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Properties of Novel Non-Silicon Materials for Photovoltaic Applications: A First-Principle Insight

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Table S1. Calculated GGA band gap values for 30 compounds with lattice parameters.

S.No	Chemical formula	Space group	Pearson symbol	Lattice Parameter(computed)			Energy gap (in eV)	Type of band gap
				a	b	c		
1	$TlBiS_2$	R-3m(166)	hR4	7.817			0.5055	Direct
2	$BaGe_2$	*Pnma* (62)	oP24	6.860	9.196	11.678	0.5235	Indirect
3	Gd_2S_3	*Pnma* (62)	oP20	3.930	10.580	10.790	0.526	Direct
4	$GaTlTe_2$	*I*4/*mcm* (140)	tI16	7.020			0.5618	Indirect
5	GeP	*C*2/*m* (12)	mS24	7.990		9.350	0.5719	Direct
6	Ca_2CuFeO_3S	*P*4/*nmm* (129)	tP16	3.88		14.94	0.6339	Indirect
7	$Fe_2Ga_2S_5$	*P*-3*m*1 (164)	hP9	3.690		15.570	0.6558	Indirect
8	$Ca_2Fe_2O_5$	*Pnma* (62)	oP36	5.538	5.6589	14.885	0.6614	Direct
9	Ba_3BiN	*P*6$_3$/*mmc*(194)	hP10	7.770		6.805	0.6705	Direct
10	Cu_2GeZnS_4	*I*-42*m* (121)	tI16	6.552			0.6729	Direct
11	$CdCu_2GeS_4$	*Pmn*2$_1$ (31)	oP16	6.359	6.627	7.779	0.6863	Direct
12	$CdGeP_2$	*I*-42*d* (122)	tI16	6.838			0.6942	Direct
13	$ZnSnP_2$	*I*-42*d* (122)	tI16	7.0146			0.6984	Direct
14	$CdMn_2O_4$	*I*4$_1$/*amd* (141)	tI28	6.5092			0.7017	Indirect
15	Ag_2BaS_2	*P*-3*m*1 (164)	hP9	4.4251		7.2810	0.7161	Direct
16	$CuKZrS_3$	*Cmcm* (63)	oS24	7.3557		9.8515	0.7388	Direct
17	$CuFeO_3SSr_2$	*P*4/*nmm* (129)	tP16	3.9557		15.7502	0.7516	Indirect
18	$KMnNaO_2$	*Cccm* (66)	oS40	6.8241		7.1011	0.7749	Direct
19	Cu_2GeS_4Zn	*Pmn*2$_1$ (31)	oP16	6.2223	6.5706	7.4744	0.7798	Direct
20	Fe_2MnO_4	*Fd*-3*m* (227)	cF56	6.1012			0.7842	Indirect
21	MnO_3Sr	P63/mmc(194)	hP20	5.5350		9.2802	0.8325	Indirect
22	Cu_2GeMnS_4	*Pmn*2$_1$ (31)	oP16	6.2986	6.5754	7.6952	0.886	Indirect
23	ZrSO	*P*4/*nmm* (129)	tP6	3.6280		6.4154	0.8964	Direct
24	$Mn_2Na_{14}O_9$	*P*-3 (147)	hP25	6.7098		9.4004	0.9245	Indirect
25	$FeGeO_3$	*C*2/*c* (15)	mS40	6.7799		5.2895	0.9459	Indirect
26	$K_3Ni_2O_4$	*Cmcm* (63)	oS36	5.5013		10.6834	1.0845	Indirect
27	$MnNaO_2$	*Pmmn* (59)	oP8	5.8575		6.7005	1.1331	Indirect

The initial structural parameters of a thousand compounds were directly taken from the ICSD database[1], and then GGA band gap for thousand non-silicon compounds were calculated in our DFTB database[2]. These are multinary compounds including conductors, semiconductors, and insulators. Among these thousand non-silicon compounds we considered twenty-seven of them with GGA band gap values in the range of 0.5–1.1 eV (Table S1). Among these twenty-seven compounds, we identified fourteen compounds as direct band gap semiconductors and thirteen as indirect band gap semiconductors. We carried out a study on both electronic and optical properties of twenty-seven semiconductors (both direct and indirect). Our study on the optical properties of the semiconductor

materials showed that four direct band gaps among the twenty-seven materials had higher absorption coefficients in the visible region. Due to the space constraint, the optical properties of all the twenty-seven semiconductors are not presented in the supporting information part

Table S2. Calculated structural parameters and atomic positions of $TlBiS_2$, Ba_3BiN, Ag_2BaS_2, and ZrSO.

Phase	Lattice parameter						*Atomic positions*
	a	*b*	*c*	*α(deg)*	*β(deg)*	*γ(deg)*	
$TlBiS_2$ -R-3m ;166	7.817(7.711[a])			30.83	30.83	30.83	[a]Bi(3a): 0.000 0.000 0.000 [a]Tl(9d): ½ ½ ½ [a]S(36i) : 0.237 0.237 0.237
Ba_3BiN-$P6_3/mmc$;194	7.770 (7.6128[b])		6.805 (6.6805[b])	90	90	120	[b]Ba(6h): 0.1605 -0.1605 ¼ [b]Bi(2d): 1/3 2/3 ¾ [b]N(2a): 0.000 0.000 0.000
Ag_2BaS_2- *P*-3*m*1 ;164	4.4251(4.3861[c])		7.2810(7.1942[c])	90	90	120	[c]S(2d) : 1/3 2/3 0.25296 [c]Ba(1a) : 0.000 0.000 0.000 [c]Ag(2d) : 1/3 2/3 0.62252
ZrSO-P4/nmm; 129	3.6280		6.4154	90	90	90	[d]Zr(*2c*): 0, ½, 0.1950 [d]S(*2c*): 0, ½, 0.6330 [d]O(*2a*): 0, 0, 0
ZrSO-$P2_13$; 198	5.6960						[e]Zr(*4a*): 0.071, 0.071, 0.071 [e]S(*4a*): 0.3335, 0.3335, 0.3335 [e]O(*4a*): 0.6535, 0.6535, 0.6535

[a]Reference [3]; [b]Reference [4]; [c]Reference [5]; [d]Reference [6]; [e]Reference [7].

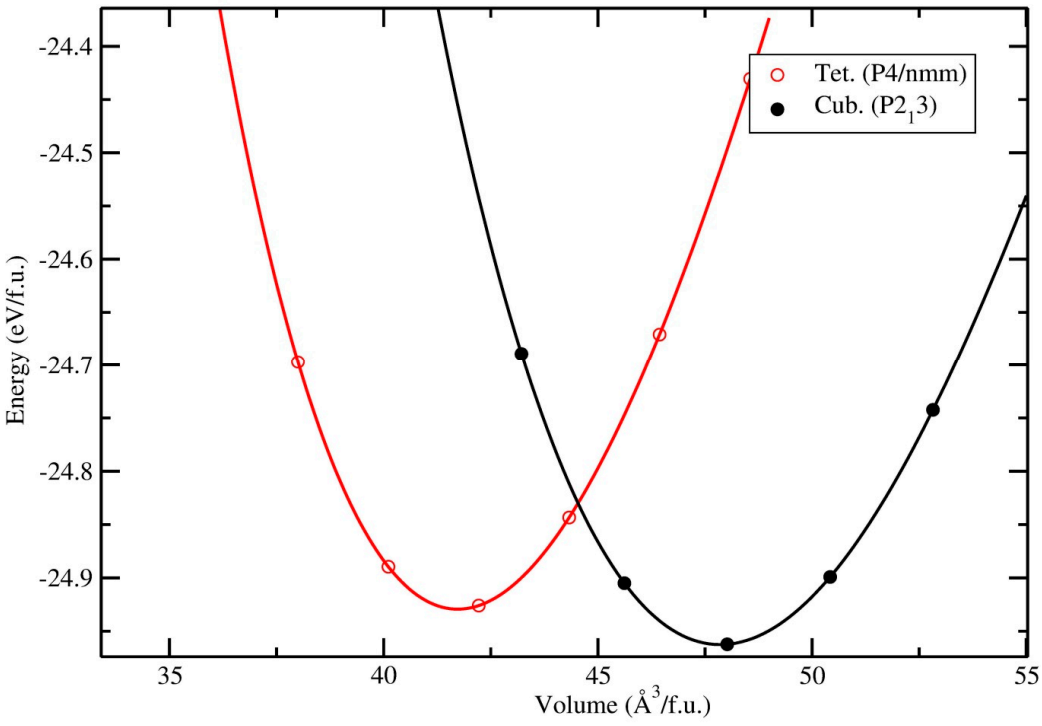

Figure S1. Calculated total energy as a function of unit cell volume for cubic- and tetragonal-ZrSO.

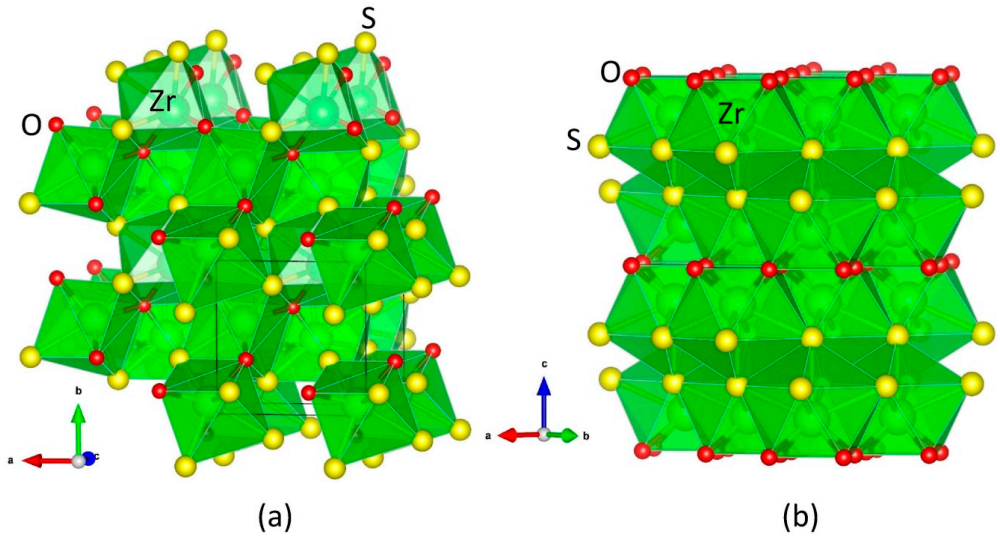

Figure S2. Crystal structures for (**a**) cubic-ZrSO; (**b**) tetragonal-ZrSO. The legends for the different kinds of atoms shown in the illustration.

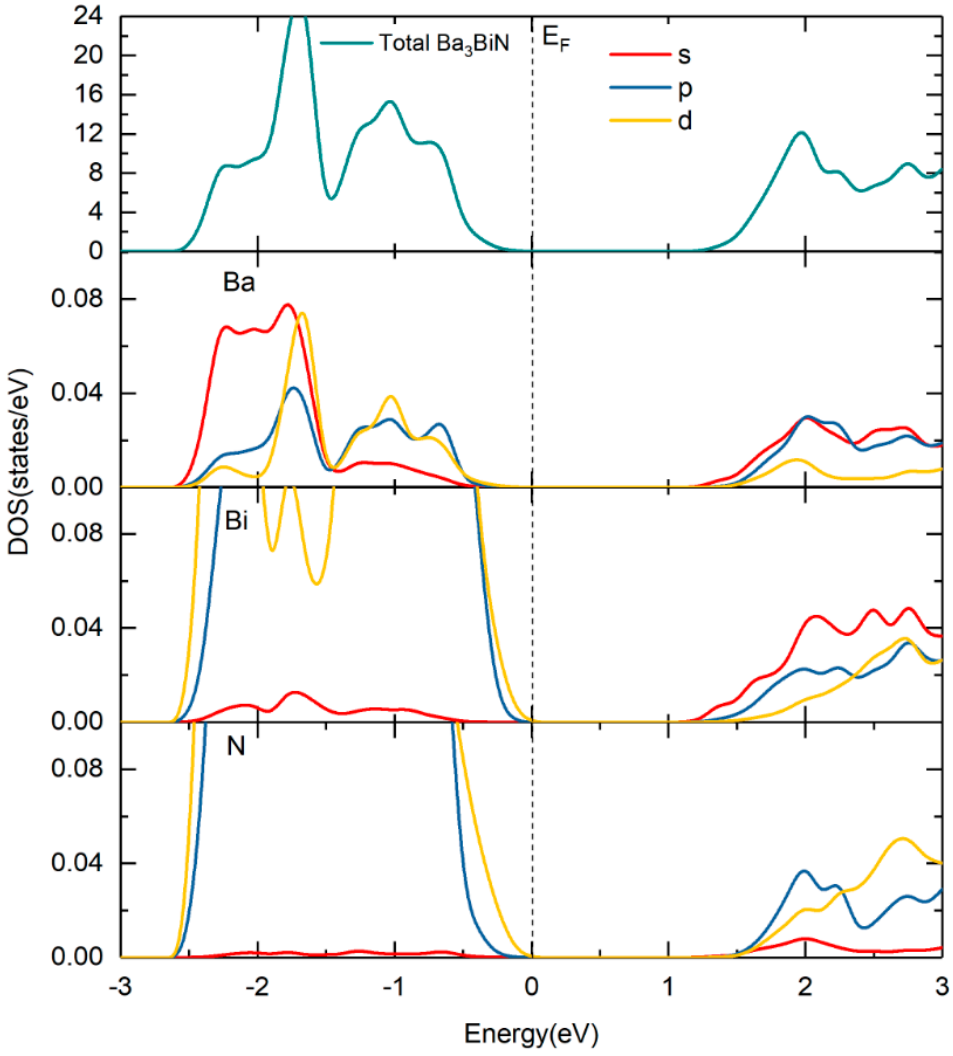

Figure S3. Total and site projected density of states of Ba_3BiN. The Fermi level is set to zero and marked by a vertical dotted line.

The total and site projected density of states of Ba_3BiN, Ag_2BaS_2, and ZrSO are presented in Figure S3, S4 and S5 respectively. From **Error! Reference source not found.**, we observe that the valence band derived from Bi-p and hybridized Ni-d states and conduction bands are mainly composed of Bi-*s* and Ba-*s* states. From Figure S4, we observe that the valence band maximum is derived from S-*p* states and the conduction band derived from Ag-*s* states. In the case of ZrSO, we observe that the valence bands derived from S-*p* states, and conduction bands derived from O-*s* states as shown in Figure S5.

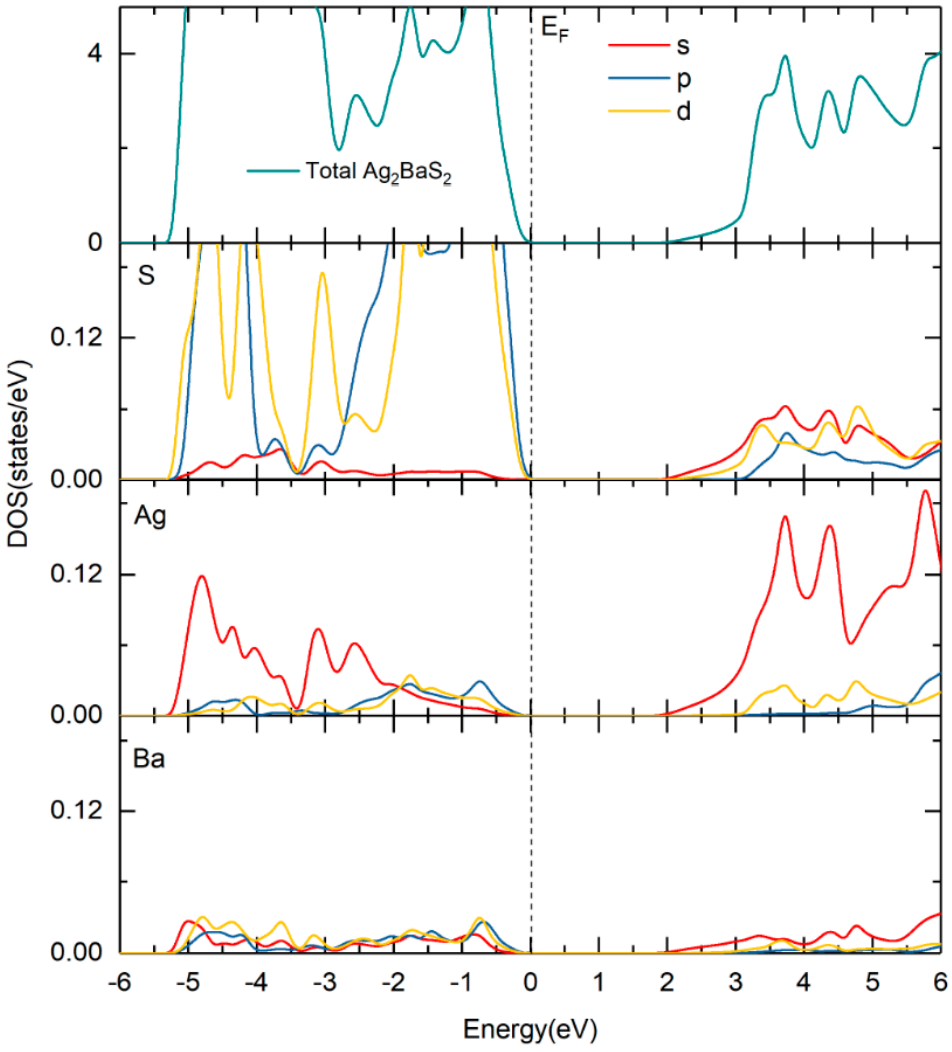

Figure S4. Total and site projected density of states of Ag_2BaS_2. The Fermi level is set to zero and marked by a vertical dotted line.

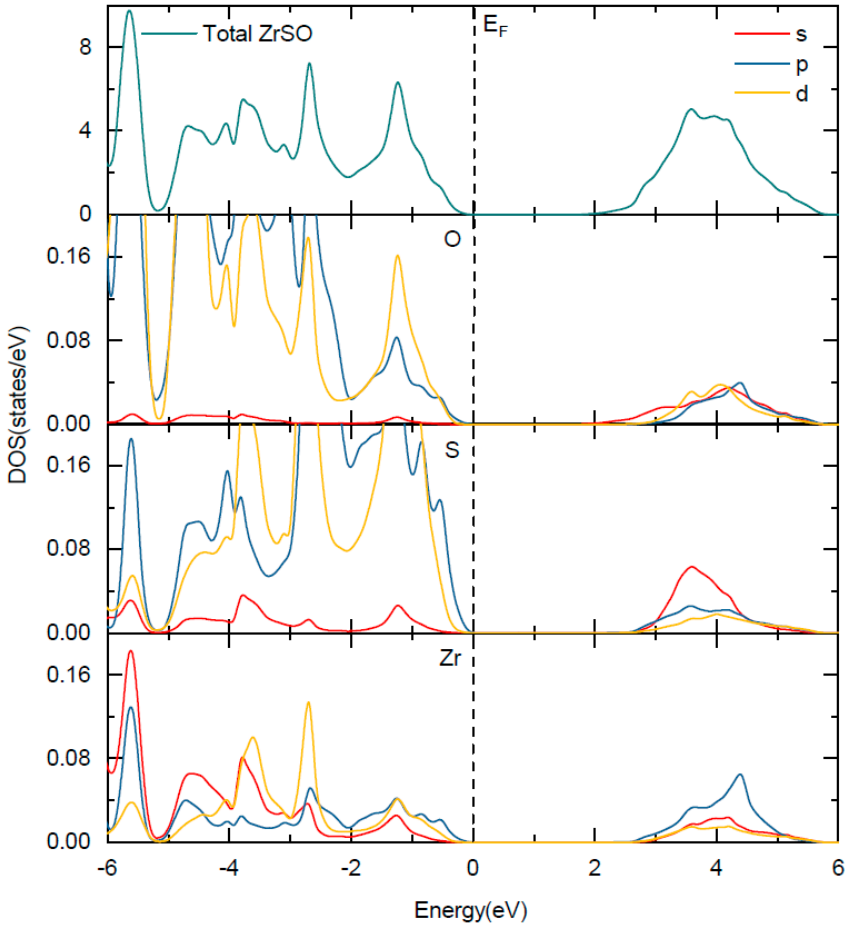

Figure S5. Total and site projected density of states of ZrSO. The Fermi level is set to zero and marked by a vertical dotted line.

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