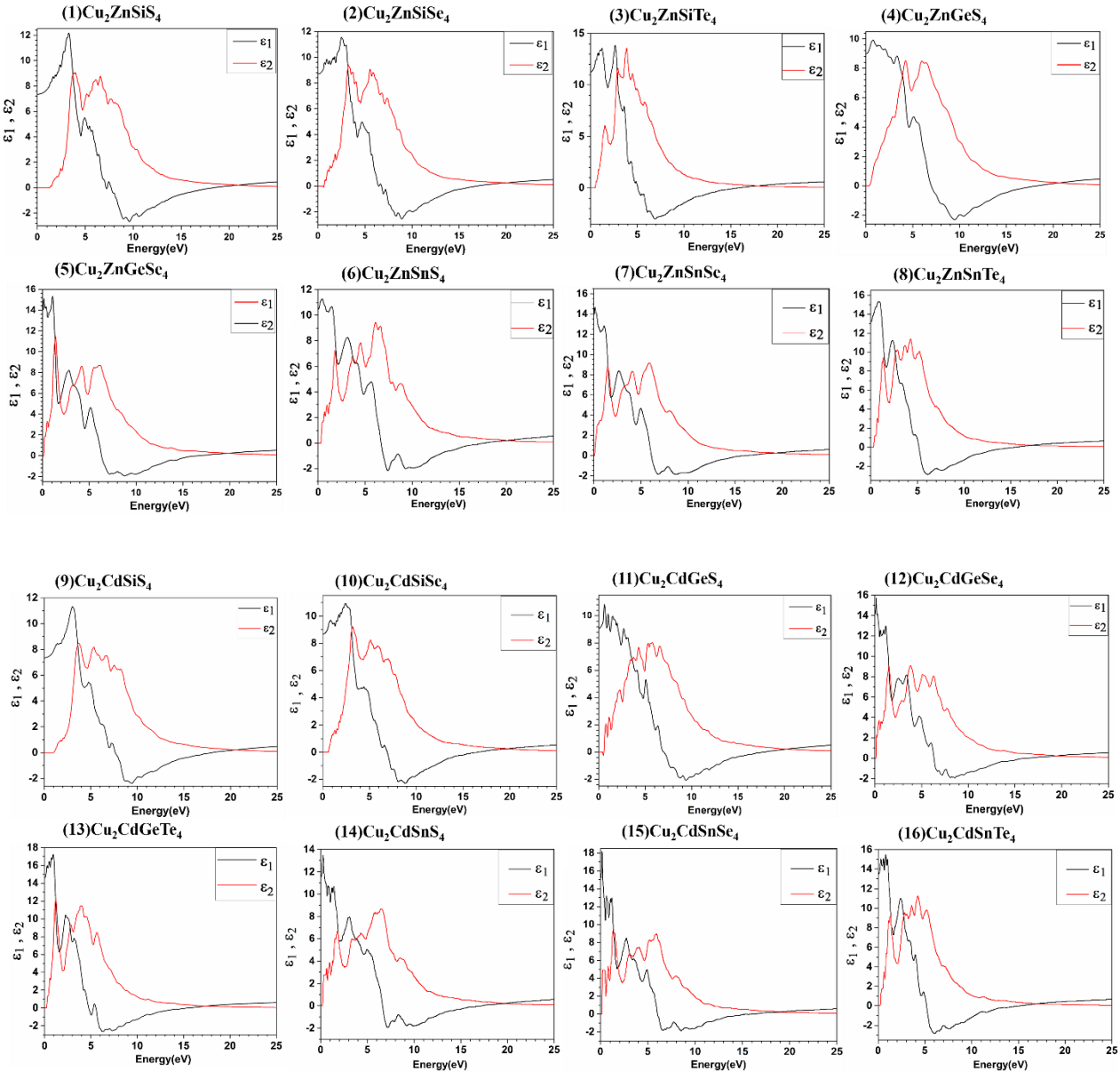
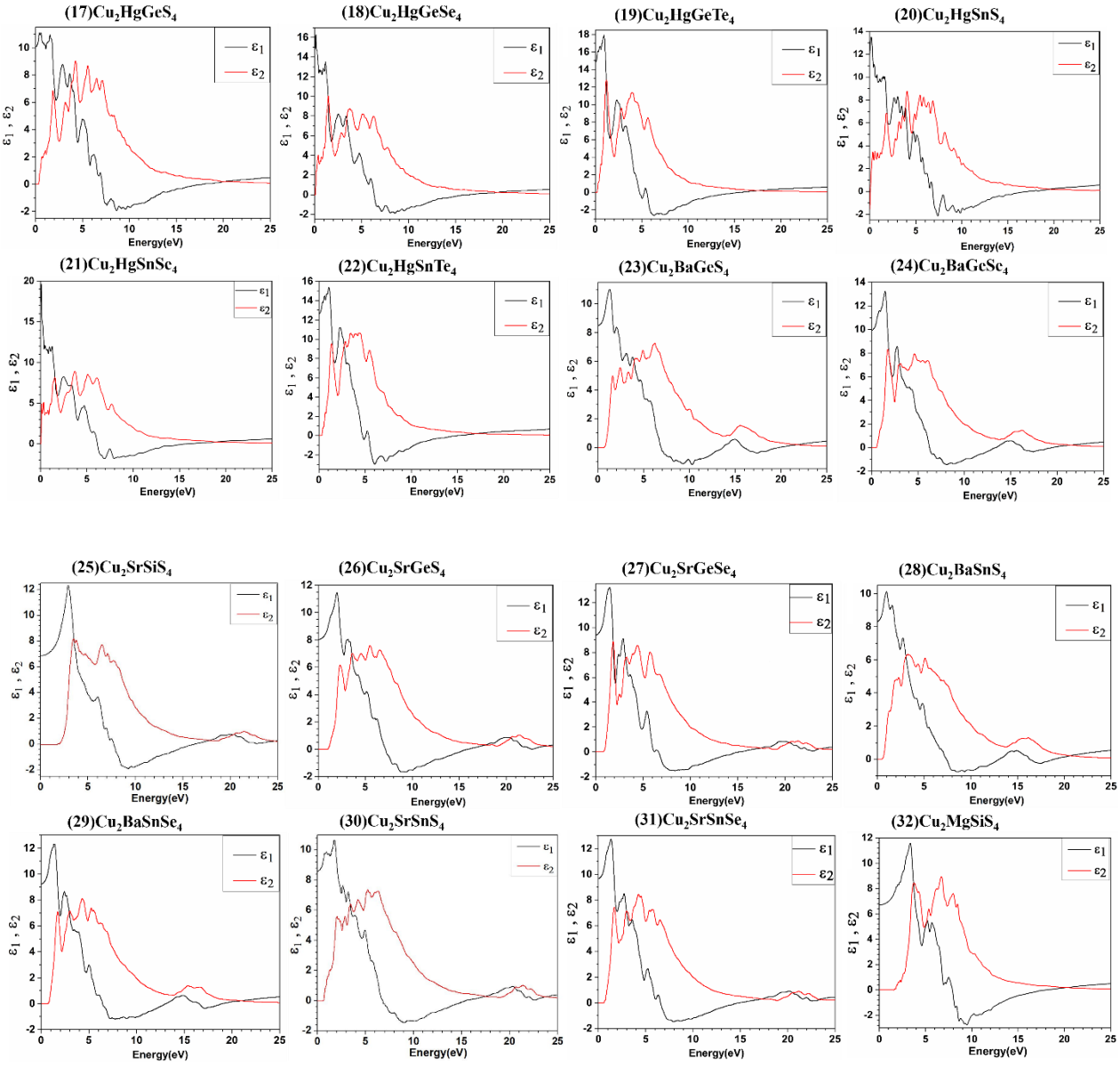
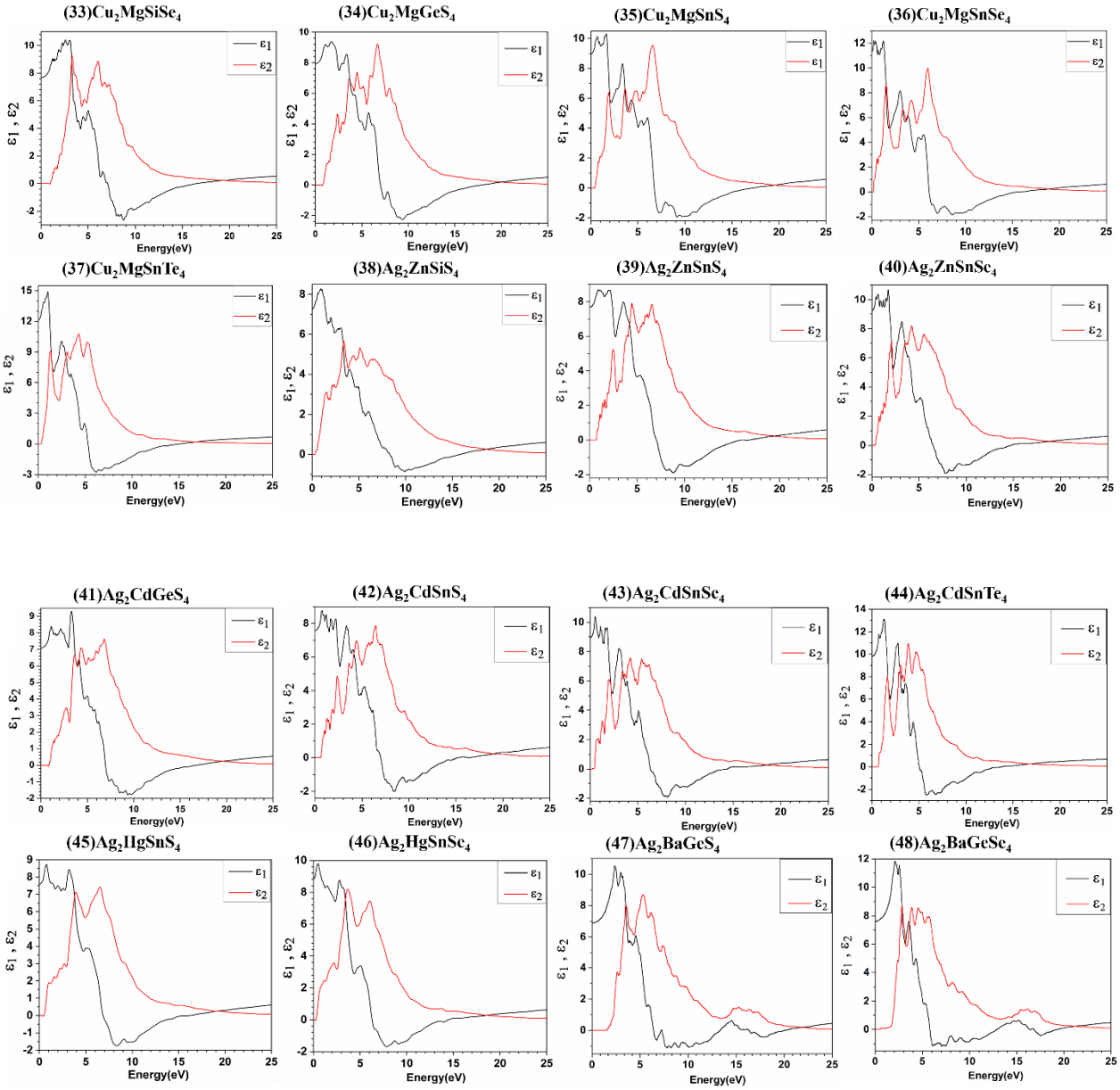
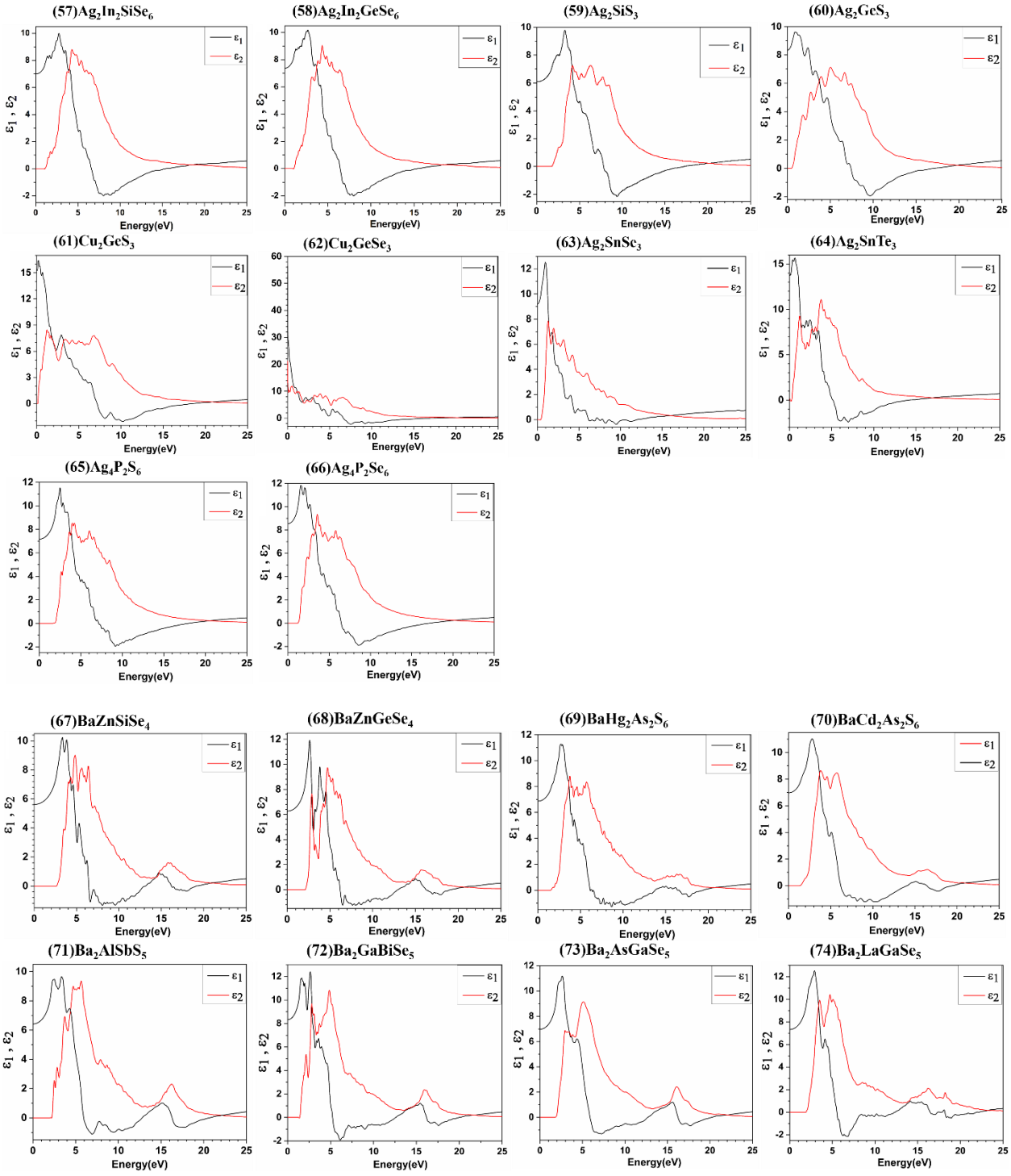


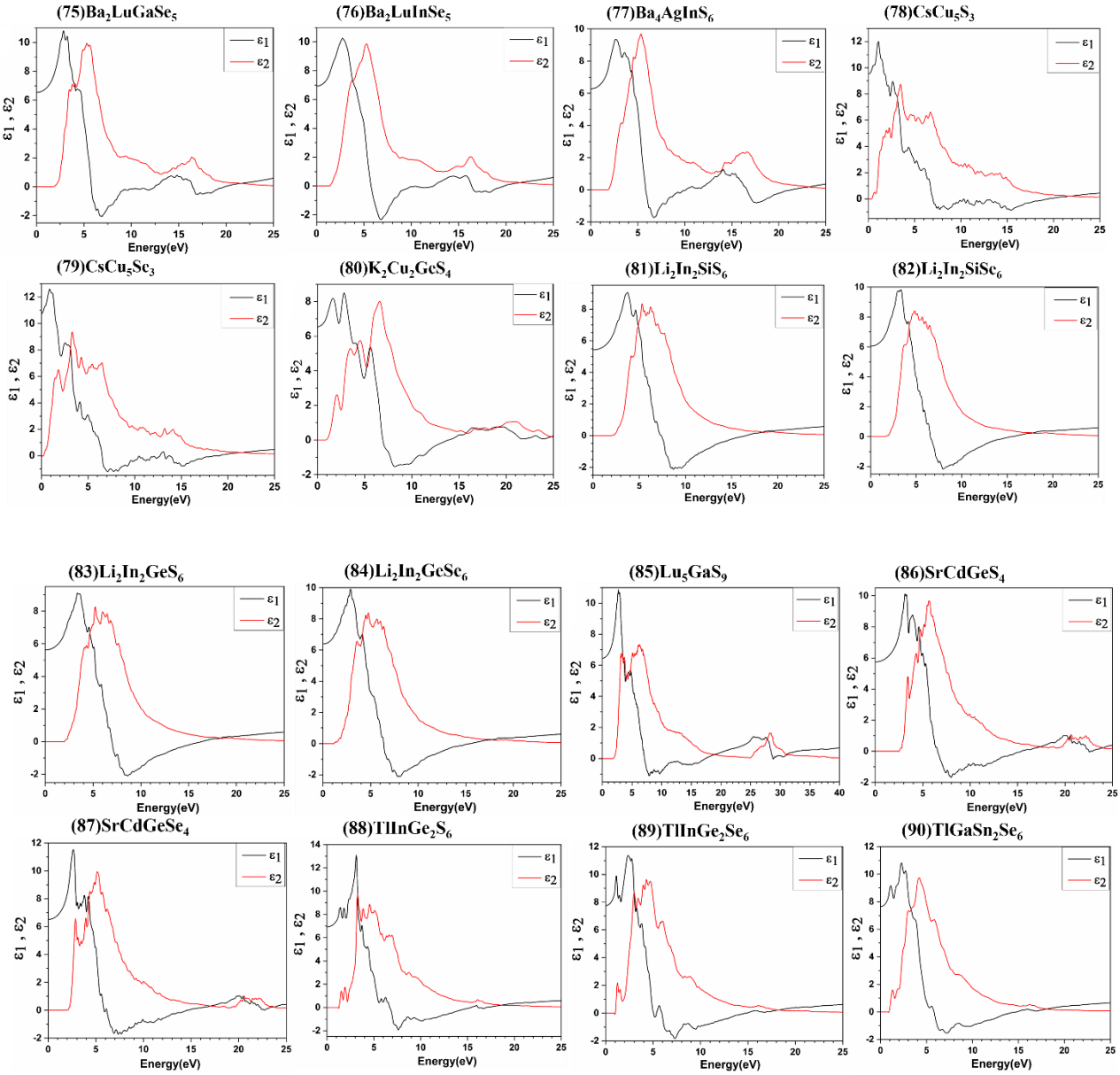
Fig. S5. Distribution of partial charge of the chalcogene elements(S, Se, Te).


(1)Cu2ZnSiS4
(2)Cu2ZnSiSe4
(3)Cu2ZnSiTe4
(4)Cu2ZnGeS4
(5)Cu2ZnGeSe4
(6)Cu2ZnSnS4
(7)Cu2ZnSnSe4
(8)Cu2ZnSnTe4
(9)Cu2CdSiS4
(10)Cu2CdSiSe4
(11)Cu2CdGeS4
(12)Cu2CdGeSe4
(13)Cu2CdGeTe4
(14)Cu2CdSnS4
(15)Cu2CdSnSe4
(16)Cu2CdSnTe4
ε1 , ε2
Energy(eV)
ε1
ε2


(17)Cu2HgGeS4
(18)Cu2HgGeSe4
(19)Cu2HgGeTe4
(20)Cu2HgSnS4
(21)Cu2HgSnSc4
(22)Cu2HgSnTe4
(23)Cu2BaGeS4
(24)Cu2BaGeSc4
(25)Cu2SrSiS4
(26)Cu2SrGeS4
(27)Cu2SrGeSe4
(28)Cu2BaSnS4
(29)Cu2BaSnSe4
(30)Cu2SrSnS4
(31)Cu2SrSnSe4
(32)Cu2MgSiS4
ε1 , ε2
Energy(eV)


(33)Cu2MgSiSe4
(34)Cu2MgGeS4
(35)Cu2MgSnS4
(36)Cu2MgSnSe4
(37)Cu2MgSnTe4
(38)Ag2ZnSiS4
(39)Ag2ZnSnS4
(40)Ag2ZnSnSc4
(41)Ag2CdGeS4
(42)Ag2CdSnS4
(43)Ag2CdSnSc4
(44)Ag2CdSnTe4
(45)Ag2IIgSnS4
(46)Ag2HgSnSc4
(47)Ag2BaGeS4
(48)Ag2BaGeSc4
ε1 , ε2
Energy(eV)
ε1
ε2


(57)Ag2In2SiSe6
(58)Ag2In2GeSe6
(59)Ag2SiS3
(60)Ag2GeS3
(61)Cu2GeS3
(62)Cu2GeSe3
(63)Ag2SnSc3
(64)Ag2SnTe3
(65)Ag4P2S6
(66)Ag4P2Se6
(67)BaZnSiSe4
(68)BaZnGeSe4
(69)BaHg2As2S6
(70)BaCd2As2S6
(71)Ba2AlSbS5
(72)Ba2GaBiSe5
(73)Ba2AsGaSe5
(74)Ba2LaGaSe5
ε1 , ε2
Energy(eV)


(75)Ba2LuGaSe5
(76)Ba2LuInSe5
(77)Ba4AgInS6
(78)CsCu5S3
(79)CsCu5Se3
(80)K2Cu2GeS4
(81)Li2In2SiS6
(82)Li2In2SiSc6
(83)Li2In2GeS6
(84)Li2In2GeSe6
(85)Lu5GaS9
(86)SrCdGeS4
(87)SrCdGeSe4
(88)TlInGe2S6
(89)TlInGe2Se6
(90)TlGaSn2Se6
ε1
ε2
ε1 , ε2
Energy(eV)

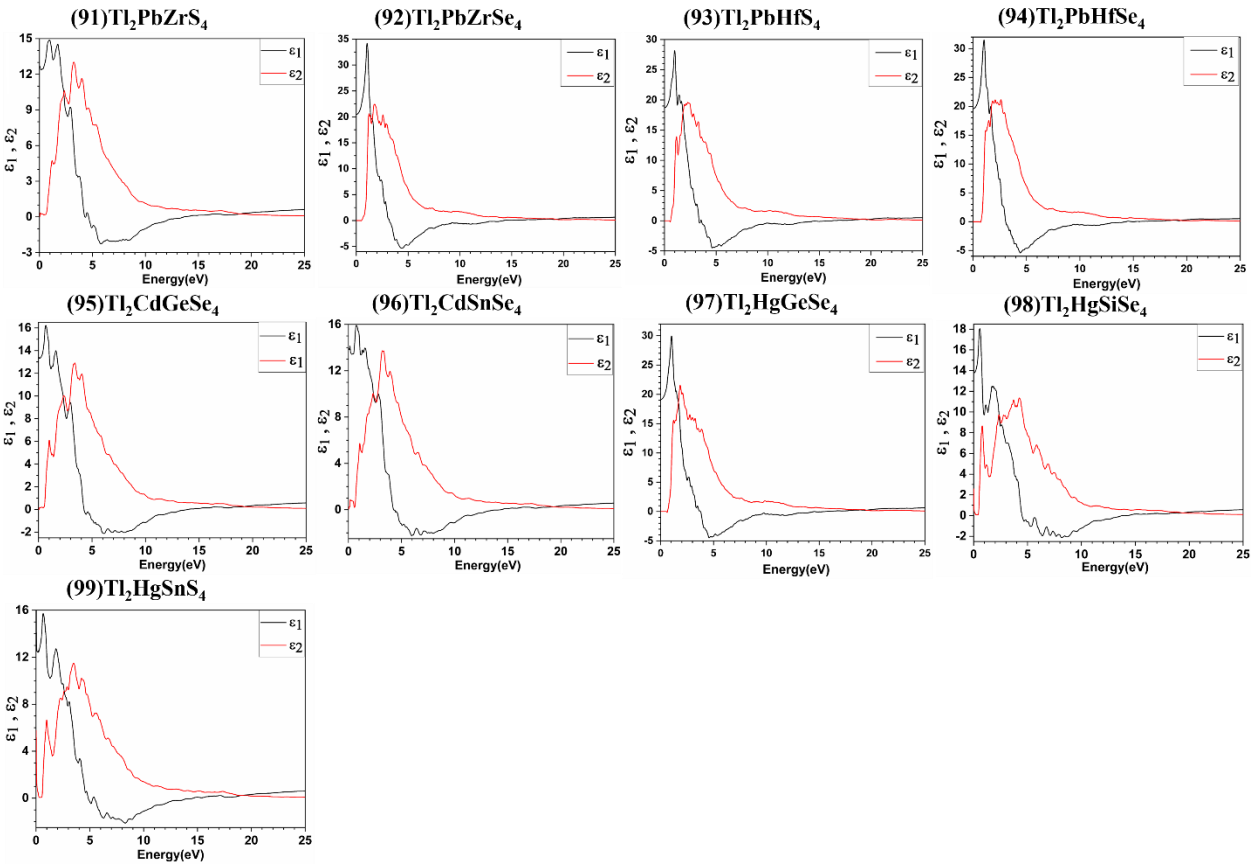
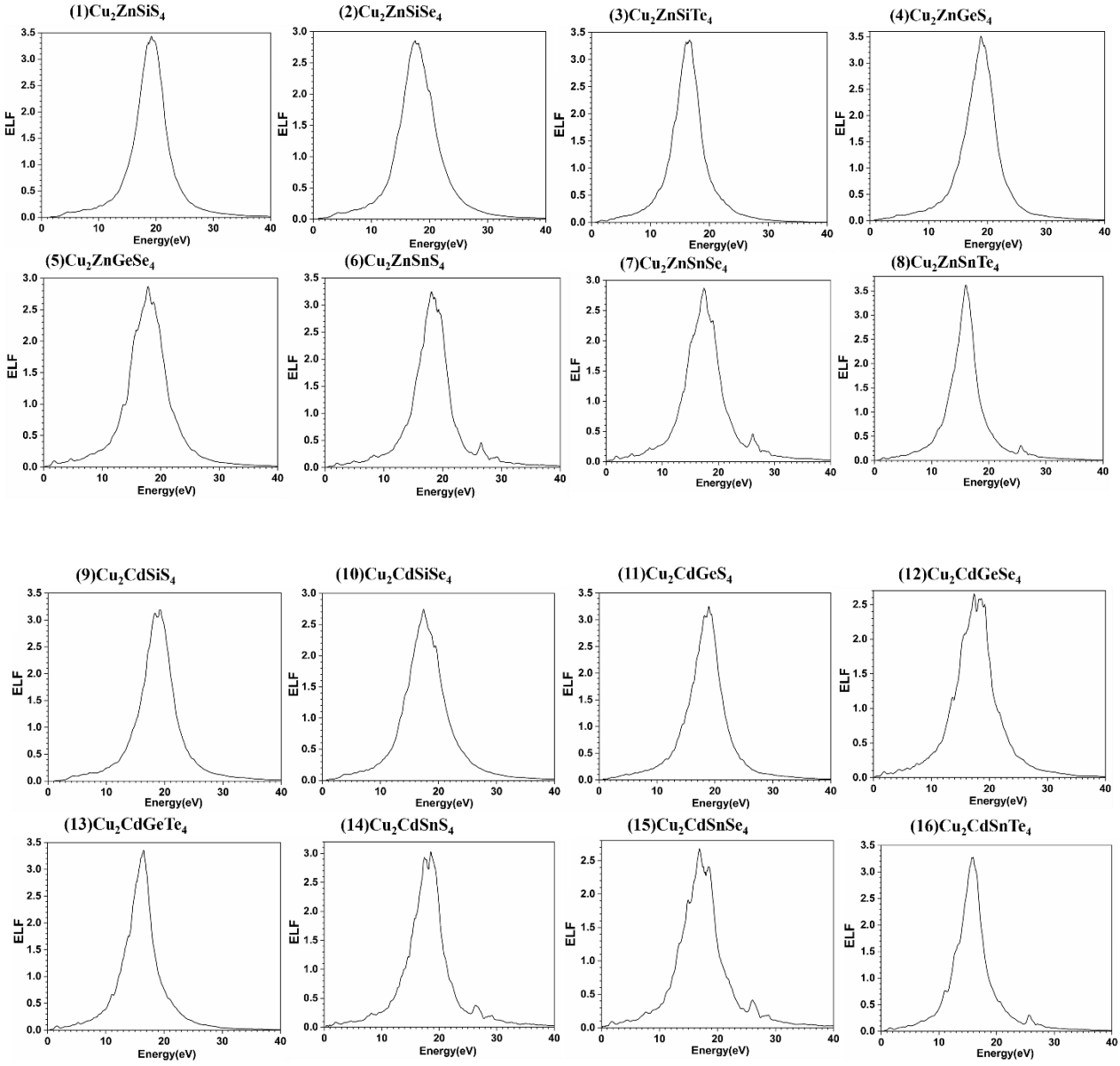
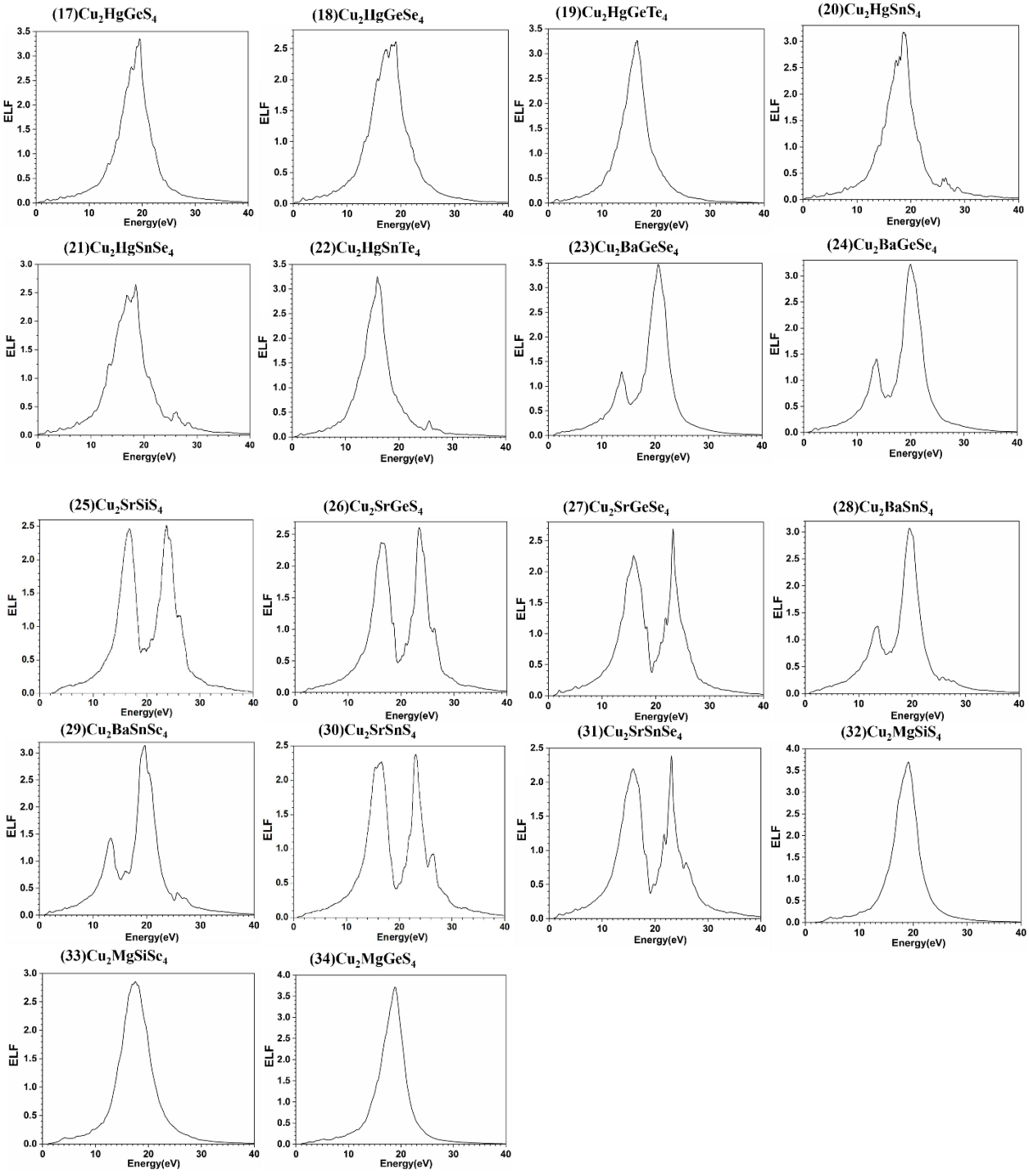
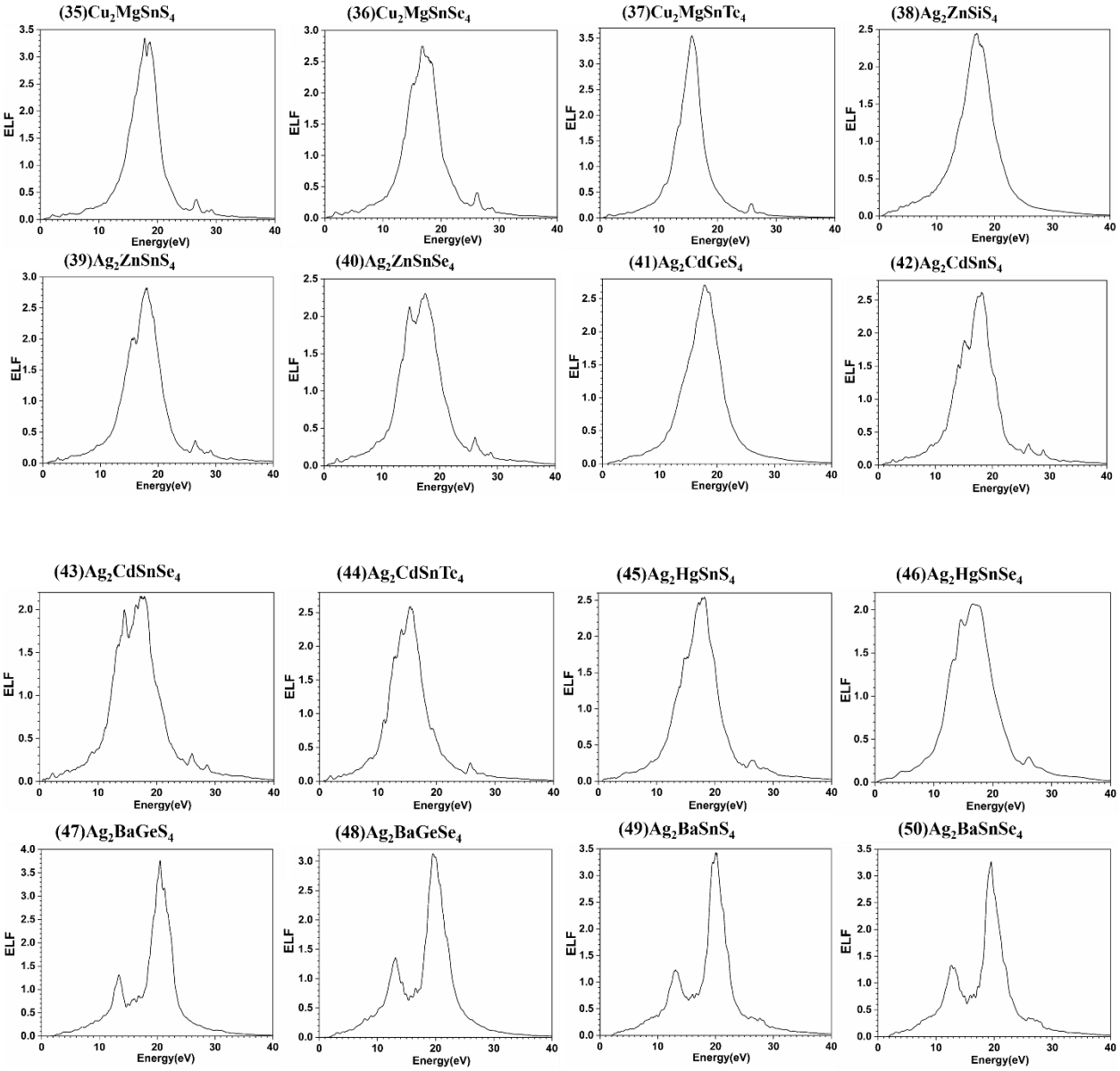
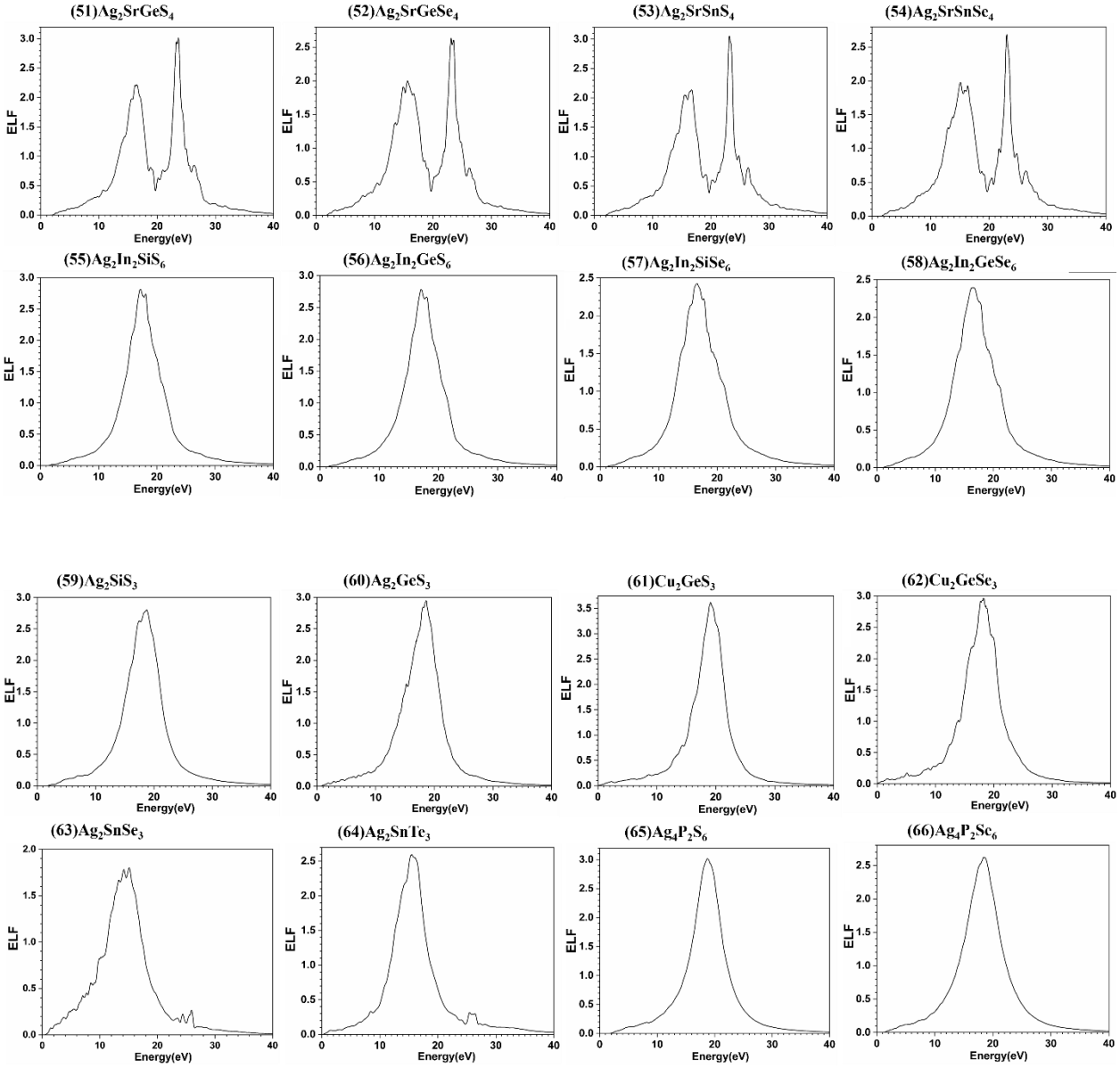


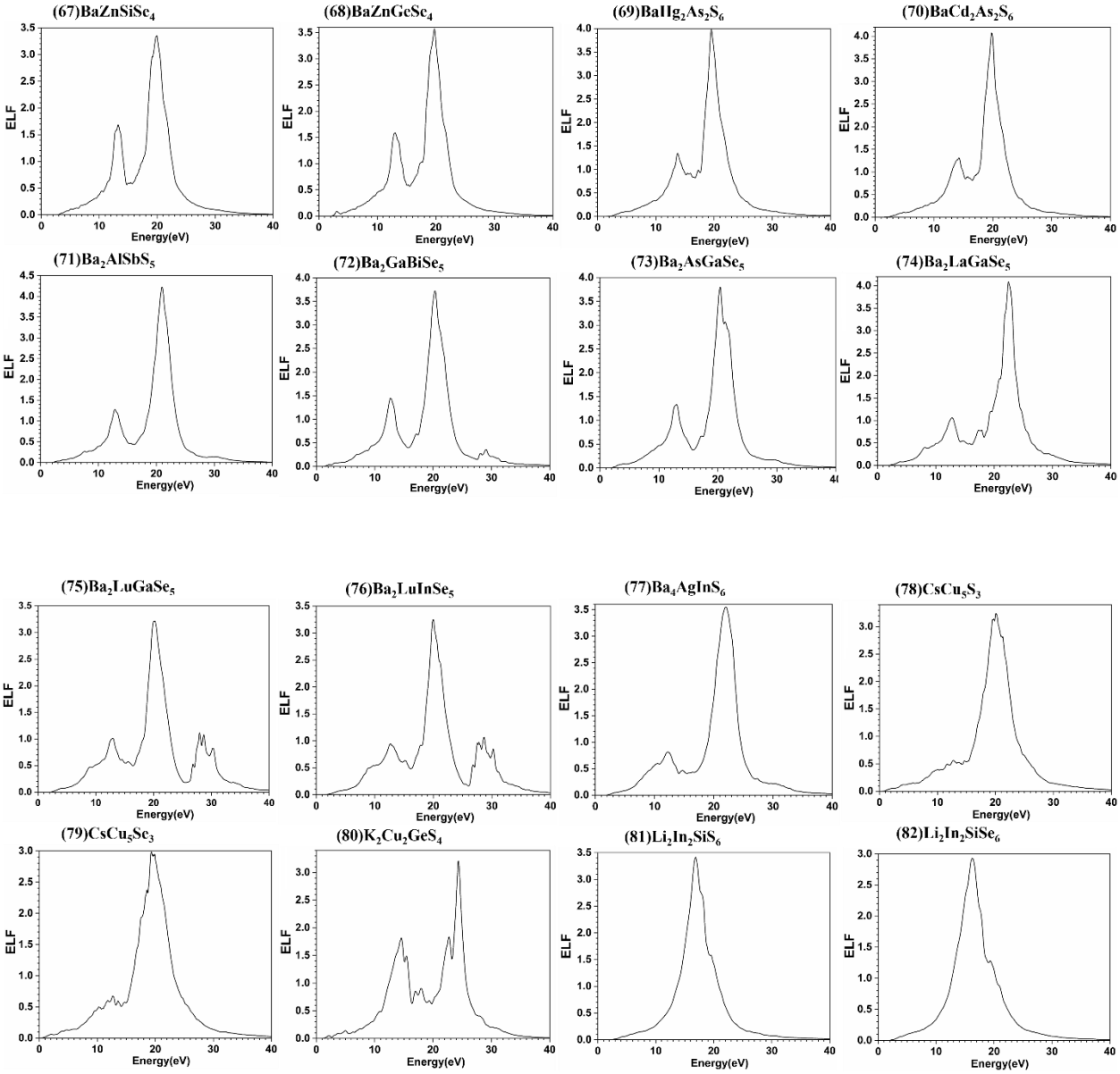
Fig. S6. Optical dielectric function for the chalcogenide crystals. The black curve for the real part (ε_1), the red curve for the imaginary part (ε_2).


(1)Cu2ZnSiS4
(2)Cu2ZnSiSe4
(3)Cu2ZnSiTe4
(4)Cu2ZnGeS4
(5)Cu2ZnGeSe4
(6)Cu2ZnSnS4
(7)Cu2ZnSnSe4
(8)Cu2ZnSnTe4
(9)Cu2CdSiS4
(10)Cu2CdSiSe4
(11)Cu2CdGeS4
(12)Cu2CdGeSe4
(13)Cu2CdGeTe4
(14)Cu2CdSnS4
(15)Cu2CdSnSe4
(16)Cu2CdSnTe4
ELF
Energy(eV)


(17)Cu2HgGeS4
(18)Cu2HgGeSe4
(19)Cu2HgGeTe4
(20)Cu2HgSnS4
(21)Cu2HgSnSe4
(22)Cu2HgSnTe4
(23)Cu2BaGeSe4
(24)Cu2BaGeSe4
(25)Cu2SrSiS4
(26)Cu2SrGeS4
(27)Cu2SrGeSe4
(28)Cu2BaSnS4
(29)Cu2BaSnSe4
(30)Cu2SrSnS4
(31)Cu2SrSnSe4
(32)Cu2MgSiS4
(33)Cu2MgSiSe4
(34)Cu2MgGeS4
ELF
Energy(eV)


(35)Cu2MgSnS4
(36)Cu2MgSnSe4
(37)Cu2MgSnTe4
(38)Ag2ZnSiS4
(39)Ag2ZnSnS4
(40)Ag2ZnSnSe4
(41)Ag2CdGeS4
(42)Ag2CdSnS4
(43)Ag2CdSnSe4
(44)Ag2CdSnTe4
(45)Ag2HgSnS4
(46)Ag2HgSnSe4
(47)Ag2BaGeS4
(48)Ag2BaGeSe4
(49)Ag2BaSnS4
(50)Ag2BaSnSe4
ELF
Energy(eV)


(51)Ag2SrGeS4
(52)Ag2SrGeSe4
(53)Ag2SrSnS4
(54)Ag2SrSnSe4
(55)Ag2In2SiS6
(56)Ag2In2GeS6
(57)Ag2In2SiSe6
(58)Ag2In2GeSe6
(59)Ag2SiS3
(60)Ag2GeS3
(61)Cu2GeS3
(62)Cu2GeSe3
(63)Ag2SnSe3
(64)Ag2SnTe3
(65)Ag4P2S6
(66)Ag4P2Sc6
ELF
Energy(eV)


(67)BaZnSiSe4
(68)BaZnGeSe4
(69)BaHg2As2S6
(70)BaCd2As2S6
(71)Ba2AlSbS5
(72)Ba2GaBiSe5
(73)Ba2AsGaSe5
(74)Ba2LaGaSe5
(75)Ba2LuGaSe5
(76)Ba2LuInSe5
(77)Ba4AgInS6
(78)CsCu5S3
(79)CsCu5Se3
(80)K2Cu2GeS4
(81)Li2In2SiS6
(82)Li2In2SiSe6
ELF
Energy(eV)

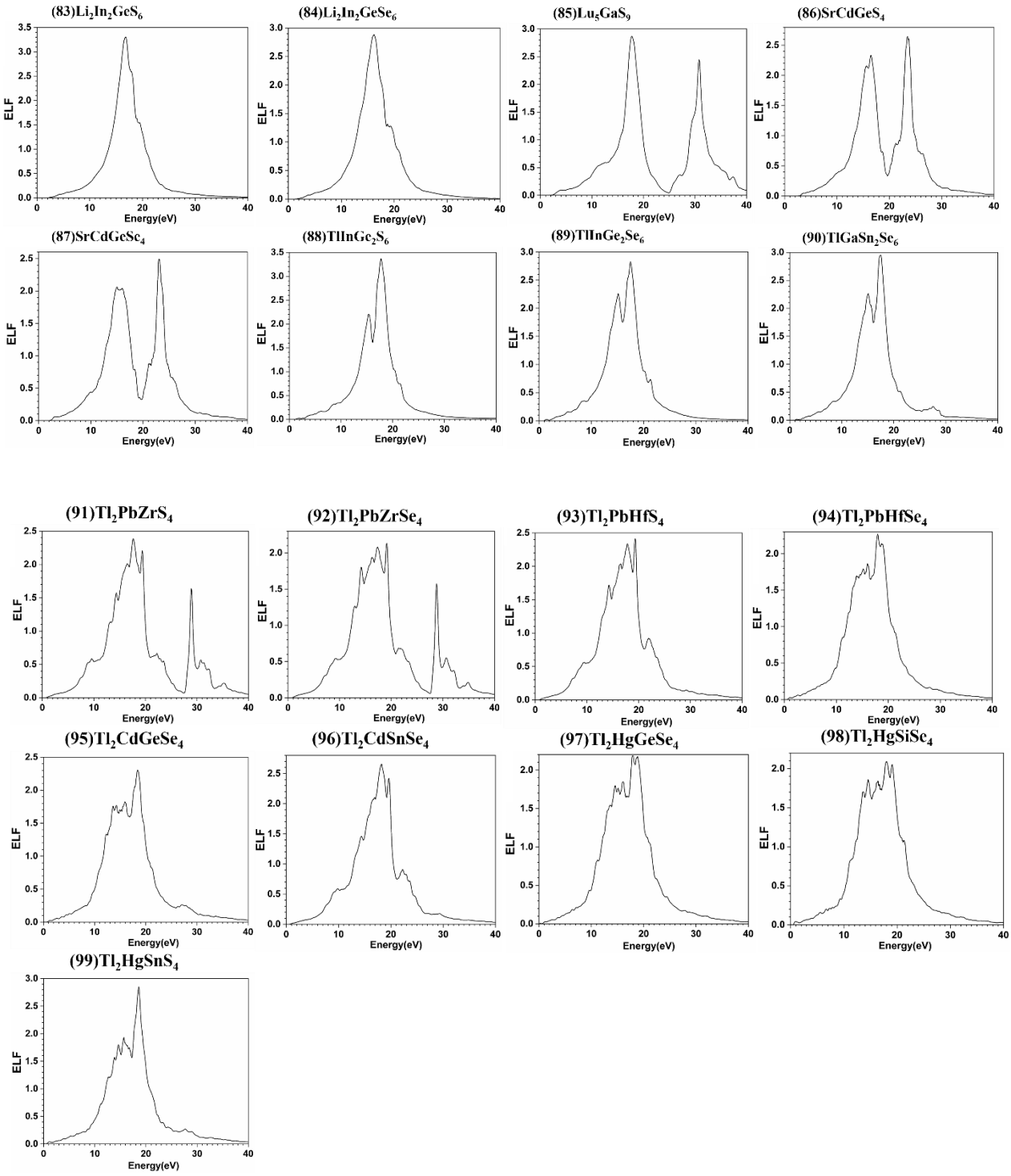


Fig. S7. The Optical Loss function for the chalcogenide crystals

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