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Trends in opto-electronic properties of $Mg_xZn_{1-x}SnN_2$ using first principles methods

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Supplementary Material

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Table S1: Average value of bond lengths up to the first nearest neighbors around an element in the $Mg_xZn_{1-x}SnN_2$ alloy system. The values are given in Å.

Material	Element			
	Mg	Zn	Sn	N
$ZnSnN_2$	-	2.09	2.14	2.11
$Mg_{0.25}Zn_{0.75}SnN_2$	2.09	2.08	2.10	2.09
$Mg_{0.50}Zn_{0.50}SnN_2$	2.09	2.08	2.10	2.09
$Mg_{0.75}Zn_{0.25}SnN_2$	2.10	2.08	2.10	2.10
$MgSnN_2$	2.09	-	2.12	2.11

Table S2: Independent elastic and mechanical parameters, in GPa, of $Mg_xZn_{1-x}SnN_2$ alloys, computed using the GGA functional.

Parameters (GPa)	Material				
	$ZnSnN_2$	$Mg_{0.25}Zn_{0.75}SnN_2$	$Mg_{0.50}Zn_{0.50}SnN_2$	$Mg_{0.75}Zn_{0.25}SnN_2$	$MgSnN_2$
C_{11}	215.20	223.41	235.98	234.34	236.76
C_{12}	104.14	93.97	97.00	98.47	99.30
C_{13}	84.35	76.70	79.82	82.46	75.94
C_{14}	0.00	-1.20	-0.60	-0.58	0.00
C_{15}	1.49	-0.33	-0.47	0.21	-0.10
C_{16}	0.00	1.13	-0.09	-1.39	0.00
C_{22}	$= C_{11}$	220.07	231.16	230.43	$= C_{11}$
C_{23}	$= C_{13}$	78.20	80.46	82.80	$= C_{13}$
C_{24}	0.00	-1.03	0.31	-0.47	0.00
C_{25}	$= -C_{15}$	0.20	-0.89	0.73	$= -C_{15}$
C_{26}	0.00	0.37	-0.38	-0.77	0.00
C_{33}	147.34	232.49	232.53	228.44	229.17
C_{34}	0.00	-1.03	-0.53	-0.80	0.00
C_{35}	0.00	1.36	1.68	1.70	0.00
C_{36}	0.00	0.81	0.05	-0.52	0.00
C_{44}	55.53	62.88	66.16	67.22	68.73
C_{45}	0.00	0.28	0.16	-0.15	0.00
C_{46}	$= C_{15}$	0.42	0.05	0.56	$= C_{15}$
C_{55}	51.15	56.93	60.98	62.73	58.21
C_{56}	0.00	-0.08	-0.54	0.33	0.00
C_{66}	$= C_{55}$	56.76	60.67	63.63	$= C_{55}$
Mechanical Stability	Yes	Yes	Yes	Yes	Yes

Bulk Modulus (B_V)	124.82	130.41	134.91	135.63	133.89
Bulk Modulus (B_R)	118.65	130.36	134.76	135.40	133.46
Bulk Modulus (B)	121.74	130.39	134.83	135.52	133.68
Shear Modulus (G_V)	51.89	63.79	67.06	67.35	67.13
Shear Modulus (G_R)	51.03	62.89	66.40	67.00	66.03
Shear Modulus (G)	51.46	63.34	66.73	67.17	66.58
Pugh's Ratio (κ)	2.37	2.06	2.02	2.02	2.01
Vickers hardness (H_V)	28.73	38.98	41.31	41.58	41.54

Table S3: Charge transfer, in elementary charge units *e*, from Mg, Zn, and Sn, to N in $Mg_xZn_{1-x}SnN_2$ calculated using the Bader charge partitioning scheme under GGA functional.

Material	Mg to N	Zn to N	Sn to N	M to N
$ZnSnN_2$	-	1.02	1.80	1.41
$Mg_{0.25}Zn_{0.75}SnN_2$	1.65	1.02	1.80	1.50
$Mg_{0.50}Zn_{0.50}SnN_2$	1.65	1.02	1.80	1.57
$Mg_{0.75}Zn_{0.25}SnN_2$	1.65	1.02	1.80	1.65
$MgSnN_2$	1.65	-	1.70	1.68

Table S4: Average ($\overline{X}$) and standard deviation (σ) of band structure effective masses (m^*) of electrons and holes of $Mg_xZn_{1-x}SnN_2$ alloys. Values are given in units of electron mass (m_o).

Material	Space Group	Electron Effective Mass (m_e^*)		Hole Effective Mass (m_h^*)	
		$\overline{X}$	σ	$\overline{X}$	σ
$ZnSnN_2$	$P3m1$	9.45	5.81	0.91	0.63
$Mg_{0.25}Zn_{0.75}SnN_2$	$P1$	17.94	12.59	1.31	1.65
$Mg_{0.50}Zn_{0.50}SnN_2$	$P1$	17.12	15.54	0.79	0.59
$Mg_{0.75}Zn_{0.25}SnN_2$	$P1$	23.14	14.84	0.82	0.63
$MgSnN_2$	$P3m1$	4.47	4.46	0.76	0.41

Table S5: Dielectric constants of $Mg_xZn_{1-x}SnN_2$ alloys calculated using the hybrid HSE06 functional.

Material	Space Group	Dielectric Constant
$ZnSnN_2$	$P3m1$	2.65
$Mg_{0.25}Zn_{0.75}SnN_2$	$P1$	2.59
$Mg_{0.50}Zn_{0.50}SnN_2$	$P1$	2.32
$Mg_{0.75}Zn_{0.25}SnN_2$	$P1$	2.28
$MgSnN_2$	$P3m1$	2.28

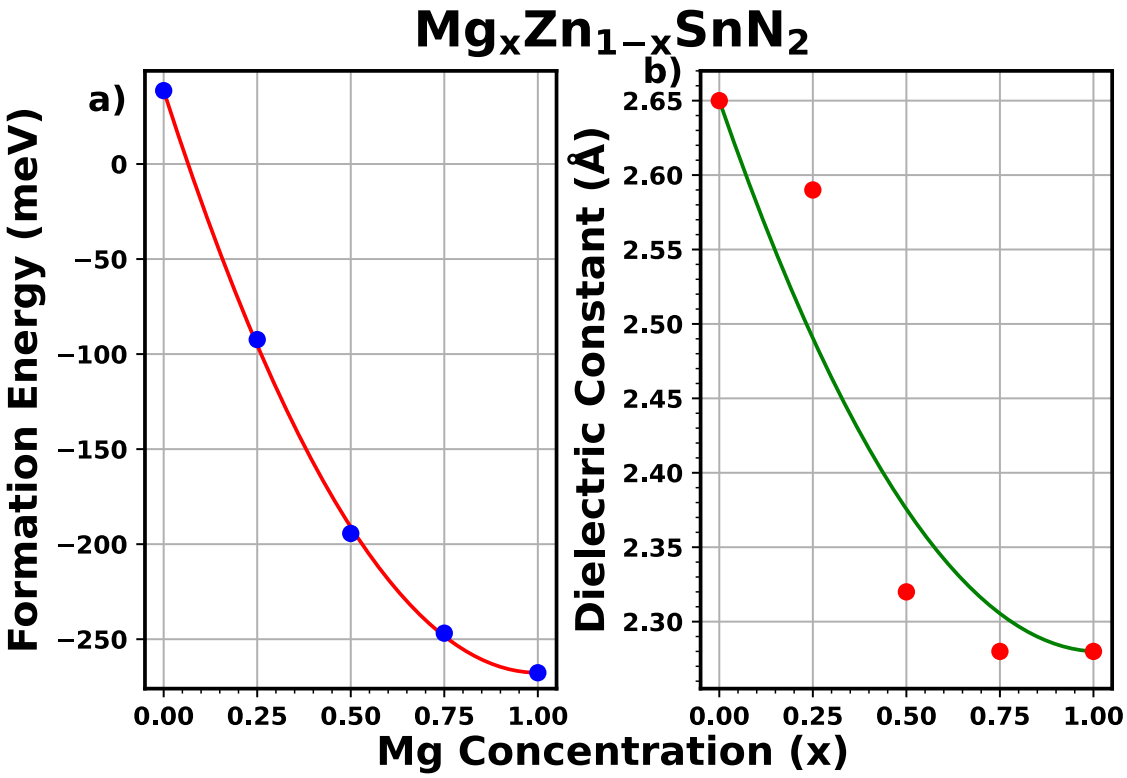

Figure S1: a) Formation energies calculated using the GGA functional, and b) dielectric constants calculated using the hybrid HSEO6 functional of $Mg_xZn_{1-x}SnN_2$ alloys. Here, points denote calculated values whereas curves sketch fitting based on a bowing parameter defined in Eq. (2).

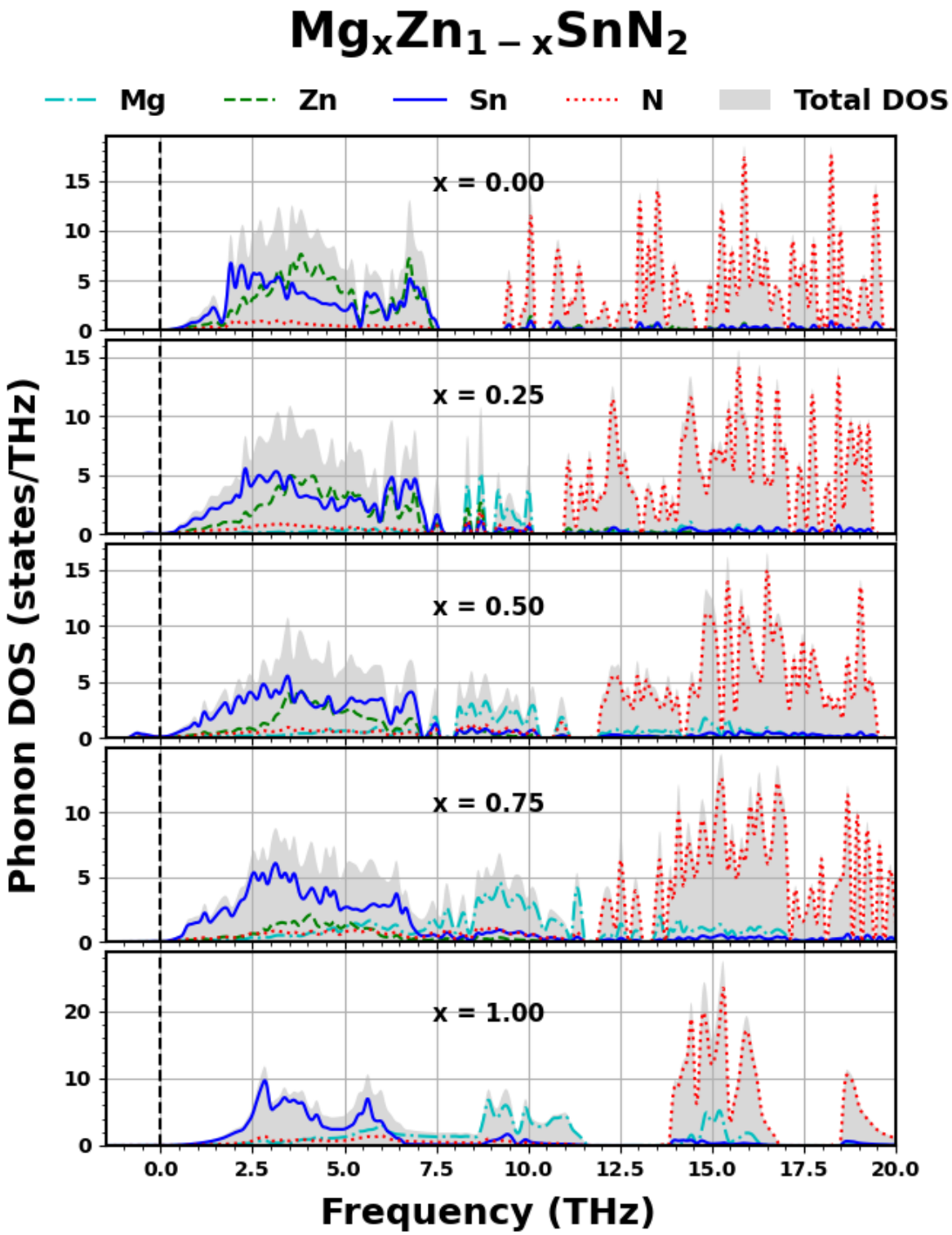

Figure S2. Comparison of the phonon densities of states (DOS) per unit cell of $Mg_xZn_{1-x}SnN_2$ alloys, computed using the GGA functional.

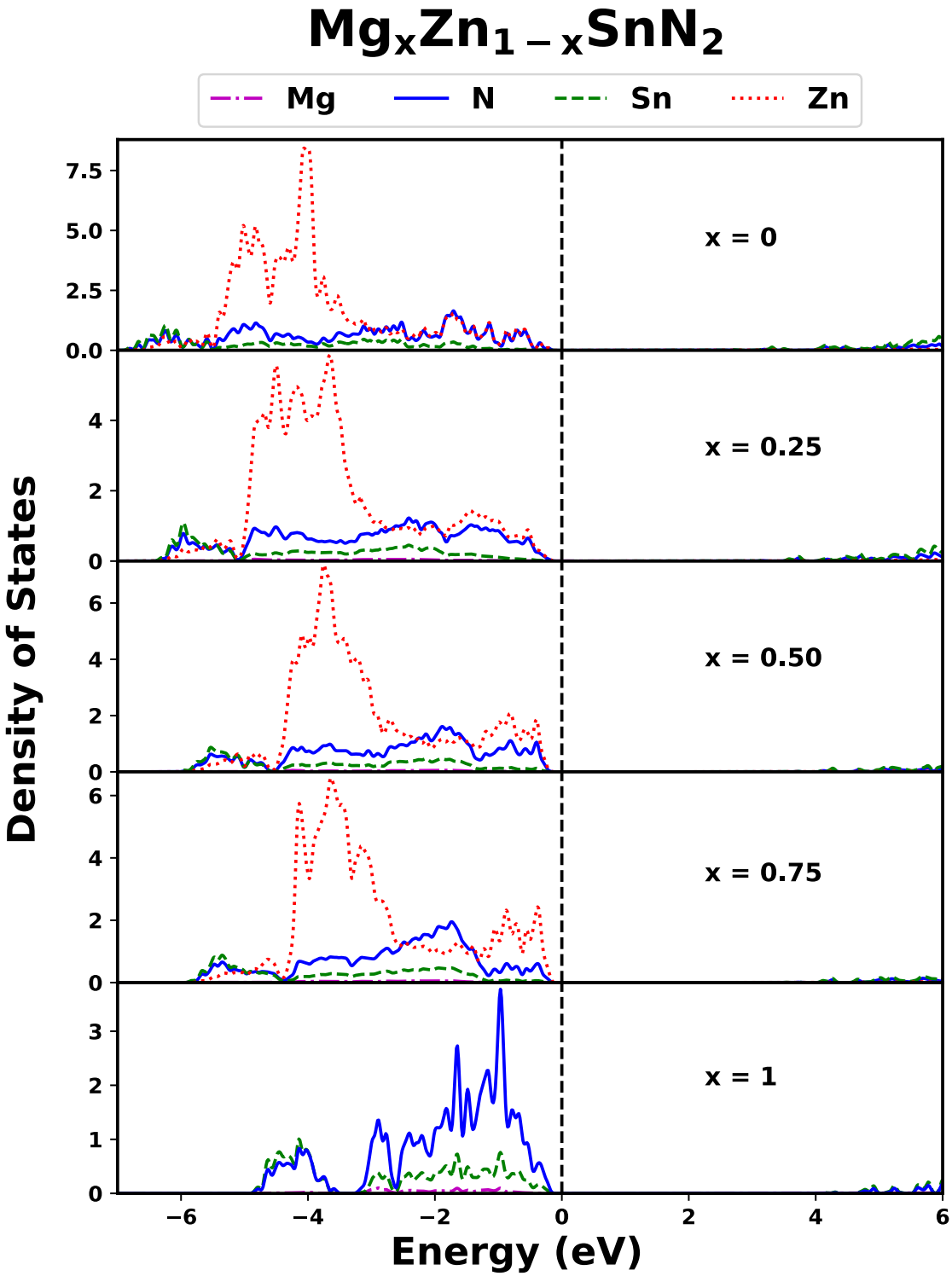

Figure S3: On-site local electronic density of states (LDOS) per formula unit of $Mg_xZn_{1-x}SnN_2$ alloys calculated using the HSE06 functional. The Fermi level is set to 0 eV.

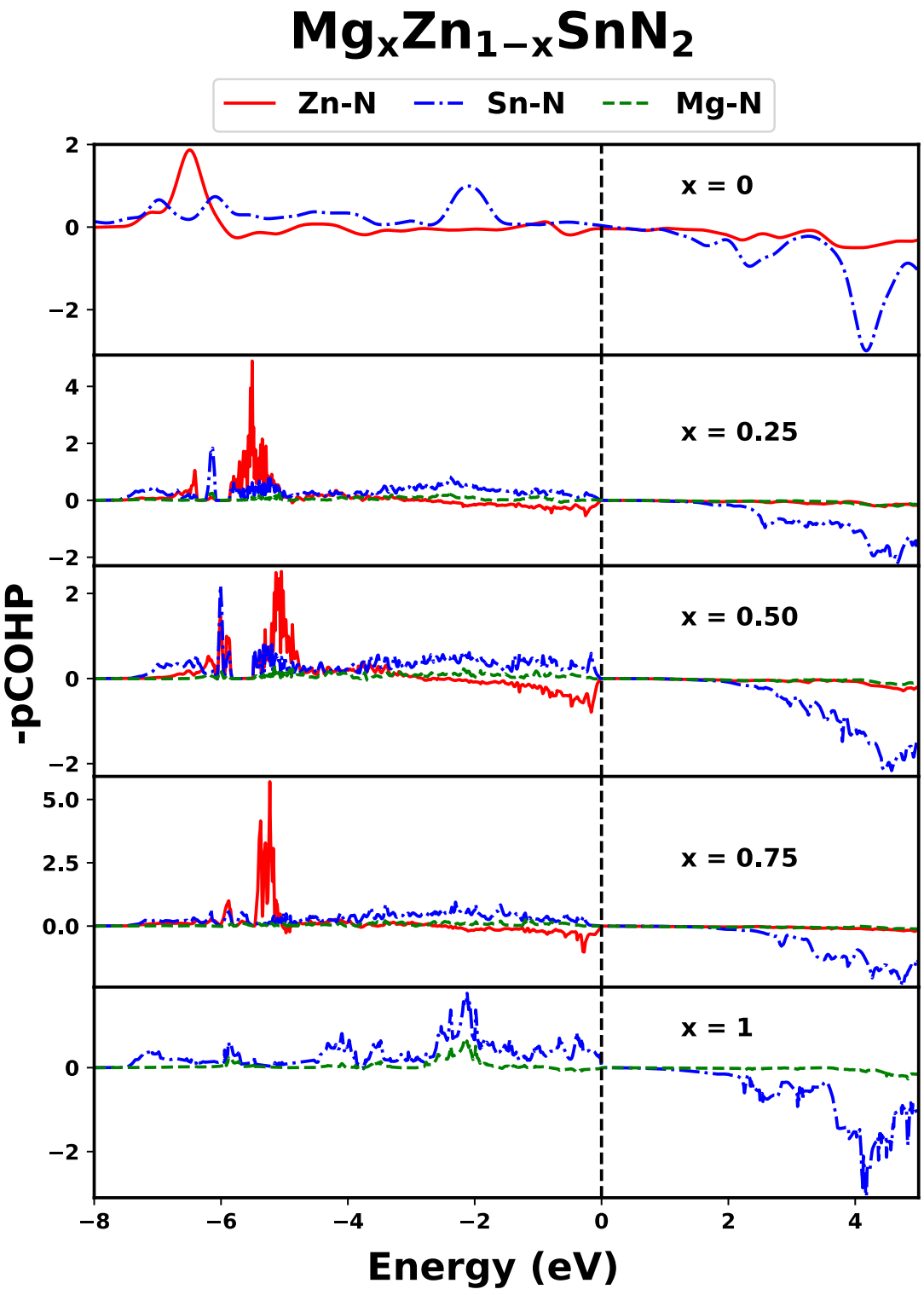

Figure S4: Negative Projected Crystal Orbital Hamiltonian Populations (-pCOHP) of nearest-neighbors' interactions of $Mg_xZn_{1-x}SnN_2$ alloys. All other covalent interactions are negligible compared to atomic pairs displayed here. Positive and negative values of -pCOHP correspond to bonding and antibonding interactions respectively. The Fermi level is set to 0 eV.

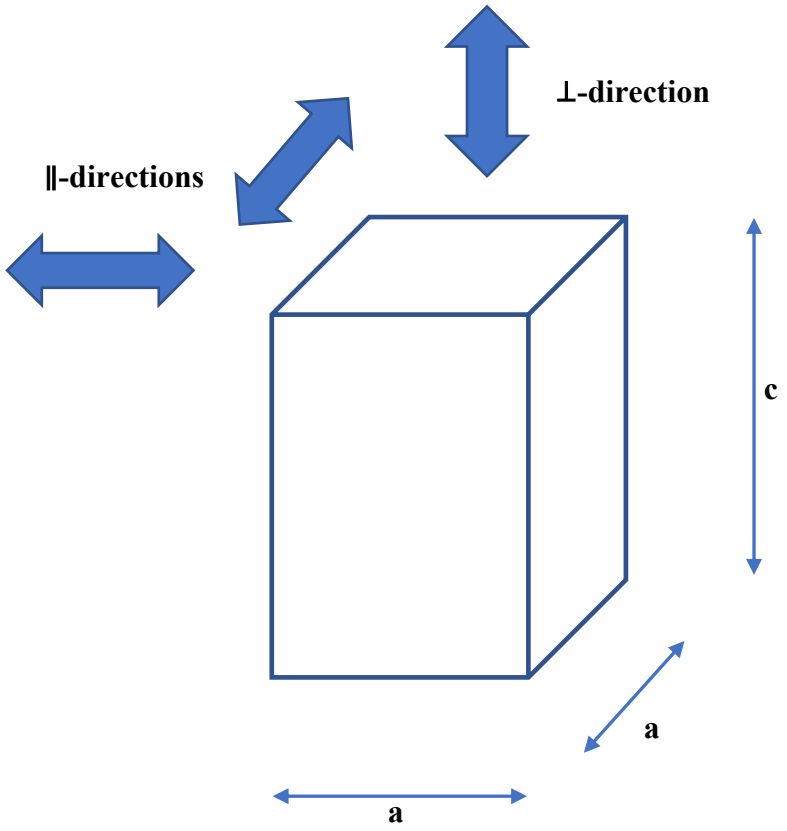

Figure S5: ∥- and ⊥-directions in a wurtzite crystal structure.

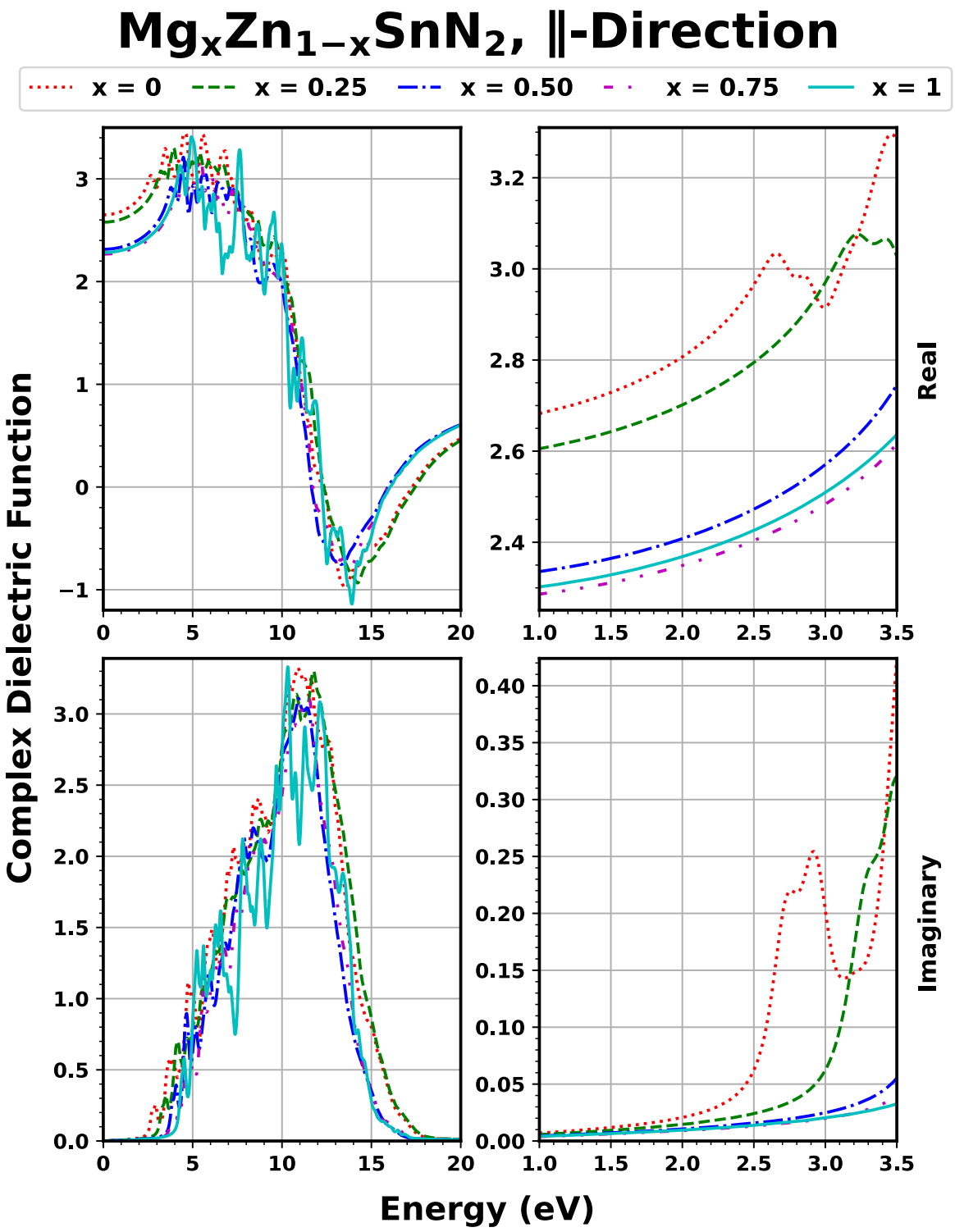

Figure S6: Variation of complex dielectric functions of $Mg_xZn_{1-x}SnN_2$ alloys in ∥-direction (shown in Figure S3) calculated using the hybrid HSEO6 functional. Left side shows wide range in photon energies whereas right side shows photon energies in the visible range only. Similarly, top row shows real part whereas bottom row shows imaginary part of the dielectric function.

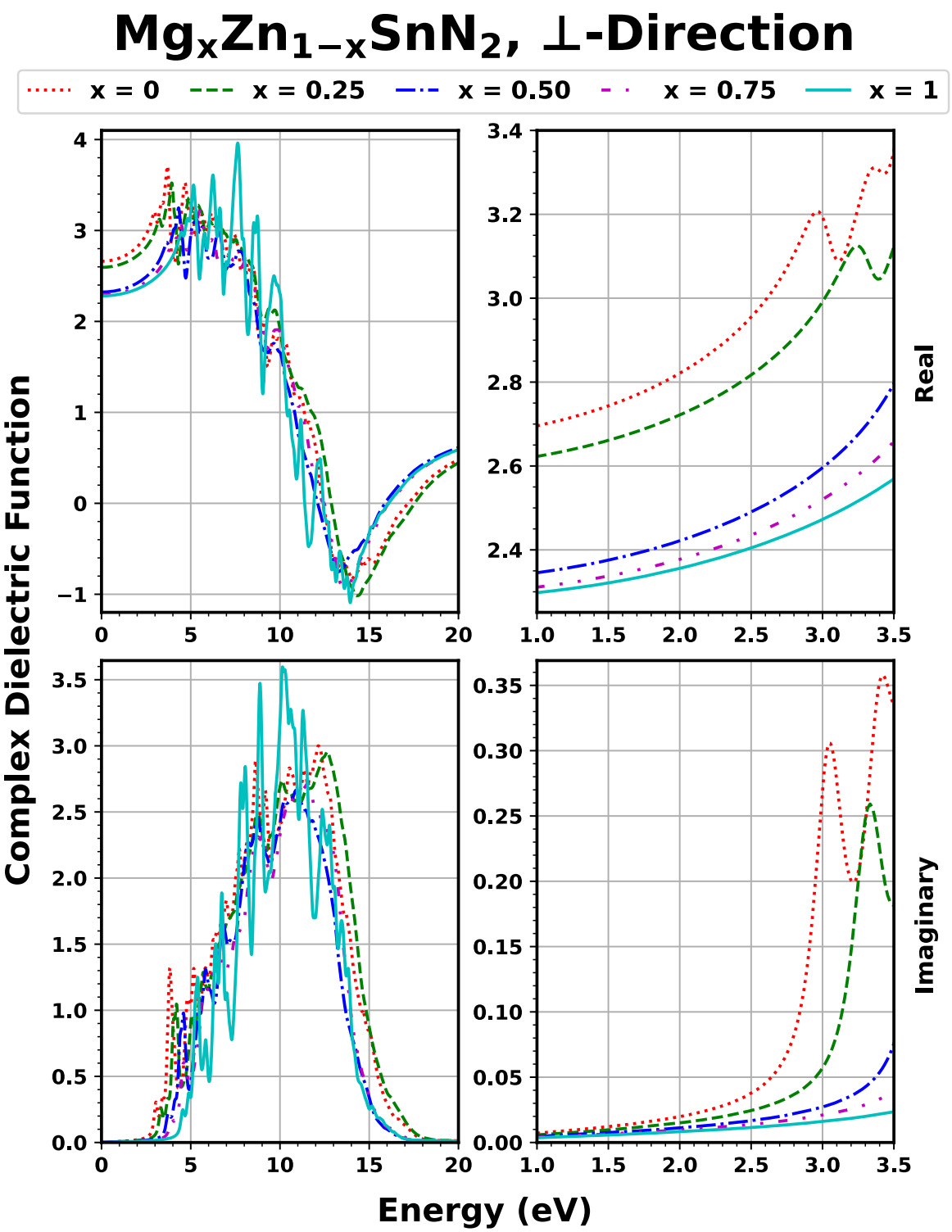

Figure S7: Variation of complex dielectric functions of $Mg_xZn_{1-x}SnN_2$ alloys in ⊥-direction (shown in Figure S3) calculated using the hybrid HSEO6 functional. Left side shows wide range in photon energies whereas right side shows photon energies in the visible range only. Similarly, top row shows real part whereas bottom row shows imaginary part of the dielectric function.

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References

1. *Ohio Supercomputer Center*. 1987.