

**B. B. Dumre, S. V. Khare, Physica B: Condensed Matter 637, 413896, Supplementary Material (2022)**

**Interrelationship of bonding strength with structural stability of ternary oxide phases of  $\text{MgSnO}_3$ : A first-principles study**

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**Supplementary Material**

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**Table S1:** Average value of the bond lengths, up to the first nearest neighbors, between two atoms in the three different crystal structures of MgSnO<sub>3</sub>.

Crystal Structure	Space Group	Average bond length (Å)		Average of all bond lengths (Å)
		Mg-O	Sn-O	
Ilmenite	$R\bar{3}$	2.11	1.89	2.03
Perovskite	$Pm\bar{3}m$	2.84	2.01	2.42
LiNbO <sub>3</sub> type	$R3c$	2.05	2.06	2.06

**Table S2:** Independent elastic and mechanical parameters, in GPa, of MgSnO<sub>3</sub> in the Ilmenite crystal structure, computed using the GGA functional.

Elastic and Mechanical Parameters of Ilmenite (Space Group $R\bar{3}$ ) MgSnO <sub>3</sub> (GPa)	
C <sub>11</sub>	2804.6
C <sub>22</sub>	2764.1
C <sub>33</sub>	1572.6
C <sub>12</sub>	1615.9
C <sub>13</sub>	1116.4
C <sub>23</sub>	1100.8
C <sub>44</sub>	595.5
C <sub>55</sub>	485.5
C <sub>66</sub>	541.5
C <sub>14</sub>	12.9
C <sub>24</sub>	-24.9
C <sub>34</sub>	-8.9
C <sub>15</sub>	68.6
C <sub>25</sub>	-65.2
C <sub>35</sub>	9.2
C <sub>45</sub>	-146.0
C <sub>16</sub>	153.2
C <sub>26</sub>	-149.5

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C <sub>36</sub>	12.0
C <sub>46</sub>	69.4
C <sub>56</sub>	0.7
Mechanical Stability	Yes
Bulk Modulus (B <sub>V</sub> )	1645.3
Bulk Modulus (B <sub>R</sub> )	1433.8
Bulk Modulus (B)	1539.6
Shear Modulus (G <sub>V</sub> )	545.0
Shear Modulus (G <sub>R</sub> )	488.9
Shear Modulus (G)	517.0
Pugh's Ratio ( $\kappa$ )	2.98
Vickers hardness (H <sub>V</sub> )	22.2

**Table S3:** Independent elastic and mechanical parameters, in GPa, of MgSnO<sub>3</sub> in the Perovskite crystal structure, computed using the GGA functional.

Elastic and Mechanical Parameters of Perovskite (Space Group $Pm\bar{3}m$ ) MgSnO <sub>3</sub> (GPa)	
C <sub>11</sub>	3051.8
C <sub>12</sub>	848.4
C <sub>44</sub>	536.5
Mechanical Stability	Yes
Bulk Modulus (B <sub>V</sub> )	1582.8
Bulk Modulus (B <sub>R</sub> )	1582.8
Bulk Modulus (B)	1582.8
Shear Modulus (G <sub>V</sub> )	762.6
Shear Modulus (G <sub>R</sub> )	675.0
Shear Modulus (G)	718.8
Pugh's Ratio ( $\kappa$ )	2.22
Vickers hardness (H <sub>V</sub> )	39.5

**Table S4:** Independent elastic and mechanical parameters, in GPa, of MgSnO<sub>3</sub> in the LiNbO<sub>3</sub> type crystal structure, computed using the GGA functional.

Elastic and Mechanical Parameters of LiNbO <sub>3</sub> Type (Space Group <i>R3c</i> ) MgSnO <sub>3</sub> (GPa)	
C <sub>11</sub>	2864.4
C <sub>33</sub>	2561.6
C <sub>12</sub>	1139.3
C <sub>13</sub>	965.3
C <sub>44</sub>	862.6
C <sub>55</sub>	896.7
C <sub>15</sub>	28.9
C <sub>25</sub>	-28.9
Mechanical Stability	Yes
Bulk Modulus (B <sub>V</sub> )	1603.3
Bulk Modulus (B <sub>R</sub> )	1593.7
Bulk Modulus (B)	1598.5
Shear Modulus (G <sub>V</sub> )	879.2
Shear Modulus (G <sub>R</sub> )	877.1
Shear Modulus (G)	878.2
Pugh's Ratio ( $\kappa$ )	1.82
Vickers hardness (H <sub>V</sub> )	56.5

**Table S5:** IpCOHP of the interactions in between various atom pairs in all the three phases of MgSnO<sub>3</sub> computed using the GGA functional.

Material	IpCOHP (eV)						
	Mg-Mg	Mg-O	Mg-Sn	O-O	Sn-O	Sn-Sn	Total
Ilmenite	-0.090	-0.418	-0.105	-0.059	-1.875	-0.601	-0.419
Perovskite	-0.009	-0.175	-0.157	-0.051	-4.621	-0.083	-0.428
LiNbO <sub>3</sub> type	-0.016	-0.436	-0.231	-0.056	-1.730	-0.104	-0.379

**Table S6:** Charge transfer, in the elementary charge units  $e$ , from Mg and Sn to O in  $\text{MgSnO}_3$  for the three different crystal structures calculated using the Bader charge partitioning scheme under the GGA functional.

Crystal Structure	Mg to O	Sn to O
Ilmenite	1.73	2.46
Perovskite	1.75	2.41
$\text{LiNbO}_3$ type	1.73	2.35



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**Table S7:** Values of photon energy, in eV, and the corresponding complex dielectric function,  $\varepsilon = \varepsilon_1 + i\varepsilon_2$ , in the two distinct directions of the Ilmenite crystal structure in Space Group  $R\bar{3}$  of  $\text{MgSnO}_3$  calculated using the hybrid HSE06 functional. The direction parallel to the a-b plane in the crystal is denoted by “||”, whereas the direction perpendicular to the a-b plane in the crystal is denoted by “ $\perp$ ”. See Fig. S4 for the directions inside the crystal structure.

Ilmenite (Space Group: $R\bar{3}$ )				
Photon Energy (eV)	-direction		$\perp$ -direction	
	$\varepsilon_1$	$\varepsilon_2$	$\varepsilon_1$	$\varepsilon_2$
0	2.393	0	2.1822	0
0.0182	2.393	0	2.1822	0
0.0365	2.393	0.0001	2.1822	0.0001
0.0547	2.393	0.0001	2.1822	0.0001
0.0729	2.393	0.0002	2.1822	0.0002
0.0912	2.3931	0.0002	2.1823	0.0002
0.1094	2.3931	0.0003	2.1823	0.0003
0.1276	2.3932	0.0003	2.1824	0.0003
0.1459	2.3933	0.0004	2.1824	0.0003
0.1641	2.3933	0.0004	2.1825	0.0004
0.1823	2.3934	0.0005	2.1826	0.0004
0.2006	2.3935	0.0005	2.1827	0.0005
0.2188	2.3936	0.0006	2.1827	0.0005

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0.237	2.3937	0.0006	2.1828	0.0006
0.2553	2.3938	0.0007	2.1829	0.0006
0.2735	2.394	0.0007	2.1831	0.0007
0.2917	2.3941	0.0008	2.1832	0.0007
0.31	2.3943	0.0008	2.1833	0.0007
0.3282	2.3944	0.0009	2.1835	0.0008
0.3464	2.3946	0.0009	2.1836	0.0008
0.3647	2.3947	0.001	2.1838	0.0009
0.3829	2.3949	0.001	2.1839	0.0009
0.4011	2.3951	0.0011	2.1841	0.001
0.4194	2.3953	0.0011	2.1843	0.001
0.4376	2.3955	0.0012	2.1845	0.001
0.4558	2.3957	0.0012	2.1846	0.0011
0.4741	2.396	0.0013	2.1849	0.0011
0.4923	2.3962	0.0013	2.1851	0.0012
0.5106	2.3964	0.0014	2.1853	0.0012
0.5288	2.3967	0.0014	2.1855	0.0013
0.547	2.397	0.0015	2.1857	0.0013
0.5653	2.3972	0.0015	2.186	0.0014
0.5835	2.3975	0.0016	2.1862	0.0014
0.6017	2.3978	0.0016	2.1865	0.0014

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0.62	2.3981	0.0017	2.1868	0.0015
0.6382	2.3984	0.0017	2.187	0.0015
0.6564	2.3987	0.0018	2.1873	0.0016
0.6747	2.3991	0.0018	2.1876	0.0016
0.6929	2.3994	0.0019	2.1879	0.0017
0.7111	2.3997	0.0019	2.1882	0.0017
0.7294	2.4001	0.002	2.1885	0.0018
0.7476	2.4004	0.002	2.1889	0.0018
0.7658	2.4008	0.0021	2.1892	0.0018
0.7841	2.4012	0.0021	2.1895	0.0019
0.8023	2.4016	0.0022	2.1899	0.0019
0.8205	2.402	0.0022	2.1902	0.002
0.8388	2.4024	0.0023	2.1906	0.002
0.857	2.4028	0.0023	2.191	0.0021
0.8752	2.4032	0.0024	2.1914	0.0021
0.8935	2.4037	0.0024	2.1918	0.0022
0.9117	2.4041	0.0025	2.1922	0.0022
0.9299	2.4046	0.0025	2.1926	0.0023
0.9482	2.405	0.0026	2.193	0.0023
0.9664	2.4055	0.0026	2.1934	0.0024
0.9846	2.406	0.0027	2.1938	0.0024

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1.0029	2.4065	0.0027	2.1943	0.0025
1.0211	2.407	0.0028	2.1947	0.0025
1.0393	2.4075	0.0028	2.1952	0.0025
1.0576	2.408	0.0029	2.1957	0.0026
1.0758	2.4086	0.0029	2.1961	0.0026
1.094	2.4091	0.003	2.1966	0.0027
1.1123	2.4097	0.003	2.1971	0.0027
1.1305	2.4102	0.0031	2.1976	0.0028
1.1487	2.4108	0.0032	2.1981	0.0028
1.167	2.4114	0.0032	2.1987	0.0029
1.1852	2.412	0.0033	2.1992	0.0029
1.2034	2.4126	0.0033	2.1997	0.003
1.2217	2.4132	0.0034	2.2003	0.003
1.2399	2.4138	0.0034	2.2008	0.0031
1.2581	2.4144	0.0035	2.2014	0.0031
1.2764	2.4151	0.0035	2.202	0.0032
1.2946	2.4157	0.0036	2.2026	0.0032
1.3128	2.4164	0.0036	2.2032	0.0033
1.3311	2.417	0.0037	2.2038	0.0033
1.3493	2.4177	0.0038	2.2044	0.0034
1.3675	2.4184	0.0038	2.205	0.0034

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1.3858	2.4191	0.0039	2.2056	0.0035
1.404	2.4198	0.0039	2.2063	0.0035
1.4222	2.4205	0.004	2.2069	0.0036
1.4405	2.4213	0.004	2.2076	0.0036
1.4587	2.422	0.0041	2.2082	0.0037
1.4769	2.4228	0.0042	2.2089	0.0037
1.4952	2.4235	0.0042	2.2096	0.0038
1.5134	2.4243	0.0043	2.2103	0.0038
1.5317	2.4251	0.0043	2.211	0.0039
1.5499	2.4259	0.0044	2.2117	0.004
1.5681	2.4267	0.0044	2.2124	0.004
1.5864	2.4275	0.0045	2.2132	0.0041
1.6046	2.4283	0.0046	2.2139	0.0041
1.6228	2.4291	0.0046	2.2147	0.0042
1.6411	2.43	0.0047	2.2154	0.0042
1.6593	2.4308	0.0047	2.2162	0.0043
1.6775	2.4317	0.0048	2.217	0.0043
1.6958	2.4326	0.0049	2.2178	0.0044
1.714	2.4335	0.0049	2.2186	0.0045
1.7322	2.4344	0.005	2.2194	0.0045
1.7505	2.4353	0.005	2.2203	0.0046

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1.7687	2.4362	0.0051	2.2211	0.0046
1.7869	2.4372	0.0052	2.2219	0.0047
1.8052	2.4381	0.0052	2.2228	0.0047
1.8234	2.4391	0.0053	2.2237	0.0048
1.8416	2.44	0.0053	2.2245	0.0049
1.8599	2.441	0.0054	2.2254	0.0049
1.8781	2.442	0.0055	2.2263	0.005
1.8963	2.443	0.0055	2.2272	0.005
1.9146	2.444	0.0056	2.2282	0.0051
1.9328	2.445	0.0057	2.2291	0.0051
1.951	2.4461	0.0057	2.23	0.0052
1.9693	2.4471	0.0058	2.231	0.0053
1.9875	2.4482	0.0059	2.232	0.0053
2.0057	2.4493	0.0059	2.2329	0.0054
2.024	2.4504	0.006	2.2339	0.0055
2.0422	2.4515	0.0061	2.2349	0.0055
2.0604	2.4526	0.0061	2.2359	0.0056
2.0787	2.4537	0.0062	2.237	0.0056
2.0969	2.4548	0.0063	2.238	0.0057
2.1151	2.456	0.0063	2.239	0.0058
2.1334	2.4571	0.0064	2.2401	0.0058

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2.1516	2.4583	0.0065	2.2412	0.0059
2.1698	2.4595	0.0065	2.2422	0.006
2.1881	2.4607	0.0066	2.2433	0.006
2.2063	2.4619	0.0067	2.2444	0.0061
2.2245	2.4631	0.0068	2.2456	0.0062
2.2428	2.4644	0.0068	2.2467	0.0062
2.261	2.4656	0.0069	2.2478	0.0063
2.2792	2.4669	0.007	2.249	0.0064
2.2975	2.4682	0.007	2.2502	0.0064
2.3157	2.4694	0.0071	2.2513	0.0065
2.3339	2.4707	0.0072	2.2525	0.0066
2.3522	2.4721	0.0073	2.2537	0.0067
2.3704	2.4734	0.0073	2.255	0.0067
2.3886	2.4747	0.0074	2.2562	0.0068
2.4069	2.4761	0.0075	2.2574	0.0069
2.4251	2.4775	0.0076	2.2587	0.007
2.4433	2.4788	0.0076	2.26	0.007
2.4616	2.4802	0.0077	2.2613	0.0071
2.4798	2.4817	0.0078	2.2626	0.0072
2.498	2.4831	0.0079	2.2639	0.0073
2.5163	2.4845	0.008	2.2652	0.0073

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2.5345	2.486	0.008	2.2666	0.0074
2.5528	2.4875	0.0081	2.2679	0.0075
2.571	2.4889	0.0082	2.2693	0.0076
2.5892	2.4904	0.0083	2.2707	0.0076
2.6075	2.492	0.0084	2.2721	0.0077
2.6257	2.4935	0.0084	2.2735	0.0078
2.6439	2.495	0.0085	2.2749	0.0079
2.6622	2.4966	0.0086	2.2764	0.008
2.6804	2.4982	0.0087	2.2778	0.0081
2.6986	2.4998	0.0088	2.2793	0.0081
2.7169	2.5014	0.0089	2.2808	0.0082
2.7351	2.503	0.009	2.2823	0.0083
2.7533	2.5046	0.009	2.2838	0.0084
2.7716	2.5063	0.0091	2.2853	0.0085
2.7898	2.508	0.0092	2.2869	0.0086
2.808	2.5096	0.0093	2.2885	0.0087
2.8263	2.5113	0.0094	2.2901	0.0088
2.8445	2.5131	0.0095	2.2917	0.0089
2.8627	2.5148	0.0096	2.2933	0.0089
2.881	2.5166	0.0097	2.2949	0.009
2.8992	2.5183	0.0098	2.2966	0.0091



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2.9174	2.5201	0.0099	2.2982	0.0092
2.9357	2.5219	0.01	2.2999	0.0093
2.9539	2.5238	0.0101	2.3016	0.0094
2.9721	2.5256	0.0102	2.3034	0.0095
2.9904	2.5275	0.0103	2.3051	0.0096
3.0086	2.5293	0.0104	2.3069	0.0097
3.0268	2.5312	0.0105	2.3087	0.0098
3.0451	2.5331	0.0106	2.3105	0.0099
3.0633	2.5351	0.0107	2.3123	0.01
3.0815	2.537	0.0108	2.3141	0.0101
3.0998	2.539	0.0109	2.316	0.0103
3.118	2.541	0.011	2.3178	0.0104
3.1362	2.543	0.0111	2.3197	0.0105
3.1545	2.545	0.0112	2.3217	0.0106
3.1727	2.5471	0.0113	2.3236	0.0107
3.1909	2.5491	0.0114	2.3256	0.0108
3.2092	2.5512	0.0115	2.3275	0.0109
3.2274	2.5533	0.0116	2.3295	0.011
3.2456	2.5555	0.0117	2.3316	0.0112
3.2639	2.5576	0.0119	2.3336	0.0113
3.2821	2.5598	0.012	2.3357	0.0114

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3.3003	2.562	0.0121	2.3378	0.0115
3.3186	2.5642	0.0122	2.3399	0.0117
3.3368	2.5664	0.0123	2.342	0.0118
3.355	2.5687	0.0125	2.3442	0.0119
3.3733	2.571	0.0126	2.3463	0.0121
3.3915	2.5733	0.0127	2.3485	0.0122
3.4097	2.5756	0.0128	2.3508	0.0123
3.428	2.5779	0.013	2.353	0.0125
3.4462	2.5803	0.0131	2.3553	0.0126
3.4644	2.5827	0.0132	2.3576	0.0127
3.4827	2.5851	0.0133	2.3599	0.0129
3.5009	2.5876	0.0135	2.3623	0.013
3.5192	2.59	0.0136	2.3647	0.0132
3.5374	2.5925	0.0138	2.3671	0.0133
3.5556	2.5951	0.0139	2.3695	0.0135
3.5739	2.5976	0.014	2.372	0.0136
3.5921	2.6002	0.0142	2.3745	0.0138
3.6103	2.6028	0.0143	2.377	0.014
3.6286	2.6054	0.0145	2.3796	0.0141
3.6468	2.608	0.0146	2.3822	0.0143
3.665	2.6107	0.0148	2.3848	0.0145

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3.6833	2.6134	0.0149	2.3874	0.0146
3.7015	2.6161	0.0151	2.3901	0.0148
3.7197	2.6189	0.0152	2.3928	0.015
3.738	2.6217	0.0154	2.3956	0.0152
3.7562	2.6245	0.0155	2.3984	0.0154
3.7744	2.6273	0.0157	2.4012	0.0156
3.7927	2.6302	0.0159	2.404	0.0157
3.8109	2.6331	0.016	2.4069	0.0159
3.8291	2.636	0.0162	2.4098	0.0161
3.8474	2.639	0.0164	2.4128	0.0163
3.8656	2.642	0.0166	2.4158	0.0166
3.8838	2.645	0.0167	2.4188	0.0168
3.9021	2.6481	0.0169	2.4219	0.017
3.9203	2.6512	0.0171	2.425	0.0172
3.9385	2.6543	0.0173	2.4281	0.0174
3.9568	2.6575	0.0175	2.4313	0.0177
3.975	2.6607	0.0177	2.4345	0.0179
3.9932	2.6639	0.0179	2.4378	0.0182
4.0115	2.6672	0.0181	2.4411	0.0184
4.0297	2.6705	0.0183	2.4445	0.0187
4.0479	2.6739	0.0185	2.4479	0.0189

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4.0662	2.6772	0.0187	2.4514	0.0192
4.0844	2.6807	0.0189	2.4549	0.0195
4.1026	2.6841	0.0191	2.4585	0.0197
4.1209	2.6876	0.0193	2.4621	0.02
4.1391	2.6912	0.0196	2.4657	0.0203
4.1573	2.6947	0.0198	2.4695	0.0206
4.1756	2.6984	0.02	2.4732	0.0209
4.1938	2.702	0.0203	2.4771	0.0213
4.212	2.7057	0.0205	2.4809	0.0216
4.2303	2.7095	0.0208	2.4849	0.0219
4.2485	2.7133	0.021	2.4889	0.0223
4.2667	2.7171	0.0213	2.493	0.0226
4.285	2.721	0.0215	2.4971	0.023
4.3032	2.725	0.0218	2.5013	0.0234
4.3214	2.729	0.0221	2.5056	0.0238
4.3397	2.733	0.0224	2.51	0.0242
4.3579	2.7371	0.0227	2.5144	0.0246
4.3761	2.7412	0.023	2.5189	0.0251
4.3944	2.7454	0.0233	2.5235	0.0255
4.4126	2.7497	0.0236	2.5281	0.026
4.4308	2.754	0.0239	2.5329	0.0265

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4.4491	2.7584	0.0242	2.5377	0.027
4.4673	2.7628	0.0245	2.5426	0.0275
4.4855	2.7673	0.0249	2.5476	0.028
4.5038	2.7719	0.0252	2.5528	0.0286
4.522	2.7765	0.0256	2.558	0.0292
4.5403	2.7812	0.026	2.5633	0.0298
4.5585	2.7859	0.0263	2.5688	0.0305
4.5767	2.7907	0.0267	2.5743	0.0312
4.595	2.7956	0.0271	2.58	0.0319
4.6132	2.8006	0.0275	2.5858	0.0327
4.6314	2.8056	0.028	2.5918	0.0335
4.6497	2.8107	0.0284	2.5978	0.0343
4.6679	2.8159	0.0289	2.6041	0.0353
4.6861	2.8212	0.0293	2.6105	0.0362
4.7044	2.8266	0.0298	2.617	0.0373
4.7226	2.832	0.0303	2.6237	0.0384
4.7408	2.8376	0.0308	2.6306	0.0396
4.7591	2.8432	0.0314	2.6377	0.0409
4.7773	2.8489	0.0319	2.645	0.0423
4.7955	2.8548	0.0325	2.6525	0.0439
4.8138	2.8607	0.0331	2.6602	0.0456

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4.832	2.8667	0.0338	2.6681	0.0475
4.8502	2.8729	0.0344	2.6762	0.0495
4.8685	2.8792	0.0351	2.6845	0.0518
4.8867	2.8856	0.0358	2.6931	0.0543
4.9049	2.8921	0.0366	2.7019	0.0572
4.9232	2.8988	0.0374	2.7108	0.0603
4.9414	2.9056	0.0383	2.72	0.0638
4.9596	2.9125	0.0392	2.7293	0.0677
4.9779	2.9196	0.0401	2.7387	0.072
4.9961	2.9269	0.0411	2.7482	0.0767
5.0143	2.9343	0.0422	2.7578	0.0819
5.0326	2.9419	0.0434	2.7673	0.0876
5.0508	2.9497	0.0446	2.7768	0.0938
5.069	2.9577	0.046	2.7861	0.1005
5.0873	2.9659	0.0475	2.7952	0.1077
5.1055	2.9743	0.0491	2.804	0.1153
5.1237	2.9828	0.0509	2.8125	0.1233
5.142	2.9916	0.0528	2.8206	0.1316
5.1602	3.0006	0.0549	2.8282	0.1402
5.1784	3.0098	0.0573	2.8354	0.149
5.1967	3.0192	0.0599	2.8421	0.1578

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5.2149	3.0288	0.0627	2.8483	0.1666
5.2331	3.0386	0.0659	2.8542	0.1753
5.2514	3.0485	0.0694	2.8596	0.1837
5.2696	3.0586	0.0732	2.8648	0.1918
5.2878	3.0688	0.0774	2.8699	0.1994
5.3061	3.079	0.082	2.875	0.2066
5.3243	3.0893	0.0869	2.8802	0.2134
5.3425	3.0995	0.0923	2.8858	0.2197
5.3608	3.1098	0.098	2.8918	0.2257
5.379	3.1199	0.1041	2.8986	0.2314
5.3972	3.13	0.1106	2.9061	0.237
5.4155	3.1399	0.1173	2.9146	0.2427
5.4337	3.1496	0.1244	2.9241	0.2486
5.4519	3.1592	0.1317	2.9346	0.2552
5.4702	3.1686	0.1393	2.9463	0.2625
5.4884	3.1779	0.147	2.9589	0.271
5.5066	3.187	0.1549	2.9723	0.2809
5.5249	3.1961	0.1629	2.9864	0.2925
5.5431	3.2051	0.171	3.0009	0.3059
5.5614	3.2141	0.1793	3.0155	0.3215
5.5796	3.2231	0.1878	3.0298	0.3393

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5.5978	3.2321	0.1964	3.0434	0.3595
5.6161	3.2412	0.2053	3.0559	0.3819
5.6343	3.2505	0.2146	3.0669	0.4066
5.6525	3.2598	0.2242	3.0759	0.4333
5.6708	3.2691	0.2342	3.0824	0.4619
5.689	3.2785	0.2448	3.0862	0.4919
5.7072	3.2879	0.2561	3.087	0.5229
5.7255	3.297	0.2679	3.0844	0.5544
5.7437	3.306	0.2805	3.0784	0.5859
5.7619	3.3145	0.2938	3.0689	0.6169
5.7802	3.3225	0.3079	3.056	0.6468
5.7984	3.3299	0.3226	3.0399	0.6749
5.8166	3.3364	0.3379	3.0209	0.7009
5.8349	3.3421	0.3537	2.9993	0.7243
5.8531	3.3466	0.3698	2.9756	0.7446
5.8713	3.3501	0.3862	2.9503	0.7617
5.8896	3.3524	0.4026	2.924	0.7753
5.9078	3.3535	0.4188	2.8972	0.7854
5.926	3.3535	0.4346	2.8705	0.792
5.9443	3.3523	0.4498	2.8443	0.7954
5.9625	3.3503	0.4643	2.8191	0.7956



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5.9807	3.3473	0.4779	2.7954	0.793
5.999	3.3438	0.4904	2.7733	0.7879
6.0172	3.3397	0.5019	2.7532	0.7807
6.0354	3.3355	0.5122	2.7352	0.7717
6.0537	3.3312	0.5213	2.7195	0.7613
6.0719	3.327	0.5294	2.7059	0.7499
6.0901	3.3232	0.5364	2.6945	0.7377
6.1084	3.3199	0.5426	2.6853	0.7251
6.1266	3.3172	0.5479	2.6781	0.7121
6.1448	3.3152	0.5527	2.6728	0.6991
6.1631	3.314	0.5569	2.6694	0.6862
6.1813	3.3136	0.5609	2.6676	0.6735
6.1995	3.3139	0.5646	2.6676	0.661
6.2178	3.315	0.5682	2.669	0.6489
6.236	3.3169	0.5718	2.672	0.6372
6.2542	3.3195	0.5755	2.6765	0.626
6.2725	3.3228	0.5793	2.6825	0.6153
6.2907	3.3268	0.5835	2.6899	0.6053
6.3089	3.3315	0.5879	2.6987	0.5961
6.3272	3.3368	0.5928	2.7091	0.5877
6.3454	3.3428	0.5981	2.7208	0.5804

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6.3636	3.3493	0.6041	2.7339	0.5743
6.3819	3.3564	0.6109	2.7483	0.5697
6.4001	3.3639	0.6184	2.764	0.5666
6.4183	3.3718	0.627	2.7806	0.5654
6.4366	3.3798	0.6366	2.7981	0.5661
6.4548	3.3879	0.6474	2.8162	0.569
6.473	3.3958	0.6594	2.8346	0.5741
6.4913	3.4033	0.6725	2.8531	0.5816
6.5095	3.4102	0.6869	2.8712	0.5915
6.5278	3.4162	0.7023	2.8887	0.6037
6.546	3.4211	0.7187	2.9052	0.6182
6.5642	3.4248	0.7357	2.9203	0.6348
6.5825	3.4272	0.7533	2.9338	0.6532
6.6007	3.4281	0.7711	2.9455	0.6733
6.6189	3.4276	0.789	2.9551	0.6947
6.6372	3.4256	0.8065	2.9624	0.717
6.6554	3.4225	0.8236	2.9675	0.74
6.6736	3.4181	0.8399	2.9702	0.7633
6.6919	3.4129	0.8554	2.9707	0.7864
6.7101	3.4069	0.8701	2.9691	0.8091
6.7283	3.4003	0.8837	2.9654	0.8312

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6.7466	3.3934	0.8964	2.9601	0.8523
6.7648	3.3863	0.9083	2.9532	0.8723
6.783	3.3792	0.9194	2.9451	0.891
6.8013	3.3721	0.9298	2.936	0.9085
6.8195	3.3651	0.9397	2.9262	0.9246
6.8377	3.3581	0.9492	2.9159	0.9395
6.856	3.3512	0.9583	2.9054	0.9533
6.8742	3.3441	0.9671	2.8947	0.9661
6.8924	3.3369	0.9757	2.884	0.978
6.9107	3.3295	0.984	2.8734	0.9892
6.9289	3.3217	0.9919	2.8628	1
6.9471	3.3135	0.9993	2.8521	1.0103
6.9654	3.305	1.006	2.8414	1.0203
6.9836	3.2961	1.012	2.8304	1.0301
7.0018	3.287	1.0171	2.819	1.0396
7.0201	3.2778	1.0211	2.8072	1.0489
7.0383	3.2686	1.024	2.7947	1.0578
7.0565	3.2596	1.0258	2.7816	1.0662
7.0748	3.2511	1.0264	2.7677	1.0739
7.093	3.2433	1.0259	2.753	1.0808
7.1112	3.2363	1.0243	2.7376	1.0867

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7.1295	3.2303	1.0219	2.7215	1.0913
7.1477	3.2255	1.0188	2.705	1.0945
7.1659	3.2219	1.0152	2.6881	1.0961
7.1842	3.2195	1.0113	2.6712	1.0961
7.2024	3.2185	1.0072	2.6545	1.0943
7.2206	3.2187	1.0032	2.6381	1.0907
7.2389	3.2201	0.9995	2.6225	1.0855
7.2571	3.2226	0.996	2.6078	1.0787
7.2753	3.2261	0.9931	2.5942	1.0704
7.2936	3.2305	0.9907	2.5819	1.0608
7.3118	3.2357	0.9889	2.5711	1.0501
7.33	3.2416	0.9877	2.5619	1.0385
7.3483	3.2482	0.9873	2.5542	1.0262
7.3665	3.2554	0.9875	2.5482	1.0134
7.3847	3.2631	0.9884	2.5438	1.0003
7.403	3.2713	0.9901	2.5411	0.987
7.4212	3.2798	0.9925	2.5398	0.9737
7.4394	3.2888	0.9958	2.5401	0.9605
7.4577	3.2981	0.9998	2.5419	0.9475
7.4759	3.3077	1.0048	2.545	0.9348
7.4941	3.3175	1.0106	2.5495	0.9224

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7.5124	3.3275	1.0175	2.5554	0.9104
7.5306	3.3374	1.0253	2.5626	0.8989
7.5489	3.3474	1.0342	2.5711	0.8879
7.5671	3.3572	1.0442	2.5809	0.8775
7.5853	3.3667	1.0552	2.5921	0.8678
7.6036	3.3758	1.0674	2.6046	0.8589
7.6218	3.3842	1.0806	2.6185	0.8509
7.64	3.392	1.0949	2.6337	0.8439
7.6583	3.3989	1.11	2.6503	0.8381
7.6765	3.4048	1.126	2.6682	0.8336
7.6947	3.4095	1.1427	2.6875	0.8307
7.713	3.4129	1.16	2.7079	0.8295
7.7312	3.415	1.1776	2.7295	0.8304
7.7494	3.4157	1.1954	2.7521	0.8334
7.7677	3.415	1.2131	2.7755	0.8389
7.7859	3.4128	1.2306	2.7994	0.847
7.8041	3.4093	1.2476	2.8235	0.8581
7.8224	3.4045	1.2639	2.8476	0.8722
7.8406	3.3985	1.2793	2.8711	0.8896
7.8588	3.3916	1.2936	2.8936	0.9102
7.8771	3.3838	1.3068	2.9146	0.934

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7.8953	3.3755	1.3187	2.9335	0.961
7.9135	3.3669	1.3293	2.9498	0.9908
7.9318	3.3582	1.3386	2.9631	1.0233
7.95	3.3495	1.3466	2.9728	1.058
7.9682	3.3411	1.3534	2.9785	1.0943
7.9865	3.3332	1.3592	2.98	1.1316
8.0047	3.3259	1.3641	2.977	1.1693
8.0229	3.3192	1.3683	2.9695	1.2066
8.0412	3.3133	1.3718	2.9575	1.2428
8.0594	3.3081	1.3749	2.9413	1.2772
8.0776	3.3037	1.3777	2.9213	1.309
8.0959	3.2998	1.3803	2.8979	1.3378
8.1141	3.2966	1.3828	2.8717	1.3631
8.1323	3.294	1.3853	2.8433	1.3844
8.1506	3.2917	1.3878	2.8136	1.4017
8.1688	3.2899	1.3903	2.7831	1.4148
8.187	3.2885	1.3928	2.7527	1.4238
8.2053	3.2873	1.3953	2.723	1.429
8.2235	3.2864	1.3978	2.6944	1.4306
8.2417	3.2859	1.4002	2.6676	1.4292
8.26	3.2856	1.4025	2.6428	1.4253

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8.2782	3.2858	1.4048	2.6202	1.4192
8.2964	3.2862	1.4069	2.6	1.4116
8.3147	3.2871	1.4091	2.582	1.4029
8.3329	3.2885	1.4112	2.5663	1.3936
8.3511	3.2902	1.4134	2.5526	1.384
8.3694	3.2924	1.4156	2.5406	1.3744
8.3876	3.2951	1.4179	2.5301	1.365
8.4058	3.2981	1.4204	2.5208	1.3559
8.4241	3.3015	1.4231	2.5125	1.347
8.4423	3.3053	1.426	2.5049	1.3383
8.4605	3.3094	1.4292	2.4979	1.3298
8.4788	3.3138	1.4325	2.4914	1.3212
8.497	3.3185	1.436	2.4853	1.3125
8.5152	3.3234	1.4397	2.4798	1.3035
8.5335	3.3286	1.4436	2.4748	1.294
8.5517	3.3341	1.4477	2.4705	1.2841
8.57	3.3398	1.4518	2.4671	1.2737
8.5882	3.3459	1.4562	2.4646	1.2627
8.6064	3.3523	1.4607	2.4634	1.2514
8.6247	3.3592	1.4654	2.4634	1.2398
8.6429	3.3664	1.4703	2.4649	1.2281

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8.6611	3.374	1.4755	2.4679	1.2166
8.6794	3.3821	1.4809	2.4723	1.2053
8.6976	3.3906	1.4867	2.4782	1.1946
8.7158	3.3996	1.4929	2.4855	1.1847
8.7341	3.409	1.4996	2.494	1.1757
8.7523	3.4188	1.5067	2.5036	1.1678
8.7705	3.429	1.5144	2.5141	1.1612
8.7888	3.4396	1.5226	2.5252	1.1558
8.807	3.4505	1.5315	2.5367	1.1518
8.8252	3.4618	1.541	2.5484	1.1491
8.8435	3.4735	1.5513	2.56	1.1476
8.8617	3.4854	1.5623	2.5714	1.1471
8.8799	3.4976	1.5742	2.5824	1.1476
8.8982	3.5099	1.587	2.5929	1.1488
8.9164	3.5224	1.6008	2.6028	1.1505
8.9346	3.5349	1.6156	2.6122	1.1524
8.9529	3.5473	1.6315	2.621	1.1544
8.9711	3.5595	1.6486	2.6294	1.1561
8.9893	3.5714	1.6667	2.6376	1.1575
9.0076	3.5827	1.686	2.6458	1.1584
9.0258	3.5933	1.7063	2.6542	1.1586



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9.044	3.6031	1.7275	2.6632	1.1582
9.0623	3.6119	1.7496	2.6729	1.1573
9.0805	3.6197	1.7723	2.6838	1.1559
9.0987	3.6263	1.7955	2.6959	1.1542
9.117	3.6318	1.819	2.7097	1.1525
9.1352	3.6362	1.8425	2.7251	1.1512
9.1534	3.6395	1.8659	2.7424	1.1504
9.1717	3.6419	1.889	2.7614	1.1507
9.1899	3.6434	1.9117	2.7822	1.1524
9.2081	3.6444	1.9338	2.8045	1.1558
9.2264	3.6449	1.9553	2.8282	1.1612
9.2446	3.6452	1.9762	2.8531	1.169
9.2628	3.6456	1.9965	2.8786	1.1793
9.2811	3.6461	2.0163	2.9046	1.1923
9.2993	3.6471	2.0357	2.9306	1.208
9.3175	3.6485	2.055	2.9562	1.2265
9.3358	3.6505	2.0743	2.9811	1.2477
9.354	3.6531	2.0939	3.0049	1.2714
9.3722	3.6563	2.1139	3.0274	1.2974
9.3905	3.66	2.1346	3.0482	1.3255
9.4087	3.6642	2.1561	3.0673	1.3556

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9.4269	3.6687	2.1786	3.0844	1.3871
9.4452	3.6732	2.2022	3.0995	1.42
9.4634	3.6777	2.2271	3.1127	1.454
9.4816	3.6819	2.2532	3.1239	1.4888
9.4999	3.6856	2.2805	3.1331	1.5242
9.5181	3.6885	2.3091	3.1405	1.5601
9.5364	3.6906	2.3389	3.1463	1.5964
9.5546	3.6916	2.3697	3.1504	1.633
9.5728	3.6915	2.4014	3.153	1.6699
9.5911	3.6899	2.4339	3.1541	1.7071
9.6093	3.687	2.467	3.1538	1.7445
9.6275	3.6826	2.5005	3.1522	1.7824
9.6458	3.6766	2.5343	3.1491	1.8207
9.664	3.6692	2.5683	3.1444	1.8595
9.6822	3.6602	2.6022	3.1382	1.8988
9.7005	3.6498	2.6358	3.1302	1.9386
9.7187	3.638	2.6692	3.1201	1.979
9.7369	3.6249	2.7021	3.108	2.0198
9.7552	3.6105	2.7345	3.0934	2.0608
9.7734	3.5949	2.7663	3.0762	2.1021
9.7916	3.5783	2.7973	3.0563	2.1431

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9.8099	3.5606	2.8277	3.0333	2.1838
9.8281	3.5421	2.8572	3.0073	2.2237
9.8463	3.5227	2.8859	2.9782	2.2624
9.8646	3.5025	2.9138	2.946	2.2995
9.8828	3.4817	2.9407	2.9107	2.3345
9.901	3.4603	2.9667	2.8726	2.367
9.9193	3.4383	2.9918	2.8319	2.3966
9.9375	3.416	3.0159	2.7889	2.4229
9.9557	3.3933	3.039	2.7442	2.4455
9.974	3.3703	3.0612	2.6981	2.4642
9.9922	3.3472	3.0824	2.6513	2.4789
10.0104	3.3241	3.1027	2.6042	2.4895

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**Table S8:** Values of photon energy, in eV, and the corresponding complex dielectric function,  $\epsilon = \epsilon_1 + i\epsilon_2$ , in the two distinct directions of the LiNbO<sub>3</sub> type (Space Group  $R3c$ ) and one isotropic direction of the Perovskite (Space Group  $Pm\bar{3}m$ ) crystal structures in MgSnO<sub>3</sub> calculated using the hybrid HSE06 functional. The direction parallel to the a-b plane in the crystal is denoted by “||”, whereas the direction perpendicular to the a-b plane in the crystal is denoted by “⊥”. See Fig. S4 for the directions inside the crystal structure.

LiNbO <sub>3</sub> type (Space Group: $R3c$ )					Perovskite (Space Group: $Pm\bar{3}m$ )		
Photon	-direction		⊥-direction		Photon	Isotropic	
Energy (eV)	$\epsilon_1$	$\epsilon_2$	$\epsilon_1$	$\epsilon_2$	Energy (eV)	$\epsilon_1$	$\epsilon_2$
0	2.7356	0	2.5927	0	0	2.9203	0
0.0181	2.7356	0.0001	2.5928	0.0001	0.0197	2.9203	0.0001
0.0361	2.7357	0.0002	2.5928	0.0002	0.0394	2.9203	0.0002
0.0542	2.7357	0.0003	2.5928	0.0003	0.0592	2.9204	0.0004
0.0722	2.7358	0.0004	2.5929	0.0004	0.0789	2.9205	0.0005
0.0903	2.7358	0.0005	2.5929	0.0004	0.0986	2.9206	0.0006
0.1083	2.7359	0.0006	2.593	0.0005	0.1183	2.9207	0.0007
0.1264	2.736	0.0006	2.5931	0.0006	0.138	2.9209	0.0008
0.1445	2.7362	0.0007	2.5933	0.0007	0.1577	2.921	0.001
0.1625	2.7363	0.0008	2.5934	0.0008	0.1775	2.9212	0.0011
0.1806	2.7365	0.0009	2.5935	0.0009	0.1972	2.9215	0.0012

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0.1986	2.7366	0.001	2.5937	0.001	0.2169	2.9217	0.0013
0.2167	2.7368	0.0011	2.5939	0.0011	0.2366	2.922	0.0014
0.2347	2.737	0.0012	2.5941	0.0011	0.2563	2.9223	0.0016
0.2528	2.7373	0.0013	2.5943	0.0012	0.2761	2.9226	0.0017
0.2709	2.7375	0.0014	2.5945	0.0013	0.2958	2.923	0.0018
0.2889	2.7378	0.0015	2.5948	0.0014	0.3155	2.9233	0.0019
0.307	2.738	0.0016	2.595	0.0015	0.3352	2.9237	0.0021
0.325	2.7383	0.0017	2.5953	0.0016	0.3549	2.9241	0.0022
0.3431	2.7387	0.0018	2.5956	0.0017	0.3746	2.9246	0.0023
0.3611	2.739	0.0019	2.5959	0.0018	0.3944	2.925	0.0024
0.3792	2.7393	0.002	2.5963	0.0019	0.4141	2.9255	0.0025
0.3972	2.7397	0.002	2.5966	0.002	0.4338	2.926	0.0027
0.4153	2.7401	0.0021	2.597	0.002	0.4535	2.9266	0.0028
0.4334	2.7405	0.0022	2.5973	0.0021	0.4732	2.9271	0.0029
0.4514	2.7409	0.0023	2.5977	0.0022	0.493	2.9277	0.003
0.4695	2.7413	0.0024	2.5981	0.0023	0.5127	2.9283	0.0032
0.4875	2.7417	0.0025	2.5986	0.0024	0.5324	2.929	0.0033
0.5056	2.7422	0.0026	2.599	0.0025	0.5521	2.9296	0.0034
0.5236	2.7427	0.0027	2.5995	0.0026	0.5718	2.9303	0.0035
0.5417	2.7432	0.0028	2.5999	0.0027	0.5915	2.931	0.0037
0.5598	2.7437	0.0029	2.6004	0.0028	0.6113	2.9318	0.0038

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0.5778	2.7442	0.003	2.6009	0.0029	0.631	2.9325	0.0039
0.5959	2.7448	0.0031	2.6015	0.003	0.6507	2.9333	0.0041
0.6139	2.7454	0.0032	2.602	0.003	0.6704	2.9341	0.0042
0.632	2.7459	0.0033	2.6026	0.0031	0.6901	2.9349	0.0043
0.65	2.7465	0.0034	2.6031	0.0032	0.7099	2.9358	0.0044
0.6681	2.7472	0.0035	2.6037	0.0033	0.7296	2.9367	0.0046
0.6862	2.7478	0.0036	2.6043	0.0034	0.7493	2.9376	0.0047
0.7042	2.7485	0.0037	2.605	0.0035	0.769	2.9385	0.0048
0.7223	2.7491	0.0038	2.6056	0.0036	0.7887	2.9395	0.005
0.7403	2.7498	0.0039	2.6063	0.0037	0.8084	2.9405	0.0051
0.7584	2.7505	0.004	2.607	0.0038	0.8282	2.9415	0.0052
0.7764	2.7513	0.0041	2.6076	0.0039	0.8479	2.9426	0.0054
0.7945	2.752	0.0042	2.6084	0.004	0.8676	2.9436	0.0055
0.8126	2.7528	0.0043	2.6091	0.0041	0.8873	2.9447	0.0056
0.8306	2.7536	0.0044	2.6098	0.0042	0.907	2.9459	0.0058
0.8487	2.7544	0.0045	2.6106	0.0043	0.9268	2.947	0.0059
0.8667	2.7552	0.0046	2.6114	0.0044	0.9465	2.9482	0.0061
0.8848	2.756	0.0047	2.6122	0.0045	0.9662	2.9494	0.0062
0.9028	2.7569	0.0048	2.613	0.0046	0.9859	2.9506	0.0063
0.9209	2.7578	0.0049	2.6138	0.0047	1.0056	2.9519	0.0065
0.9389	2.7587	0.005	2.6147	0.0048	1.0254	2.9532	0.0066

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0.957	2.7596	0.0051	2.6156	0.0049	1.0451	2.9545	0.0068
0.9751	2.7605	0.0052	2.6165	0.005	1.0648	2.9558	0.0069
0.9931	2.7615	0.0053	2.6174	0.0051	1.0845	2.9572	0.0071
1.0112	2.7624	0.0054	2.6183	0.0052	1.1042	2.9586	0.0072
1.0292	2.7634	0.0055	2.6192	0.0053	1.1239	2.9601	0.0073
1.0473	2.7644	0.0056	2.6202	0.0054	1.1437	2.9615	0.0075
1.0653	2.7655	0.0058	2.6212	0.0055	1.1634	2.963	0.0076
1.0834	2.7665	0.0059	2.6222	0.0056	1.1831	2.9645	0.0078
1.1015	2.7676	0.006	2.6232	0.0057	1.2028	2.9661	0.008
1.1195	2.7687	0.0061	2.6242	0.0058	1.2225	2.9677	0.0081
1.1376	2.7698	0.0062	2.6253	0.0059	1.2423	2.9693	0.0083
1.1556	2.7709	0.0063	2.6264	0.006	1.262	2.9709	0.0084
1.1737	2.772	0.0064	2.6275	0.0061	1.2817	2.9726	0.0086
1.1917	2.7732	0.0065	2.6286	0.0062	1.3014	2.9743	0.0087
1.2098	2.7744	0.0066	2.6297	0.0064	1.3211	2.976	0.0089
1.2279	2.7756	0.0068	2.6309	0.0065	1.3408	2.9778	0.0091
1.2459	2.7768	0.0069	2.6321	0.0066	1.3606	2.9796	0.0092
1.264	2.7781	0.007	2.6333	0.0067	1.3803	2.9814	0.0094
1.282	2.7794	0.0071	2.6345	0.0068	1.4	2.9833	0.0096
1.3001	2.7806	0.0072	2.6357	0.0069	1.4197	2.9852	0.0097
1.3181	2.782	0.0073	2.637	0.007	1.4394	2.9871	0.0099

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1.3362	2.7833	0.0075	2.6382	0.0071	1.4592	2.9891	0.0101
1.3543	2.7847	0.0076	2.6395	0.0073	1.4789	2.9911	0.0102
1.3723	2.786	0.0077	2.6409	0.0074	1.4986	2.9931	0.0104
1.3904	2.7874	0.0078	2.6422	0.0075	1.5183	2.9952	0.0106
1.4084	2.7889	0.0079	2.6436	0.0076	1.538	2.9973	0.0108
1.4265	2.7903	0.0081	2.6449	0.0077	1.5577	2.9994	0.011
1.4445	2.7918	0.0082	2.6463	0.0078	1.5775	3.0016	0.0111
1.4626	2.7932	0.0083	2.6478	0.008	1.5972	3.0038	0.0113
1.4807	2.7948	0.0084	2.6492	0.0081	1.6169	3.0061	0.0115
1.4987	2.7963	0.0086	2.6507	0.0082	1.6366	3.0084	0.0117
1.5168	2.7978	0.0087	2.6522	0.0083	1.6563	3.0107	0.0119
1.5348	2.7994	0.0088	2.6537	0.0085	1.6761	3.0131	0.0121
1.5529	2.801	0.009	2.6552	0.0086	1.6958	3.0155	0.0123
1.5709	2.8027	0.0091	2.6568	0.0087	1.7155	3.0179	0.0125
1.589	2.8043	0.0092	2.6584	0.0089	1.7352	3.0204	0.0127
1.607	2.806	0.0094	2.66	0.009	1.7549	3.0229	0.0129
1.6251	2.8077	0.0095	2.6616	0.0091	1.7746	3.0255	0.0131
1.6432	2.8094	0.0096	2.6633	0.0092	1.7944	3.0281	0.0133
1.6612	2.8112	0.0098	2.665	0.0094	1.8141	3.0307	0.0135
1.6793	2.8129	0.0099	2.6667	0.0095	1.8338	3.0334	0.0138
1.6973	2.8147	0.01	2.6684	0.0097	1.8535	3.0361	0.014



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1.7154	2.8165	0.0102	2.6701	0.0098	1.8732	3.0389	0.0142
1.7334	2.8184	0.0103	2.6719	0.0099	1.893	3.0417	0.0144
1.7515	2.8203	0.0105	2.6737	0.0101	1.9127	3.0446	0.0147
1.7696	2.8222	0.0106	2.6755	0.0102	1.9324	3.0475	0.0149
1.7876	2.8241	0.0108	2.6774	0.0104	1.9521	3.0504	0.0151
1.8057	2.826	0.0109	2.6793	0.0105	1.9718	3.0534	0.0154
1.8237	2.828	0.0111	2.6812	0.0106	1.9915	3.0565	0.0156
1.8418	2.83	0.0112	2.6831	0.0108	2.0113	3.0596	0.0159
1.8598	2.8321	0.0114	2.6851	0.0109	2.031	3.0627	0.0161
1.8779	2.8341	0.0115	2.6871	0.0111	2.0507	3.0659	0.0164
1.896	2.8362	0.0117	2.6891	0.0112	2.0704	3.0692	0.0166
1.914	2.8383	0.0118	2.6911	0.0114	2.0901	3.0725	0.0169
1.9321	2.8405	0.012	2.6932	0.0116	2.1099	3.0758	0.0172
1.9501	2.8426	0.0121	2.6953	0.0117	2.1296	3.0792	0.0174
1.9682	2.8449	0.0123	2.6974	0.0119	2.1493	3.0827	0.0177
1.9862	2.8471	0.0125	2.6996	0.012	2.169	3.0862	0.018
2.0043	2.8493	0.0126	2.7018	0.0122	2.1887	3.0898	0.0183
2.0224	2.8516	0.0128	2.704	0.0124	2.2084	3.0934	0.0186
2.0404	2.854	0.013	2.7062	0.0125	2.2282	3.0971	0.0189
2.0585	2.8563	0.0131	2.7085	0.0127	2.2479	3.1008	0.0192
2.0765	2.8587	0.0133	2.7108	0.0129	2.2676	3.1046	0.0195

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2.0946	2.8611	0.0135	2.7131	0.0131	2.2873	3.1085	0.0198
2.1126	2.8636	0.0137	2.7155	0.0132	2.307	3.1124	0.0202
2.1307	2.8661	0.0139	2.7179	0.0134	2.3268	3.1164	0.0205
2.1488	2.8686	0.014	2.7204	0.0136	2.3465	3.1205	0.0208
2.1668	2.8711	0.0142	2.7228	0.0138	2.3662	3.1246	0.0212
2.1849	2.8737	0.0144	2.7253	0.014	2.3859	3.1288	0.0215
2.2029	2.8763	0.0146	2.7279	0.0142	2.4056	3.1331	0.0219
2.221	2.879	0.0148	2.7304	0.0144	2.4253	3.1374	0.0223
2.239	2.8816	0.015	2.733	0.0146	2.4451	3.1418	0.0227
2.2571	2.8844	0.0152	2.7357	0.0148	2.4648	3.1463	0.0231
2.2751	2.8871	0.0154	2.7384	0.015	2.4845	3.1509	0.0235
2.2932	2.8899	0.0156	2.7411	0.0152	2.5042	3.1556	0.0239
2.3113	2.8927	0.0158	2.7438	0.0154	2.5239	3.1603	0.0243
2.3293	2.8956	0.016	2.7466	0.0156	2.5437	3.1651	0.0247
2.3474	2.8985	0.0162	2.7494	0.0158	2.5634	3.17	0.0252
2.3654	2.9015	0.0164	2.7523	0.016	2.5831	3.175	0.0256
2.3835	2.9044	0.0167	2.7552	0.0162	2.6028	3.1801	0.0261
2.4015	2.9075	0.0169	2.7581	0.0165	2.6225	3.1852	0.0266
2.4196	2.9105	0.0171	2.7611	0.0167	2.6422	3.1905	0.027
2.4377	2.9136	0.0173	2.7642	0.0169	2.662	3.1958	0.0276
2.4557	2.9168	0.0176	2.7672	0.0172	2.6817	3.2013	0.0281

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2.4738	2.92	0.0178	2.7703	0.0174	2.7014	3.2069	0.0286
2.4918	2.9232	0.0181	2.7735	0.0176	2.7211	3.2125	0.0292
2.5099	2.9265	0.0183	2.7767	0.0179	2.7408	3.2183	0.0297
2.5279	2.9298	0.0186	2.7799	0.0182	2.7606	3.2242	0.0303
2.546	2.9332	0.0188	2.7832	0.0184	2.7803	3.2302	0.0309
2.5641	2.9366	0.0191	2.7866	0.0187	2.8	3.2363	0.0316
2.5821	2.94	0.0193	2.79	0.0189	2.8197	3.2426	0.0322
2.6002	2.9435	0.0196	2.7934	0.0192	2.8394	3.249	0.0329
2.6182	2.9471	0.0199	2.7969	0.0195	2.8591	3.2555	0.0336
2.6363	2.9507	0.0202	2.8004	0.0198	2.8789	3.2621	0.0343
2.6543	2.9543	0.0204	2.804	0.0201	2.8986	3.2689	0.0351
2.6724	2.9581	0.0207	2.8077	0.0204	2.9183	3.2759	0.0359
2.6905	2.9618	0.021	2.8113	0.0207	2.938	3.283	0.0367
2.7085	2.9656	0.0213	2.8151	0.021	2.9577	3.2902	0.0376
2.7266	2.9695	0.0216	2.8189	0.0213	2.9775	3.2976	0.0385
2.7446	2.9734	0.0219	2.8228	0.0216	2.9972	3.3052	0.0394
2.7627	2.9774	0.0223	2.8267	0.022	3.0169	3.313	0.0404
2.7807	2.9814	0.0226	2.8307	0.0223	3.0366	3.321	0.0414
2.7988	2.9855	0.0229	2.8347	0.0226	3.0563	3.3292	0.0425
2.8168	2.9897	0.0233	2.8388	0.023	3.0761	3.3376	0.0436
2.8349	2.9939	0.0236	2.843	0.0233	3.0958	3.3462	0.0449

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2.853	2.9982	0.024	2.8472	0.0237	3.1155	3.355	0.0461
2.871	3.0025	0.0243	2.8515	0.0241	3.1352	3.3641	0.0475
2.8891	3.0069	0.0247	2.8559	0.0245	3.1549	3.3734	0.0489
2.9071	3.0114	0.0251	2.8603	0.0249	3.1746	3.383	0.0505
2.9252	3.016	0.0255	2.8648	0.0253	3.1944	3.3929	0.0522
2.9432	3.0206	0.0259	2.8694	0.0257	3.2141	3.4031	0.0539
2.9613	3.0253	0.0263	2.8741	0.0261	3.2338	3.4136	0.0559
2.9794	3.0301	0.0267	2.8788	0.0266	3.2535	3.4244	0.058
2.9974	3.0349	0.0272	2.8836	0.0271	3.2732	3.4355	0.0603
3.0155	3.0398	0.0276	2.8885	0.0275	3.293	3.4471	0.0628
3.0335	3.0448	0.0281	2.8935	0.028	3.3127	3.459	0.0655
3.0516	3.0499	0.0286	2.8986	0.0285	3.3324	3.4712	0.0685
3.0696	3.0551	0.0291	2.9038	0.029	3.3521	3.4839	0.0719
3.0877	3.0604	0.0296	2.909	0.0295	3.3718	3.4969	0.0756
3.1058	3.0657	0.0301	2.9144	0.0301	3.3915	3.5104	0.0797
3.1238	3.0712	0.0306	2.9198	0.0307	3.4113	3.5242	0.0843
3.1419	3.0767	0.0312	2.9254	0.0312	3.431	3.5384	0.0893
3.1599	3.0824	0.0318	2.931	0.0318	3.4507	3.553	0.0949
3.178	3.0881	0.0324	2.9368	0.0325	3.4704	3.5679	0.1012
3.196	3.094	0.033	2.9427	0.0331	3.4901	3.5831	0.108
3.2141	3.0999	0.0336	2.9487	0.0338	3.5099	3.5985	0.1156

**B. B. Dumre, S. V. Khare, Physica B: Condensed Matter 637, 413896, Supplementary Material (2022)**

3.2322	3.106	0.0343	2.9548	0.0345	3.5296	3.6142	0.1238
3.2502	3.1122	0.035	2.961	0.0352	3.5493	3.6301	0.1329
3.2683	3.1185	0.0357	2.9674	0.036	3.569	3.6462	0.1427
3.2863	3.125	0.0365	2.9739	0.0368	3.5887	3.6624	0.1534
3.3044	3.1316	0.0372	2.9805	0.0376	3.6084	3.6786	0.1649
3.3224	3.1383	0.0381	2.9873	0.0385	3.6282	3.6949	0.1774
3.3405	3.1451	0.0389	2.9943	0.0394	3.6479	3.7111	0.1907
3.3586	3.1522	0.0398	3.0014	0.0403	3.6676	3.7273	0.2051
3.3766	3.1593	0.0408	3.0086	0.0413	3.6873	3.7433	0.2204
3.3947	3.1667	0.0418	3.0161	0.0424	3.707	3.7592	0.2368
3.4127	3.1742	0.0429	3.0237	0.0435	3.7268	3.7748	0.2544
3.4308	3.1819	0.0441	3.0315	0.0447	3.7465	3.79	0.2731
3.4488	3.1898	0.0453	3.0396	0.0459	3.7662	3.8047	0.293
3.4669	3.1979	0.0466	3.0478	0.0473	3.7859	3.8188	0.3142
3.4849	3.2062	0.048	3.0562	0.0487	3.8056	3.8321	0.3367
3.503	3.2147	0.0495	3.0649	0.0502	3.8253	3.8444	0.3604
3.5211	3.2234	0.0512	3.0739	0.0519	3.8451	3.8555	0.3853
3.5391	3.2324	0.053	3.083	0.0536	3.8648	3.8653	0.4114
3.5572	3.2416	0.055	3.0925	0.0556	3.8845	3.8734	0.4385
3.5752	3.251	0.0571	3.1022	0.0577	3.9042	3.8798	0.4665
3.5933	3.2607	0.0595	3.1122	0.0599	3.9239	3.8841	0.4951

**B. B. Dumre, S. V. Khare, Physica B: Condensed Matter 637, 413896, Supplementary Material (2022)**

3.6113	3.2707	0.0621	3.1226	0.0625	3.9437	3.8864	0.5242
3.6294	3.2808	0.065	3.1332	0.0652	3.9634	3.8864	0.5533
3.6475	3.2913	0.0683	3.1441	0.0683	3.9831	3.884	0.5823
3.6655	3.3019	0.0718	3.1553	0.0717	4.0028	3.8793	0.6107
3.6836	3.3127	0.0758	3.1669	0.0755	4.0225	3.8722	0.6381
3.7016	3.3237	0.0801	3.1787	0.0796	4.0422	3.863	0.6643
3.7197	3.3348	0.0849	3.1908	0.0843	4.062	3.8516	0.6887
3.7377	3.3461	0.0902	3.2031	0.0894	4.0817	3.8386	0.711
3.7558	3.3573	0.096	3.2156	0.0951	4.1014	3.8241	0.7309
3.7739	3.3686	0.1023	3.2283	0.1013	4.1211	3.8087	0.7482
3.7919	3.3797	0.109	3.2411	0.1082	4.1408	3.7928	0.7626
3.81	3.3908	0.1163	3.2539	0.1158	4.1606	3.777	0.774
3.828	3.4016	0.124	3.2667	0.124	4.1803	3.7619	0.7826
3.8461	3.4122	0.1322	3.2794	0.1329	4.2	3.7482	0.7884
3.8641	3.4225	0.1408	3.292	0.1425	4.2197	3.7363	0.7918
3.8822	3.4324	0.1497	3.3042	0.1527	4.2394	3.7268	0.7933
3.9003	3.442	0.1588	3.3161	0.1635	4.2591	3.7201	0.7934
3.9183	3.4512	0.1681	3.3276	0.1748	4.2789	3.7164	0.7928
3.9364	3.46	0.1776	3.3386	0.1867	4.2986	3.7159	0.7922
3.9544	3.4685	0.187	3.3491	0.1988	4.3183	3.7186	0.7924
3.9725	3.4767	0.1964	3.359	0.2113	4.338	3.7242	0.7941

**B. B. Dumre, S. V. Khare, Physica B: Condensed Matter 637, 413896, Supplementary Material (2022)**

3.9905	3.4846	0.2058	3.3684	0.2239	4.3577	3.7322	0.7981
4.0086	3.4924	0.2149	3.3774	0.2365	4.3775	3.7422	0.8048
4.0266	3.5001	0.224	3.3859	0.2491	4.3972	3.7535	0.8149
4.0447	3.5078	0.2328	3.394	0.2615	4.4169	3.7652	0.8285
4.0628	3.5155	0.2415	3.4019	0.2738	4.4366	3.7765	0.8457
4.0808	3.5235	0.2501	3.4098	0.2858	4.4563	3.7866	0.8666
4.0989	3.5318	0.2586	3.4177	0.2975	4.476	3.7946	0.8907
4.1169	3.5404	0.2672	3.4258	0.309	4.4958	3.7998	0.9177
4.135	3.5493	0.2759	3.4344	0.3204	4.5155	3.8014	0.9469
4.153	3.5587	0.2849	3.4435	0.3318	4.5352	3.7991	0.9775
4.1711	3.5686	0.2942	3.4533	0.3434	4.5549	3.7925	1.0087
4.1892	3.5788	0.304	3.4638	0.3555	4.5746	3.7815	1.0395
4.2072	3.5893	0.3144	3.4752	0.3682	4.5944	3.7661	1.0691
4.2253	3.6002	0.3256	3.4872	0.3818	4.6141	3.7466	1.0964
4.2433	3.6112	0.3376	3.4999	0.3967	4.6338	3.7235	1.1207
4.2614	3.6223	0.3506	3.5132	0.4132	4.6535	3.6975	1.1412
4.2794	3.6333	0.3645	3.5266	0.4314	4.6732	3.6694	1.1573
4.2975	3.6441	0.3795	3.54	0.4516	4.6929	3.6401	1.1688
4.3156	3.6544	0.3955	3.5529	0.4739	4.7127	3.6105	1.1753
4.3336	3.6642	0.4126	3.565	0.4984	4.7324	3.5817	1.177
4.3517	3.6731	0.4307	3.5757	0.5251	4.7521	3.5546	1.1741

**B. B. Dumre, S. V. Khare, Physica B: Condensed Matter 637, 413896, Supplementary Material (2022)**

4.3697	3.6811	0.4496	3.5847	0.5539	4.7718	3.5302	1.1671
4.3878	3.6879	0.4693	3.5915	0.5845	4.7915	3.5091	1.1565
4.4058	3.6935	0.4896	3.5957	0.6166	4.8113	3.492	1.1433
4.4239	3.6978	0.5103	3.5969	0.65	4.831	3.4792	1.1282
4.442	3.7006	0.5312	3.5949	0.6839	4.8507	3.471	1.1122
4.46	3.702	0.5521	3.5895	0.7181	4.8704	3.4674	1.0963
4.4781	3.702	0.5728	3.5806	0.7518	4.8901	3.4682	1.0813
4.4961	3.7005	0.593	3.5683	0.7844	4.9098	3.4729	1.068
4.5142	3.6978	0.6125	3.5526	0.8156	4.9296	3.4811	1.0572
4.5322	3.694	0.6312	3.534	0.8446	4.9493	3.4921	1.0494
4.5503	3.6892	0.649	3.5127	0.871	4.969	3.5052	1.0449
4.5684	3.6835	0.6657	3.4892	0.8944	4.9887	3.5197	1.0441
4.5864	3.6772	0.6812	3.4639	0.9145	5.0084	3.5347	1.0468
4.6045	3.6705	0.6956	3.4376	0.9311	5.0282	3.5497	1.0531
4.6225	3.6635	0.7087	3.4106	0.9441	5.0479	3.5639	1.0628
4.6406	3.6565	0.7207	3.3836	0.9535	5.0676	3.5767	1.0754
4.6586	3.6495	0.7315	3.3572	0.9594	5.0873	3.5878	1.0906
4.6767	3.6428	0.7413	3.3319	0.962	5.107	3.5967	1.1079
4.6947	3.6364	0.7501	3.3081	0.9617	5.1268	3.6033	1.1268
4.7128	3.6305	0.758	3.2862	0.9586	5.1465	3.6073	1.1468
4.7309	3.6251	0.7651	3.2665	0.9534	5.1662	3.6087	1.1673



**B. B. Dumre, S. V. Khare, Physica B: Condensed Matter 637, 413896, Supplementary Material (2022)**

4.7489	3.6204	0.7716	3.2493	0.9463	5.1859	3.6077	1.188
4.767	3.6163	0.7775	3.2346	0.9378	5.2056	3.6043	1.2083
4.785	3.613	0.783	3.2225	0.9285	5.2253	3.5986	1.2279
4.8031	3.6104	0.7881	3.213	0.9186	5.2451	3.5911	1.2465
4.8211	3.6086	0.7929	3.2059	0.9085	5.2648	3.582	1.2636
4.8392	3.6076	0.7976	3.2012	0.8986	5.2845	3.5716	1.2793
4.8573	3.6073	0.8023	3.1986	0.8892	5.3042	3.5603	1.2933
4.8753	3.6079	0.807	3.198	0.8804	5.3239	3.5484	1.3055
4.8934	3.6092	0.8118	3.1991	0.8725	5.3437	3.5365	1.3161
4.9114	3.6113	0.8169	3.2017	0.8654	5.3634	3.5246	1.3252
4.9295	3.6141	0.8224	3.2057	0.8594	5.3831	3.5133	1.3328
4.9475	3.6176	0.8283	3.2108	0.8543	5.4028	3.5026	1.3394
4.9656	3.6217	0.8348	3.217	0.8504	5.4225	3.4928	1.3451
4.9837	3.6265	0.842	3.2242	0.8475	5.4422	3.4839	1.3502
5.0017	3.6317	0.8499	3.2321	0.8457	5.462	3.4759	1.3551
5.0198	3.6372	0.8587	3.2409	0.845	5.4817	3.4686	1.3601
5.0378	3.6431	0.8685	3.2503	0.8454	5.5014	3.462	1.3652
5.0559	3.649	0.8793	3.2605	0.8471	5.5211	3.4557	1.3707
5.0739	3.6549	0.8912	3.2711	0.8502	5.5408	3.4496	1.3765
5.092	3.6605	0.9041	3.2823	0.8546	5.5606	3.4433	1.3827
5.1101	3.6657	0.9181	3.2938	0.8606	5.5803	3.4367	1.3891

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5.1281	3.6703	0.9332	3.3054	0.8681	5.6	3.4296	1.3955
5.1462	3.674	0.9491	3.317	0.8774	5.6197	3.422	1.4015
5.1642	3.6768	0.9658	3.3283	0.8883	5.6394	3.414	1.4069
5.1823	3.6785	0.9831	3.3391	0.9009	5.6591	3.4057	1.4115
5.2003	3.679	1.0008	3.3491	0.9151	5.6789	3.3975	1.4151
5.2184	3.6782	1.0188	3.3581	0.9309	5.6986	3.3896	1.4176
5.2365	3.6762	1.0366	3.3658	0.948	5.7183	3.3825	1.4191
5.2545	3.673	1.0542	3.3722	0.9662	5.738	3.3765	1.4196
5.2726	3.6686	1.0714	3.3769	0.9854	5.7577	3.3721	1.4195
5.2906	3.6633	1.088	3.3799	1.0051	5.7775	3.3693	1.4193
5.3087	3.6571	1.1038	3.3812	1.0253	5.7972	3.3684	1.4195
5.3267	3.6503	1.1189	3.3808	1.0456	5.8169	3.3693	1.4205
5.3448	3.643	1.1331	3.3787	1.0657	5.8366	3.3717	1.423
5.3628	3.6354	1.1464	3.375	1.0855	5.8563	3.3754	1.4274
5.3809	3.6276	1.1591	3.37	1.1047	5.876	3.3797	1.4341
5.399	3.6198	1.171	3.3636	1.1232	5.8958	3.3842	1.4432
5.417	3.612	1.1823	3.3561	1.1409	5.9155	3.3881	1.4549
5.4351	3.6042	1.1932	3.3477	1.1577	5.9352	3.3909	1.469
5.4531	3.5964	1.2037	3.3384	1.1736	5.9549	3.3919	1.4853
5.4712	3.5886	1.2139	3.3285	1.1886	5.9746	3.3905	1.5032
5.4892	3.5806	1.2238	3.318	1.2027	5.9944	3.3865	1.5222

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5.5073	3.5725	1.2333	3.3071	1.2159	6.0141	3.3797	1.5418
5.5254	3.5642	1.2426	3.2957	1.2283	6.0338	3.37	1.5612
5.5434	3.5555	1.2514	3.284	1.2398	6.0535	3.3574	1.5799
5.5615	3.5464	1.2596	3.272	1.2504	6.0732	3.3423	1.5973
5.5795	3.537	1.2671	3.2597	1.2603	6.0929	3.325	1.613
5.5976	3.5274	1.2737	3.2471	1.2693	6.1127	3.3059	1.6267
5.6156	3.5176	1.2794	3.2342	1.2774	6.1324	3.2855	1.6381
5.6337	3.5079	1.2839	3.2212	1.2846	6.1521	3.2642	1.6472
5.6518	3.4984	1.2871	3.2079	1.2908	6.1718	3.2424	1.654
5.6698	3.4895	1.2892	3.1946	1.2959	6.1915	3.2205	1.6586
5.6879	3.4813	1.29	3.1812	1.3	6.2113	3.1988	1.6611
5.7059	3.4741	1.2898	3.1679	1.3029	6.231	3.1775	1.6618
5.724	3.4682	1.2886	3.1547	1.3046	6.2507	3.1567	1.6608
5.742	3.4638	1.2867	3.1418	1.3051	6.2704	3.1366	1.6582
5.7601	3.4611	1.2844	3.1294	1.3042	6.2901	3.1172	1.6543
5.7782	3.4601	1.282	3.1176	1.3021	6.3098	3.0984	1.6491
5.7962	3.4608	1.2799	3.1065	1.2987	6.3296	3.0804	1.6427
5.8143	3.4633	1.2784	3.0964	1.2941	6.3493	3.0631	1.6351
5.8323	3.4673	1.2779	3.0874	1.2883	6.369	3.0466	1.6263
5.8504	3.4727	1.2785	3.0797	1.2814	6.3887	3.0311	1.6164
5.8684	3.4791	1.2807	3.0736	1.2736	6.4084	3.0165	1.6054

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5.8865	3.4863	1.2845	3.0691	1.265	6.4282	3.003	1.5933
5.9045	3.4939	1.29	3.0663	1.2558	6.4479	2.9907	1.5802
5.9226	3.5015	1.2973	3.0656	1.2462	6.4676	2.9799	1.5663
5.9407	3.5088	1.3063	3.0668	1.2364	6.4873	2.9705	1.5517
5.9587	3.5155	1.3168	3.0702	1.2267	6.507	2.9626	1.5365
5.9768	3.5212	1.3287	3.0757	1.2174	6.5267	2.9564	1.5211
5.9948	3.5257	1.3416	3.0834	1.2088	6.5465	2.9517	1.5055
6.0129	3.529	1.3553	3.0932	1.2011	6.5662	2.9485	1.4901
6.0309	3.531	1.3694	3.1051	1.1947	6.5859	2.9468	1.4749
6.049	3.5316	1.3836	3.1188	1.1899	6.6056	2.9463	1.4601
6.0671	3.5309	1.3977	3.1342	1.1869	6.6253	2.9469	1.4459
6.0851	3.5292	1.4114	3.1512	1.1861	6.6451	2.9485	1.4322
6.1032	3.5265	1.4244	3.1693	1.1876	6.6648	2.9509	1.419
6.1212	3.5232	1.4367	3.1882	1.1916	6.6845	2.9539	1.4064
6.1393	3.5193	1.4481	3.2077	1.1983	6.7042	2.9575	1.3942
6.1573	3.5153	1.4586	3.2274	1.2077	6.7239	2.9616	1.3823
6.1754	3.5113	1.4683	3.2468	1.2199	6.7436	2.9662	1.3708
6.1935	3.5076	1.4773	3.2656	1.2347	6.7634	2.9712	1.3594
6.2115	3.5043	1.4856	3.2834	1.2522	6.7831	2.9768	1.3483
6.2296	3.5015	1.4936	3.2998	1.2721	6.8028	2.9829	1.3372
6.2476	3.4994	1.5012	3.3146	1.2942	6.8225	2.9897	1.3263

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6.2657	3.498	1.5088	3.3274	1.3183	6.8422	2.9971	1.3154
6.2837	3.4972	1.5165	3.338	1.3439	6.862	3.0053	1.3048
6.3018	3.497	1.5246	3.3463	1.3708	6.8817	3.0142	1.2944
6.3199	3.4973	1.533	3.3521	1.3986	6.9014	3.0239	1.2844
6.3379	3.4979	1.5421	3.3554	1.4269	6.9211	3.0344	1.2747
6.356	3.4988	1.5518	3.3563	1.4553	6.9408	3.0456	1.2655
6.374	3.4997	1.5623	3.3547	1.4836	6.9605	3.0574	1.2569
6.3921	3.5005	1.5734	3.3509	1.5113	6.9803	3.0699	1.2489
6.4101	3.5011	1.5852	3.345	1.5383	7	3.0829	1.2416
6.4282	3.5012	1.5976	3.3373	1.5641	7.0197	3.0962	1.2348
6.4463	3.5009	1.6105	3.328	1.5888	7.0394	3.1099	1.2287
6.4643	3.4999	1.6238	3.3174	1.612	7.0591	3.1237	1.2232
6.4824	3.4983	1.6373	3.3058	1.6338	7.0789	3.1377	1.2181
6.5004	3.496	1.6509	3.2935	1.6541	7.0986	3.1517	1.2134
6.5185	3.493	1.6646	3.2807	1.673	7.1183	3.1658	1.209
6.5365	3.4894	1.678	3.2678	1.6905	7.138	3.18	1.2047
6.5546	3.4852	1.6912	3.2548	1.7068	7.1577	3.1943	1.2004
6.5726	3.4805	1.7041	3.2421	1.7221	7.1775	3.2088	1.196
6.5907	3.4754	1.7165	3.2296	1.7364	7.1972	3.2237	1.1914
6.6088	3.47	1.7285	3.2175	1.7501	7.2169	3.2391	1.1865
6.6268	3.4644	1.74	3.2058	1.7632	7.2366	3.2551	1.1815

**B. B. Dumre, S. V. Khare, Physica B: Condensed Matter 637, 413896, Supplementary Material (2022)**

6.6449	3.4588	1.7509	3.1946	1.776	7.2563	3.272	1.1762
6.6629	3.4532	1.7615	3.1836	1.7885	7.276	3.2899	1.1709
6.681	3.4476	1.7715	3.1729	1.801	7.2958	3.3089	1.1656
6.699	3.4423	1.7813	3.1624	1.8135	7.3155	3.3291	1.1604
6.7171	3.4372	1.7907	3.1519	1.826	7.3352	3.3506	1.1557
6.7352	3.4324	1.7999	3.1414	1.8386	7.3549	3.3733	1.1515
6.7532	3.4279	1.8089	3.1307	1.8512	7.3746	3.3972	1.148
6.7713	3.4236	1.8179	3.1199	1.8637	7.3944	3.4221	1.1454
6.7893	3.4197	1.8267	3.1088	1.8762	7.4141	3.4481	1.1437
6.8074	3.416	1.8356	3.0974	1.8886	7.4338	3.4748	1.143
6.8254	3.4126	1.8444	3.0857	1.9008	7.4535	3.5022	1.1432
6.8435	3.4095	1.8533	3.0738	1.9126	7.4732	3.53	1.1444
6.8616	3.4067	1.8622	3.0617	1.9242	7.4929	3.5583	1.1462
6.8796	3.4042	1.8712	3.0495	1.9354	7.5127	3.5871	1.1486
6.8977	3.402	1.8802	3.0372	1.9462	7.5324	3.6163	1.1514
6.9157	3.4002	1.8893	3.0249	1.9566	7.5521	3.6461	1.1543
6.9338	3.3988	1.8987	3.0127	1.9667	7.5718	3.6768	1.1571
6.9518	3.398	1.9083	3.0007	1.9765	7.5915	3.7086	1.1598
6.9699	3.3976	1.9182	2.9889	1.986	7.6113	3.7421	1.1624
6.988	3.3977	1.9286	2.9774	1.9955	7.631	3.7776	1.165
7.006	3.3984	1.9397	2.9662	2.0049	7.6507	3.8155	1.1677

**B. B. Dumre, S. V. Khare, Physica B: Condensed Matter 637, 413896, Supplementary Material (2022)**

7.0241	3.3995	1.9516	2.9553	2.0144	7.6704	3.8564	1.1709
7.0421	3.4009	1.9645	2.9446	2.024	7.6901	3.9005	1.1752
7.0602	3.4026	1.9784	2.9343	2.034	7.7098	3.9482	1.1811
7.0782	3.4043	1.9936	2.9241	2.0444	7.7296	3.9995	1.1894
7.0963	3.4058	2.0101	2.914	2.0553	7.7493	4.0546	1.2007
7.1143	3.4069	2.0279	2.9039	2.0669	7.769	4.1132	1.2159
7.1324	3.4072	2.047	2.8935	2.0791	7.7887	4.1751	1.2358
7.1505	3.4067	2.0674	2.8828	2.0921	7.8084	4.2397	1.261
7.1685	3.4049	2.0889	2.8716	2.1058	7.8282	4.3064	1.2922
7.1866	3.4018	2.1113	2.8596	2.1202	7.8479	4.3746	1.3299
7.2046	3.3972	2.1344	2.8467	2.1352	7.8676	4.4432	1.3745
7.2227	3.3909	2.1579	2.8327	2.1507	7.8873	4.5115	1.4262
7.2407	3.3828	2.1816	2.8174	2.1666	7.907	4.5786	1.485
7.2588	3.3732	2.2051	2.8007	2.1827	7.9267	4.6435	1.5508
7.2769	3.3619	2.2283	2.7825	2.1988	7.9465	4.7055	1.6234
7.2949	3.3492	2.2508	2.7627	2.2146	7.9662	4.7638	1.7023
7.313	3.3352	2.2725	2.7414	2.2299	7.9859	4.8177	1.7872
7.331	3.3201	2.2934	2.7185	2.2444	8.0056	4.8669	1.8774
7.3491	3.3041	2.3132	2.6941	2.2579	8.0253	4.9107	1.9726
7.3671	3.2874	2.3319	2.6683	2.2702	8.0451	4.949	2.072
7.3852	3.2703	2.3497	2.6414	2.281	8.0648	4.9815	2.1752

**B. B. Dumre, S. V. Khare, Physica B: Condensed Matter 637, 413896, Supplementary Material (2022)**

7.4033	3.253	2.3666	2.6135	2.2902	8.0845	5.0081	2.2817
7.4213	3.2354	2.3826	2.5849	2.2977	8.1042	5.0285	2.3911
7.4394	3.2178	2.3979	2.5557	2.3034	8.1239	5.0428	2.503
7.4574	3.2002	2.4127	2.5263	2.3072	8.1436	5.0507	2.6169
7.4755	3.1826	2.427	2.4969	2.3092	8.1634	5.0523	2.7326
7.4935	3.1649	2.441	2.4678	2.3094	8.1831	5.0474	2.8497
7.5116	3.1472	2.4547	2.4391	2.308	8.2028	5.0358	2.9678
7.5297	3.1293	2.4683	2.411	2.3051	8.2225	5.0175	3.0866
7.5477	3.1112	2.4817	2.3837	2.3009	8.2422	4.9924	3.2055
7.5658	3.0927	2.4951	2.3573	2.2955	8.262	4.9604	3.3242
7.5838	3.0738	2.5083	2.3319	2.2892	8.2817	4.9215	3.4421
7.6019	3.0544	2.5214	2.3073	2.2822	8.3014	4.8757	3.5589
7.6199	3.0343	2.5342	2.2837	2.2746	8.3211	4.8232	3.674
7.638	3.0137	2.5467	2.2608	2.2666	8.3408	4.764	3.7871
7.6561	2.9923	2.5588	2.2387	2.2583	8.3605	4.6985	3.8977
7.6741	2.9702	2.5704	2.2172	2.2498	8.3803	4.6268	4.0056
7.6922	2.9473	2.5815	2.1961	2.2412	8.4	4.5491	4.1106
7.7102	2.9238	2.5917	2.1753	2.2324	8.4197	4.4655	4.2125
7.7283	2.8995	2.6012	2.1547	2.2235	8.4394	4.3761	4.3111
7.7463	2.8746	2.6098	2.1341	2.2143	8.4591	4.2809	4.4063
7.7644	2.8492	2.6173	2.1136	2.2047	8.4789	4.1798	4.4979



**B. B. Dumre, S. V. Khare, Physica B: Condensed Matter 637, 413896, Supplementary Material (2022)**

7.7824	2.8231	2.6238	2.093	2.1947	8.4986	4.0725	4.5857
7.8005	2.7967	2.629	2.0724	2.1841	8.5183	3.9588	4.6694
7.8186	2.7699	2.633	2.0517	2.1728	8.538	3.8384	4.7482
7.8366	2.7428	2.6356	2.031	2.1606	8.5577	3.711	4.8215
7.8547	2.7156	2.6368	2.0104	2.1476	8.5774	3.5765	4.8884
7.8727	2.6884	2.6366	1.9901	2.1335	8.5972	3.4349	4.9477
7.8908	2.6613	2.6348	1.97	2.1184	8.6169	3.2863	4.9981
7.9088	2.6345	2.6314	1.9505	2.1023	8.6366	3.1313	5.0383
7.9269	2.6081	2.6264	1.9315	2.085	8.6563	2.9707	5.0668
7.945	2.5824	2.6198	1.9132	2.0667	8.676	2.8059	5.0823
7.963	2.5575	2.6117	1.8958	2.0475	8.6958	2.6382	5.0837
7.9811	2.5337	2.6021	1.8794	2.0273	8.7155	2.4698	5.0702
7.9991	2.5111	2.591	1.864	2.0063	8.7352	2.3025	5.0411
8.0172	2.4901	2.5787	1.8497	1.9846	8.7549	2.1389	4.9964
8.0352	2.4707	2.5654	1.8365	1.9623	8.7746	1.9812	4.9367
8.0533	2.4531	2.5511	1.8246	1.9395	8.7943	1.8318	4.8626
8.0714	2.4375	2.5363	1.8138	1.9163	8.8141	1.6926	4.7757
8.0894	2.424	2.5212	1.8042	1.8928	8.8338	1.5655	4.6778
8.1075	2.4126	2.5061	1.7957	1.8691	8.8535	1.4517	4.5709
8.1255	2.4032	2.4913	1.7884	1.8452	8.8732	1.3522	4.4573
8.1436	2.3959	2.4773	1.7822	1.8214	8.8929	1.2673	4.3395

**B. B. Dumre, S. V. Khare, Physica B: Condensed Matter 637, 413896, Supplementary Material (2022)**

8.1616	2.3904	2.4642	1.777	1.7974	8.9127	1.1968	4.2198
8.1797	2.3865	2.4524	1.7728	1.7735	8.9324	1.1402	4.1003
8.1978	2.384	2.4422	1.7695	1.7497	8.9521	1.0965	3.9828
8.2158	2.3825	2.4338	1.7672	1.7259	8.9718	1.0644	3.8691
8.2339	2.3817	2.4272	1.7657	1.7022	8.9915	1.0425	3.7601
8.2519	2.3813	2.4226	1.7651	1.6786	9.0112	1.0291	3.6567
8.27	2.3809	2.42	1.7653	1.655	9.031	1.023	3.5593
8.288	2.38	2.4193	1.7664	1.6316	9.0507	1.0226	3.4679
8.3061	2.3783	2.4204	1.7683	1.6082	9.0704	1.0268	3.3824
8.3242	2.3755	2.423	1.7709	1.585	9.0901	1.0347	3.3024
8.3422	2.3713	2.427	1.7744	1.5618	9.1098	1.0453	3.2274
8.3603	2.3655	2.4321	1.7786	1.5388	9.1296	1.0583	3.157
8.3783	2.3579	2.4378	1.7836	1.5158	9.1493	1.0733	3.0907
8.3964	2.3483	2.4439	1.7893	1.493	9.169	1.09	3.0281
8.4144	2.3368	2.45	1.7958	1.4702	9.1887	1.1084	2.9689
8.4325	2.3233	2.4558	1.803	1.4475	9.2084	1.1284	2.9129
8.4505	2.3079	2.4608	1.811	1.4249	9.2282	1.15	2.86
8.4686	2.2907	2.4648	1.8198	1.4023	9.2479	1.173	2.8102
8.4867	2.2719	2.4676	1.8293	1.3797	9.2676	1.1975	2.7634
8.5047	2.2517	2.4688	1.8397	1.3572	9.2873	1.2234	2.7197
8.5228	2.2303	2.4682	1.851	1.3346	9.307	1.2503	2.6791

**B. B. Dumre, S. V. Khare, Physica B: Condensed Matter 637, 413896, Supplementary Material (2022)**

8.5408	2.208	2.4657	1.8631	1.312	9.3267	1.2782	2.6417
8.5589	2.1849	2.4611	1.8763	1.2893	9.3465	1.3068	2.6074
8.5769	2.1613	2.4544	1.8905	1.2667	9.3662	1.3359	2.5762
8.595	2.1376	2.4454	1.9058	1.2441	9.3859	1.3652	2.548
8.6131	2.1138	2.4342	1.9223	1.2215	9.4056	1.3946	2.5226
8.6311	2.0904	2.4206	1.9402	1.1991	9.4253	1.4239	2.5
8.6492	2.0674	2.4046	1.9593	1.1769	9.4451	1.4528	2.4799
8.6672	2.0453	2.3864	1.9798	1.155	9.4648	1.4814	2.4623
8.6853	2.0241	2.3658	2.0018	1.1335	9.4845	1.5094	2.4469
8.7033	2.0043	2.343	2.0252	1.1124	9.5042	1.5368	2.4336
8.7214	1.9859	2.318	2.05	1.092	9.5239	1.5636	2.4222
8.7395	1.9693	2.2908	2.0763	1.0722	9.5436	1.5898	2.4126
8.7575	1.9547	2.2618	2.104	1.0533	9.5634	1.6154	2.4047
8.7756	1.9425	2.2309	2.1332	1.0351	9.5831	1.6403	2.3984
8.7936	1.9327	2.1983	2.1637	1.0179	9.6028	1.6646	2.3936
8.8117	1.9257	2.1644	2.1955	1.0017	9.6225	1.6883	2.3902
8.8297	1.9216	2.1293	2.2288	0.9866	9.6422	1.7114	2.3883
8.8478	1.9207	2.0934	2.2633	0.9726	9.662	1.7338	2.3878
8.8659	1.923	2.057	2.2992	0.9598	9.6817	1.7555	2.3886
8.8839	1.9286	2.0203	2.3363	0.9482	9.7014	1.7765	2.3908
8.902	1.9376	1.9839	2.3748	0.938	9.7211	1.7968	2.3942

**B. B. Dumre, S. V. Khare, Physica B: Condensed Matter 637, 413896, Supplementary Material (2022)**

8.92	1.9499	1.948	2.4146	0.9292	9.7408	1.8161	2.3988
8.9381	1.9655	1.9129	2.4556	0.9218	9.7605	1.8346	2.4046
8.9561	1.9842	1.879	2.4979	0.916	9.7803	1.852	2.4115
8.9742	2.0059	1.8467	2.5415	0.9119	9.8	1.8685	2.4192
8.9922	2.0304	1.816	2.5863	0.9096	9.8197	1.8839	2.4278
9.0103	2.0575	1.7873	2.6324	0.9092	9.8394	1.8983	2.437
9.0284	2.0868	1.7607	2.6796	0.9109	9.8591	1.9117	2.4468
9.0464	2.1183	1.7363	2.728	0.9147	9.8789	1.9241	2.457
9.0645	2.1517	1.7142	2.7774	0.9208	9.8986	1.9357	2.4675
9.0825	2.1867	1.6945	2.8279	0.9293	9.9183	1.9465	2.4783
9.1006	2.2233	1.6772	2.8792	0.9405	9.938	1.9567	2.4893
9.1186	2.2611	1.6623	2.9314	0.9544	9.9577	1.9664	2.5004
9.1367	2.3001	1.6499	2.9843	0.9712	9.9774	1.9757	2.5118
9.1548	2.3401	1.6398	3.0376	0.9911	9.9972	1.9847	2.5234
9.1728	2.3811	1.6322	3.0914	1.0143	10.0169	1.9935	2.5354
9.1909	2.4229	1.6271	3.1453	1.0408			
9.2089	2.4655	1.6244	3.1991	1.0709			
9.227	2.5087	1.6242	3.2526	1.1046			
9.245	2.5524	1.6267	3.3055	1.1421			
9.2631	2.5965	1.6317	3.3574	1.1835			
9.2812	2.6408	1.6394	3.4079	1.2288			

**B. B. Dumre, S. V. Khare, Physica B: Condensed Matter 637, 413896, Supplementary Material (2022)**

9.2992	2.6853	1.6498	3.4567	1.278
9.3173	2.7297	1.6629	3.5033	1.331
9.3353	2.774	1.6787	3.5474	1.3876
9.3534	2.8178	1.6972	3.5885	1.4478
9.3714	2.8611	1.7183	3.6263	1.5111
9.3895	2.9037	1.742	3.6604	1.5773
9.4076	2.9454	1.7682	3.6905	1.6461
9.4256	2.9863	1.7968	3.7165	1.7168
9.4437	3.0261	1.8276	3.7381	1.7891
9.4617	3.0648	1.8607	3.7552	1.8626
9.4798	3.1024	1.8959	3.768	1.9366
9.4978	3.1389	1.9332	3.7765	2.0107
9.5159	3.1743	1.9725	3.7808	2.0845
9.534	3.2085	2.0139	3.7813	2.1577
9.552	3.2416	2.0573	3.7783	2.2298
9.5701	3.2734	2.1028	3.772	2.3007
9.5881	3.304	2.1504	3.7628	2.3702
9.6062	3.3332	2.2004	3.7512	2.4383
9.6242	3.3609	2.2526	3.7373	2.5049
9.6423	3.387	2.3073	3.7216	2.5702
9.6603	3.4111	2.3644	3.7043	2.6342

**B. B. Dumre, S. V. Khare, Physica B: Condensed Matter 637, 413896, Supplementary Material (2022)**

9.6784	3.4331	2.424	3.6856	2.6972
9.6965	3.4527	2.486	3.6656	2.7594
9.7145	3.4696	2.5504	3.6442	2.821
9.7326	3.4834	2.6171	3.6216	2.8822
9.7506	3.494	2.6858	3.5975	2.9433
9.7687	3.5009	2.7563	3.5718	3.0044
9.7867	3.5041	2.8284	3.5443	3.0655
9.8048	3.5032	2.9017	3.5147	3.1267
9.8229	3.4981	2.9758	3.4827	3.1879
9.8409	3.4887	3.0504	3.4481	3.249
9.859	3.4749	3.125	3.4105	3.3098
9.877	3.4569	3.1993	3.3699	3.3699
9.8951	3.4347	3.2728	3.326	3.429
9.9131	3.4083	3.3451	3.2788	3.4867
9.9312	3.3781	3.416	3.2282	3.5425
9.9493	3.3443	3.4852	3.1745	3.5961
9.9673	3.307	3.5523	3.1178	3.6469
9.9854	3.2666	3.6173	3.0585	3.6947
10.0034	3.2235	3.6799	2.9969	3.739

# MgSnO<sub>3</sub>

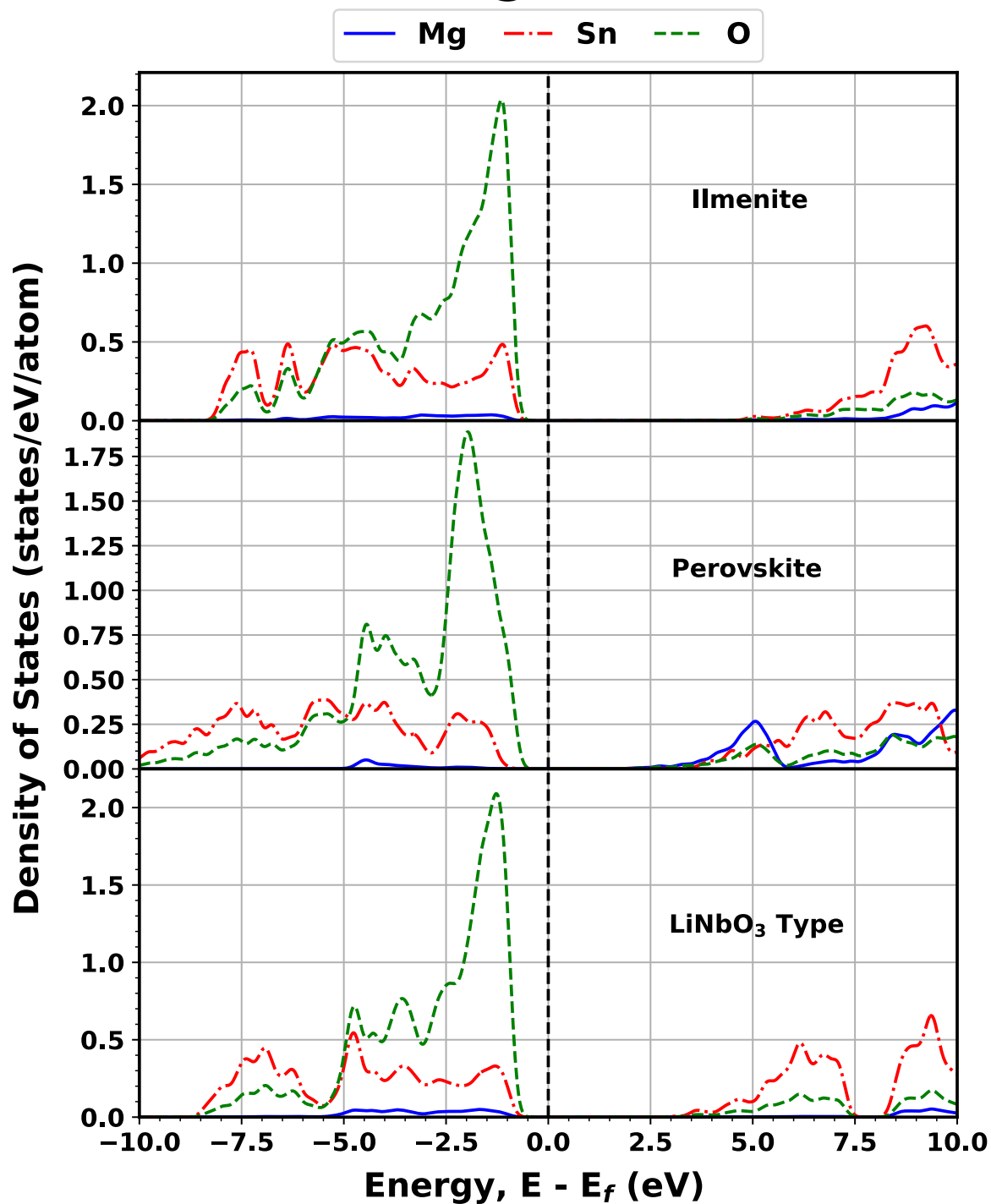
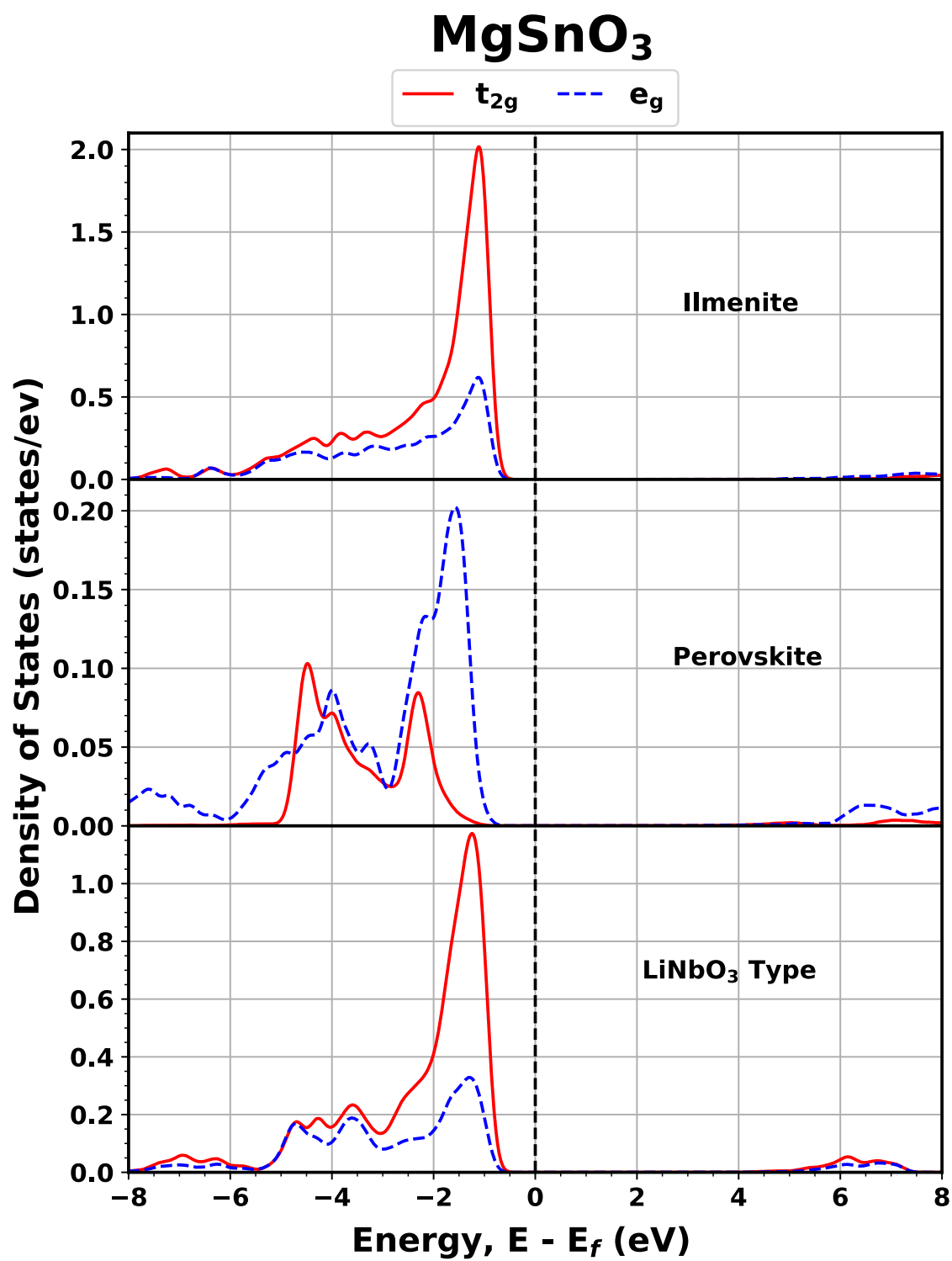
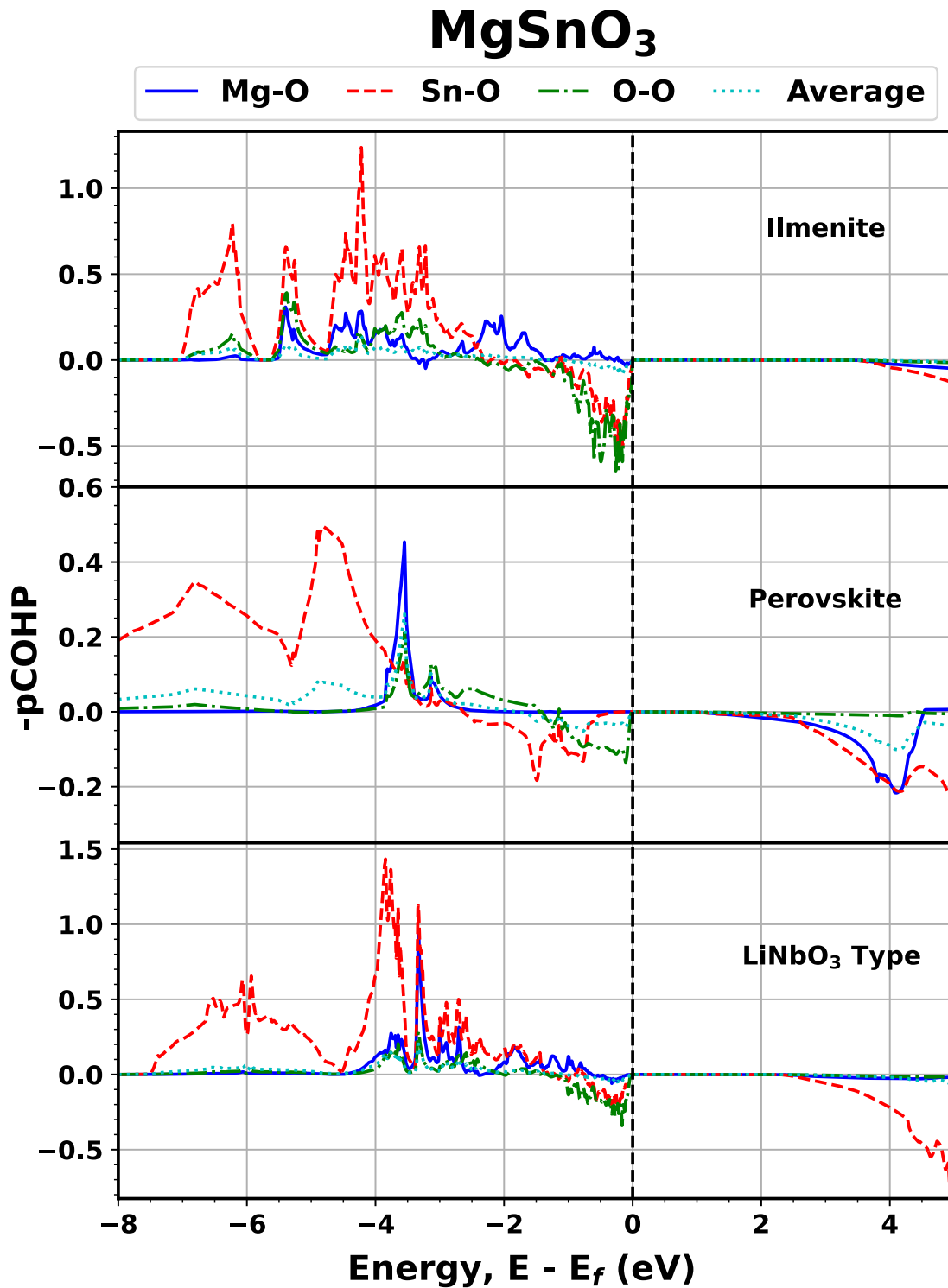


Figure S1: On-site electronic density of states (DOS) per atom of MgSnO<sub>3</sub> based on the three different crystal structures, computed using the hybrid HSE06 functional. The Fermi energy is set at 0 eV.

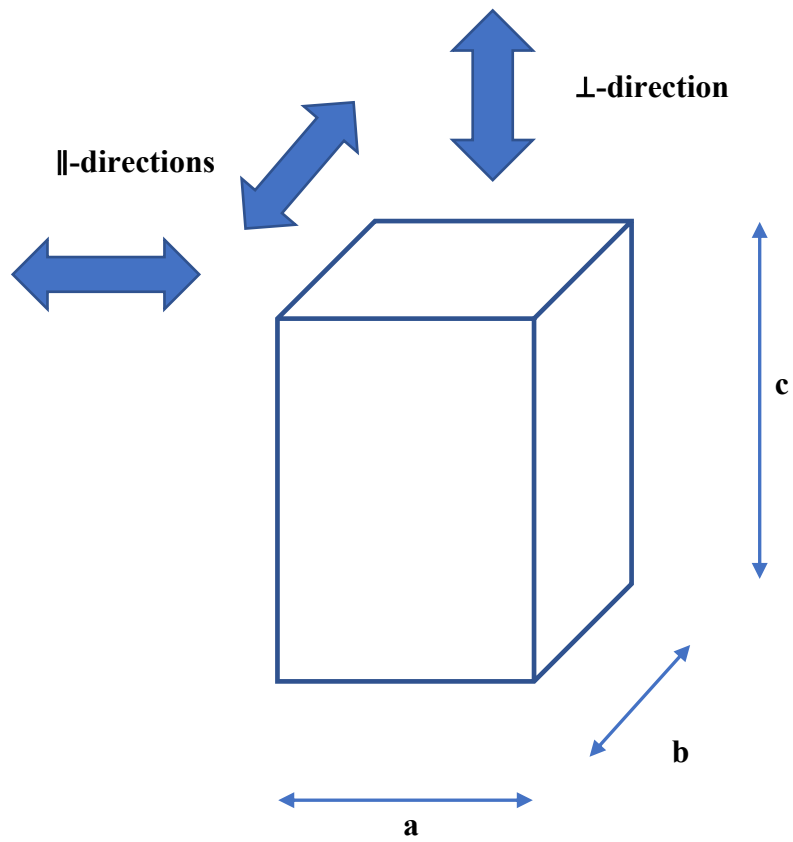


**Figure S2:** On-site electronic DOS per Sn atoms in a unit cell separated into the  $t_{2g}$  and  $e_g$  states of MgSnO<sub>3</sub> based on the three different crystal structures, computed using the hybrid HSE06 functional. The Fermi energy is set at 0 eV.



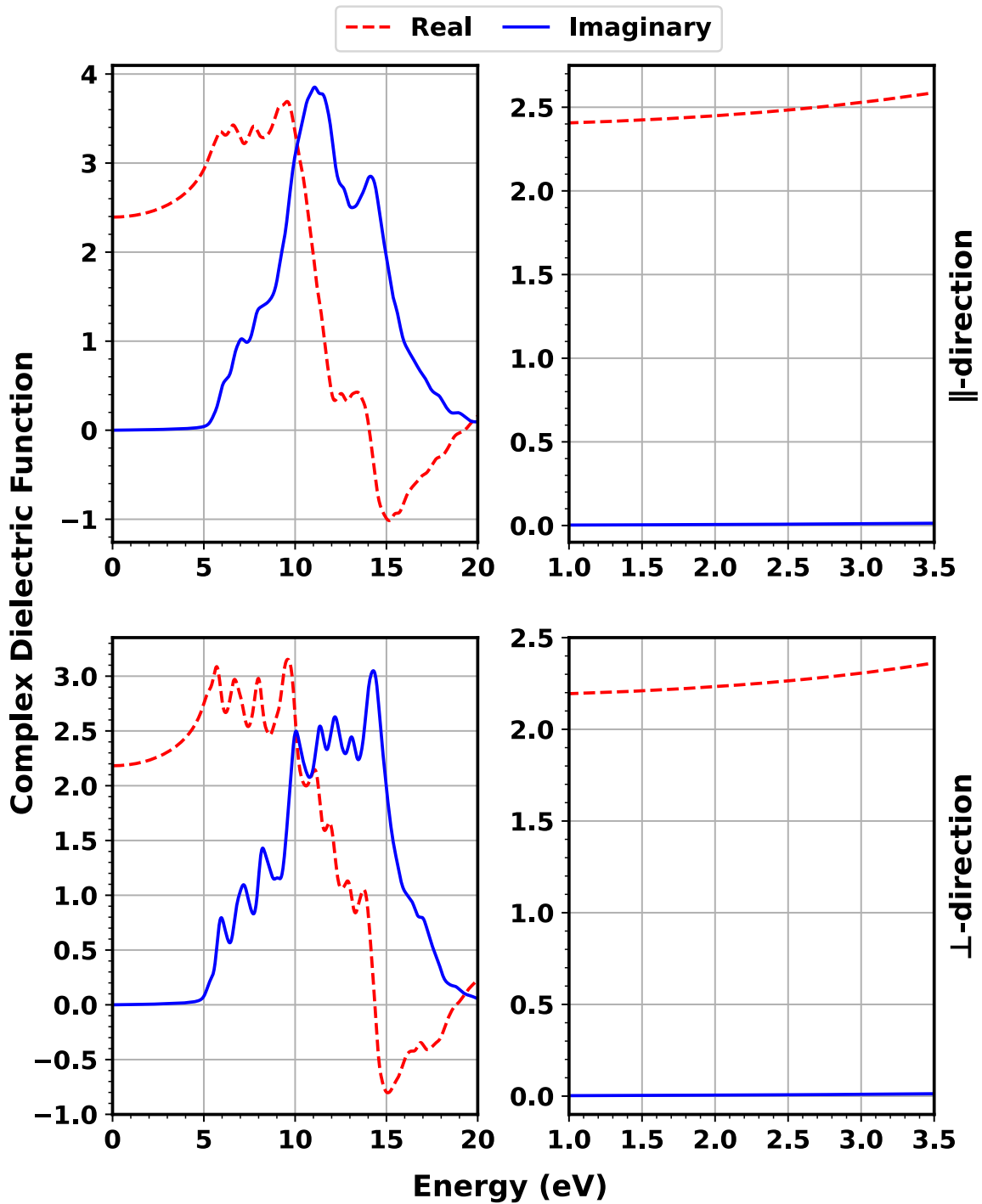


**Figure S3:** -Projected Crystal Orbital Hamilton Populations (-pCOHP) of all the nearest-neighbors' interactions in MgSnO<sub>3</sub> based on the different crystal structures computed using the GGA functional. The Fermi energy is set to 0 eV.



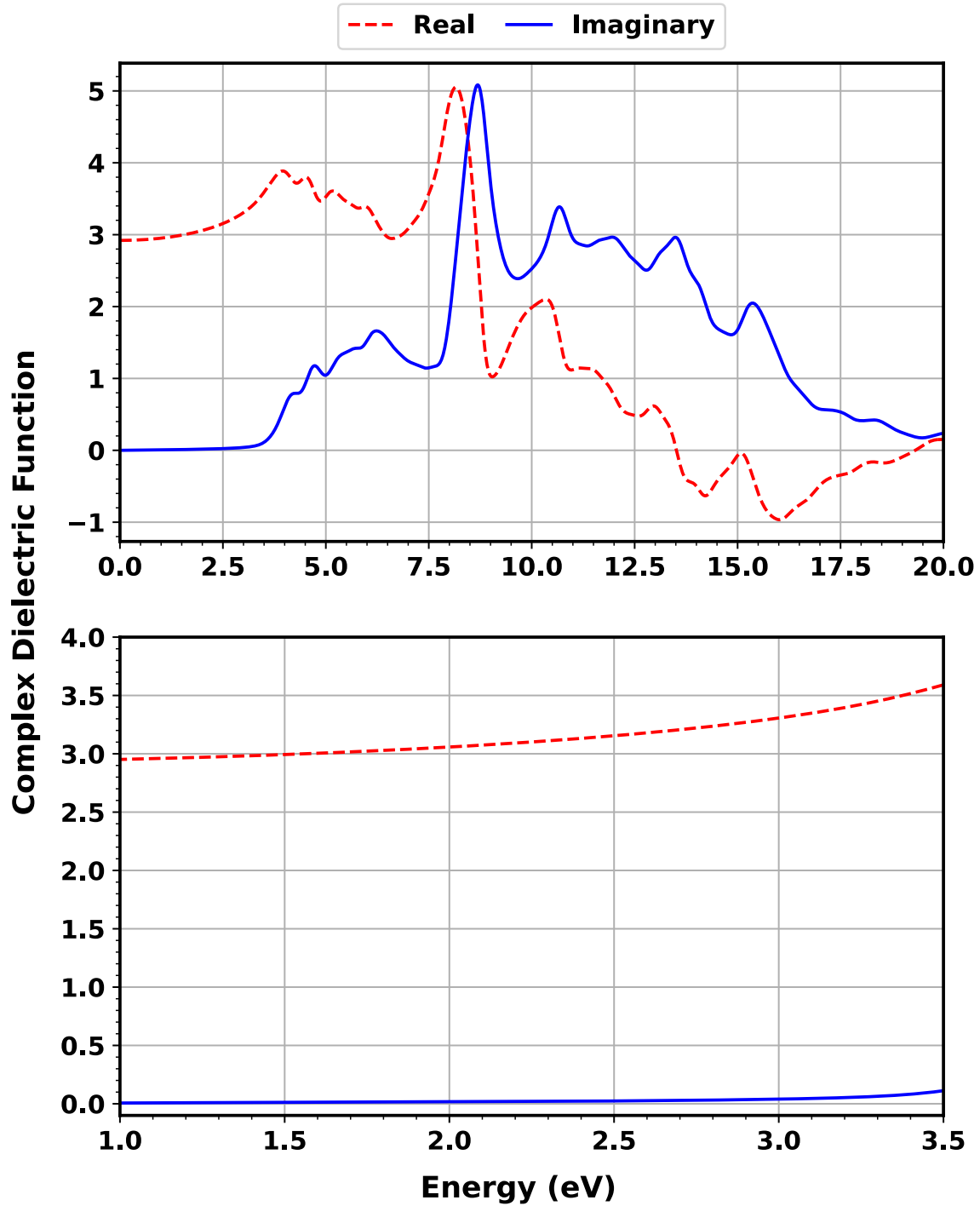
**Figure S4:** The  $\parallel$ - and  $\perp$ -directions in a rhombohedral crystal structure.

# MgSnO<sub>3</sub> Ilmenite



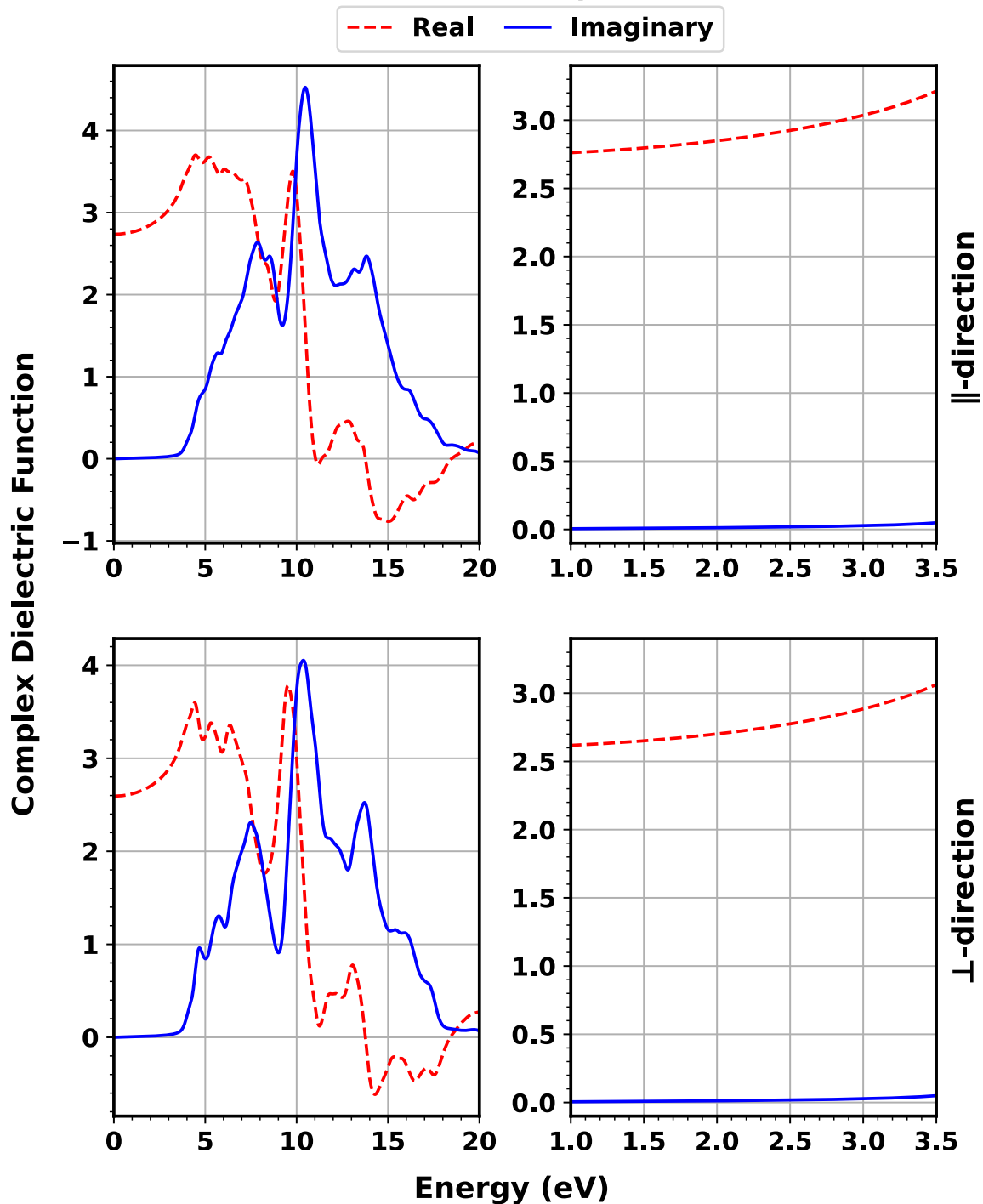
**Figure S5:** Complex dielectric functions of MgSnO<sub>3</sub> based on the Ilmenite crystal structure, computed utilizing the hybrid HSE06 functional. Left side shows a wide range in photon energies whereas right side shows photon energies in the visible range only. Similarly, top row shows values in the parallel-directions whereas bottom row shows those in the perpendicular-direction only. See Fig. S4 for the directions inside the crystal structure.

# MgSnO<sub>3</sub> Perovskite



**Figure S6:** Complex dielectric functions of MgSnO<sub>3</sub> based on the Perovskite crystal structure, computed utilizing the hybrid HSE06 functional. Top panel shows a wide range in photon energies whereas bottom panel shows photon energies in the visible range only.

# MgSnO<sub>3</sub> LiNbO<sub>3</sub>Type



**Figure S7:** Complex dielectric functions of MgSnO<sub>3</sub> based on the LiNbO<sub>3</sub> type crystal structure, computed utilizing the hybrid HSE06 functional. Left side shows a wide range in photon energies whereas right side shows photon energies in the visible range only. Similarly, top row shows values in the parallel-directions whereas bottom row shows those in the perpendicular-direction only. See Fig. S4 for the directions inside the crystal structure.