Opto-electronic and mechanical properties of $(Cd_xZn_{1-x})_2SnO_4$ in the cubic and orthorhombic phases using first-principles methods

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Supplementary Material

Table S1: Charge Transfer in units of elementary charge e from Cd, Zn, Sn to O in cubic (c-) and orthorhombic (o-) $(Cd_xZn_{1-x})_2SnO_4$, computed through Bader charge analysis using the GGA functional.

x	c- $(Cd_xZn_{1-x})_2SnO_4$			o- $(Cd_xZn_{1-x})_2SnO_4$		
	Cd-O	Zn-O	Sn-O	Cd-O	Zn-O	Sn-O
0.00	-	1.27	2.12	-	1.27	2.28
0.25	1.23	1.32	2.22	1.22	1.28	2.30
0.50	1.26	1.34	2.20	1.22	1.27	2.30
0.75	1.29	1.32	2.20	1.22	1.28	2.33
1.00	1.30	-	2.22	1.21	-	2.31

Table S2: Effective masses (m^*) and charge carrier mobilities of cubic $(Cd_xZn_{1-x})_2SnO_4$ alloys calculated using the GGA functional. Values are given in units of electron rest mass (m_0), and the mobilities are reported in cm^2/Vs.

x	m_e^* (avg)	Electron mobility cm^2/Vs	m_h^* (avg)	Hole mobility cm^2/Vs
0.00	0.18	97.71	5.46	3.22
0.25	0.17	103.45	7.24	2.43
0.50	0.16	109.92	4.72	3.73
0.75	0.15	117.25	5.17	3.4
1.00	0.14	125.62	5.70	3.09

Table S3: Effective masses (m^*) of electrons (m_e^*) and holes (m_h^*) along with their carrier mobilities of orthorhombic $(Cd_xZn_{1-x})_2SnO_4$, calculated using the GGA functional. Values are given in units of electron rest mass (m_0). Hole effective masses are reported along the crystallographic directions [100], [010], and [001]. Similarly, m_e^* (avg) represents the average electron effective mass. The carrier mobilities are reported in cm^2/Vs.

x	m_e^* (avg)	m_h^* (100)	m_h^* (010)	m_h^* (001)
0.00	0.33	1.36	8.08	26.97
0.25	0.30	1.39	7.20	147.98
0.50	0.29	1.31	7.05	187.70
0.75	0.28	1.57	9.50	293.48
1.00	0.28	2.04	15.84	15.84

x	Electron mobility cm^2/Vs	Hole mobility cm^2/Vs (100)	Hole mobility cm^2/Vs (010)	Hole mobility cm^2/Vs (001)
0.00	53.29	12.93	2.18	0.65
0.25	58.62	12.65	2.44	0.12
0.50	60.64	13.43	2.49	0.09
0.75	62.81	11.2	1.85	0.06
1.00	62.81	8.62	1.11	1.11

Table S4: Elastic constants of cubic $(Cd_xZn_{1-x})_2SnO_4$ in units of GPa.

x	C_{11}	C_{12}	C_{44}
0.00	204	141	80
0.25	193	136	69
0.50	193	132	60
0.75	193	131	53
1.00	181	116	49

Table S5: Elastic constants of orthorhombic $(Cd_xZn_{1-x})_2SnO_4$ in units of GPa.

x	C_{11}	C_{22}	C_{33}	C_{44}	C_{55}	C_{66}	C_{12}	C_{13}	C_{23}
0.00	230	300	213	47	90	76	89	124	126
0.25	213	281	195	41	81	67	90	119	121
0.50	202	261	192	37	74	64	8	119	118
0.75	118	246	195	31	70	58	88	125	119
1.00	174	222	188	29	65	56	77	117	108

Table S6: Calculated total integrated COHP in eV of cubic (c-) and orthorhombic (o-) $(Cd_xZn_{1-x})_2SnO_4$, computed using the GGA functional.

x	c- $(Cd_xZn_{1-x})_2SnO_4$	o- $(Cd_xZn_{1-x})_2SnO_4$
0.00	-2.13	-2.17
0.25	-2.08	-2.13
0.50	-2.05	-2.06
0.75	-2.02	-2.13
1.00	-1.97	-2.00

Table S7: SQS-generated structures of cubic (c-) $(Cd_xZn_{1-x})_2SnO_4$ alloy system.

Material	POSCAR
$(Cd_{0.25}Zn_{0.75})_2SnO_4$	from sqs 1.00000000000000 8.8577709656145398 -0.0170862340639907 0.0170862340639907 -0.0170095708842152 8.8834674387567745 -0.0119343762989905 0.0170095708842152 -0.0119343762989905 8.8834674387567727 Cd Zn Sn O 4 12 8 32 Direct 0.1235066806679540 0.8765385408611653 0.3781872250751328 0.3740905597860318 0.3750775608659608 0.6249224391340393 0.3779957863750225 0.8767706157904690 0.1232293842095309 0.1235066806679540 0.6218127749248674 0.1234614591388346 0.1215310285468299 0.3724606457498472 0.8749557022825905 0.6272448332376420 0.8753101822353254 0.8728403083740228 0.8721621976900222 0.1274165429571894 0.3751943017395007 0.3754508488532343 0.1255705335794735 0.8744294664205264 0.8721621976900222 0.6248056982604993 0.8725834570428107 0.8725597957095449 0.8752627668022251 0.6272138792747802 0.1215310285468299 0.1250442977174094 0.6275393542501533 0.6272448332376420 0.1271596916259771 0.1246898177646747 0.6278986397211447 0.6269536621156240 0.6254296536463760 0.6278986397211447 0.3745703463536241 0.3730463378843760 0.3820040054020891 0.6223291048764460 0.3776708951235543 0.8725597957095449 0.3727861207252199 0.1247372331977746 0.5092385481231470 0.4933873364820247 0.0011987314310778 -0.0090243009038283 0.4939012981627415 0.5060987018372588 0.5092385481231470 -0.0011987314310778 0.5066126635179752 -0.0102124012523466 0.0077097278000197 -0.0077097278000197 0.7454190029299543 0.7500621674322204 0.2499378325677795 0.2500208329802850 0.7538290624763091 0.7461283091335658 0.7538402275510908 0.2501158516076459 0.7498841483923540 0.2500208329802850 0.2538716908664345 0.2461709375236910 0.8653367002276708 0.1337101119980308 0.1325757655636916 0.1187866540386491 0.8794530329855824 0.1205469670144175 0.6306373689890145 0.1330620334716025 0.3705502000034138 0.3831435749699873 0.8623085959414963 0.3796921047520036 0.3868791916665971 0.1319131074011944 0.1148526898915998 0.1102571807604612 0.3668347561442296 0.1121396262595283 0.1168727223989454 0.1352777750098160 0.3851848905075990 0.3877295976497707 0.3837271863019351 0.3685736807113935 0.8663828717671107 0.6337271446244356 0.6325458771379615 0.1145110555735828 0.3615371011982207 0.6384628988017794 0.6306373689890145 0.6294497999965863 0.8669379665283975 0.3664814876155914 0.3657546434256914 0.8817964304256879 0.3877295976497707 0.6314263192886065 0.6162728136980653 0.1102571807604612 0.8878603737404716 0.6331652438557702 0.1168727223989454 0.6148151094924008 0.8647222249901838 0.3868791916665971 0.8851473101084001 0.8680868925988057 0.3664814876155914 0.1182035695743120 0.6342453565743089 0.6370257084162579 0.8673150667637591 0.6361971482926961 0.1304386679657102 0.1334347444642036 0.8665652555357963 0.8653367002276708 0.8674242344363083 0.8662898880019693 0.8798262588187308 0.1165488909274993 0.6172893515544223 0.6346025848453307 0.3845983257611402 0.6154016742388599 0.6196761650782152 0.1207259952461127 0.8792740047538872 0.8798262588187308 0.3827106484455774 0.8834511090725007 0.3831435749699873 0.6203078952479966 0.1376914040585035 0.6370257084162579 0.3638028517073040 0.1326849332362408 0.1361978840136670 0.6160935472818660 0.3839064527181340 0.8663828717671107 0.3674541228620384 0.3662728553755645 0.8651850689604975 0.6146060709901682 0.1148787934818066 0.6348845566444747 0.8881880621914793 0.1118119378085207 0.6214981252647110 0.6159128776157009 0.3840871223842992 0.8651850689604975 0.8851212065181935 0.3853939290098318

Material	POSCAR
$(Cd_{0.50}Zn_{0.50})_2SnO_4$	from sqs 1.00000000000000 9.0151514035774376 -0.0060664460491308 -0.0230953777825161 -0.0061043460519853 8.9837081876543756 0.0042809137438836 -0.0231457295777443 0.0042494522818318 8.9963320688757644 Cd Zn Sn O 8 8 8 32 Direct 0.6297875522032743 0.8736651544455117 0.8731682858261871 0.8749141444252847 0.1223879760256845 0.3766687566473154 0.3733437753911520 0.1293786016827401 0.8728280395090857 0.3723590787321075 0.8721634380199629 0.1287044520304889 0.1248952396224643 0.1247059880304962 0.6248876757411760 0.6251531174876244 0.1265143221719287 0.1264998654023172 0.6245203611308665 0.6246815236760116 0.6245581055383325 0.8756517775875643 0.3768299424011000 0.1223171543242873 0.1255312336617496 0.3807143080753509 0.8745582973404767 0.1248340130358943 0.8679530227831692 0.3752599807154784 0.8811744635535838 0.6247252809488936 0.8748316280824593 0.3737980463028422 0.3784775772822356 0.6224068961565047 0.8785565682185073 0.8711288146265328 0.6243090042140573 0.6182058246517322 0.3784910006935779 0.3775008088421566 0.3715432334738143 0.6227660426891024 0.3752813149239647 0.1248610407493076 0.6241151124649613 0.1255910576901247 0.4932044146224373 0.5021742294595821 0.0040871144149559 0.0056404405809848 0.5096706342314168 0.5038617123715108 0.4974003253471057 0.0019565526882187 0.4986332934314698 0.0039344765937295 -0.0081730542955911 -0.0011969165424772 0.7569304755111091 0.7396481131680682 0.2534790085541999 0.2397051659366811 0.7371696946261868 0.7437241727865050 0.7528630417310169 0.2562921153004682 0.7426390327018931 0.2503740089527700 0.2598110280137422 0.2532458371203759 0.8776058118703199 0.1215839193374219 0.1232068411904528 0.1199413230564710 0.8611345478837968 0.1370019050126905 0.6207257949743014 0.1408592310320346 0.3777274228078383 0.3644075974081298 0.8626961137909305 0.3856011630431008 0.3723933603818928 0.1274699212193720 0.1263840832808981 0.1298334848260071 0.3877467850988900 0.1161249918423064 0.1294326313902758 0.1143865858433017 0.3691996089328437 0.3786592055358546 0.3866730836993663 0.3855486673928454 0.8808832328898942 0.6360898903434458 0.6375594489733032 0.1353654326383492 0.3824164988875997 0.6338911867329927 0.6378937912996560 0.6177191890824086 0.8819899447794560 0.3640554128415913 0.3868300971424509 0.8626768396989910 0.3689062510892252 0.6135824683092129 0.6124650768561061 0.1147134028493451 0.8673078762398336 0.6121518324430729 0.1171904670105964 0.6158941164597038 0.8854524168584880 0.3698132625521680 0.8680694253562081 0.8674569557222155 0.3761424224764390 0.1404997838678155 0.6205255904598493 0.6385067645474657 0.8786235975057266 0.6177012225742301 0.1205067516250026 0.1389004434714215 0.8806113463335596 0.8853328154271854 0.8613421519147137 0.8619676906783984 0.8735551288956155 0.1101583979238296 0.6291168905891099 0.6135633814531642 0.3722347609918268 0.6133761292112526 0.6274095712330597 0.1308267460224800 0.8738627195388747 0.8866012557551252 0.3877165734115629 0.8637690384321499 0.3606716205650762 0.6196513447742058 0.1374480287409208 0.6201356145792286 0.3806237371093360 0.1404499951736073 0.1330004935134311 0.6299832193261393 0.3652127446434053 0.8659760448035787 0.3840489108921319 0.3839441069536159 0.8890068972322955 0.6295182793810907 0.1134444527081746 0.6278924658039529 0.8708131834211882 0.1300373532402146 0.6139249178945058 0.6143972889378571 0.3690096421744358 0.8867715720771912 0.8629544121133463 0.3872400851577533

Material	POSCAR
$(Cd_{0.75}Zn_{0.25})_2SnO_4$	from sqs 1.00000000000000 9.1271045547439353 -0.0005195549988187 -0.0149907021855051 -0.0005343897484354 9.1000037282532720 -0.0206388007568268 -0.0149687042028271 -0.0205394288225944 9.1338731380345166 Cd Zn Sn O 12 4 8 32 Direct 0.1247847756727358 0.3749261163233699 0.8751437968512046 0.1239266037293344 0.8757239327194564 0.3753342075545577 0.3764651126178471 0.1228409831797938 0.8765291579604461 0.8738299816775663 0.6280228635049011 0.8729914100622777 0.3749913170267977 0.3750782117378206 0.6248852087108654 0.1222035656368562 0.1234205041924401 0.6235729921778855 0.6247505937926856 0.1233311419094953 0.1247756232723228 0.6262948722783379 0.6277370287556083 0.6262447373334716 0.6262682535247527 0.3734250323011272 0.3748244129149573 0.3749253464652784 0.6264084209371972 0.3735173834950615 0.8750598873317124 0.3728476222239679 0.1271222986139104 0.1262152677956960 0.6267704250426146 0.1251119244272033 0.6257628938721459 0.8757699732264644 0.8750821566842182 0.8740284659342566 0.1205839781954814 0.3772660956635667 0.8719081618257867 0.8774028495093874 0.6252133560439930 0.3784214302818987 0.8752895483210400 0.1220942077707294 0.5014663241874756 0.5121197751623803 -0.0002114367993486 -0.0045603288908436 0.5014210730830193 0.5001131151680754 0.5106725322422098 -0.0038261799471587 0.4997706165791603 -0.0031339374104289 -0.0039617341286467 0.0006240318497443 0.7464093450364109 0.7607523818672238 0.2495580942310779 0.2506921389074124 0.7570208227107772 0.7543071591506125 0.7510457926018794 0.2363326022744210 0.7457634713417944 0.2460583967237058 0.2402123558294397 0.2501708766957006 0.8771238224306446 0.1167528187718034 0.1397634979250048 0.1381496895847385 0.8783108247200981 0.1204159508728283 0.6414039589860587 0.1208445215603255 0.3764680281292029 0.3818477443315974 0.8805655820415728 0.3634294417898009 0.3725434812767277 0.1085759385225020 0.1292308835842660 0.1268253364600181 0.3731401431042933 0.1251629374470580 0.1080482496651564 0.1253238903441627 0.3733657548251363 0.3738703224995645 0.3698937798687782 0.3721030669376790 0.8769499489675635 0.6412647255481910 0.6201703940806889 0.1227969235746647 0.3763240338424605 0.6251666499121050 0.6244492016556039 0.6427139151954993 0.8762548612970464 0.3787871421144320 0.3777899368310589 0.8776398890779061 0.3739857842732569 0.6309896574609404 0.6251696639040544 0.1118201341948734 0.8722834067284196 0.6301770165330560 0.1245476603975471 0.6274825154562398 0.8750992992896661 0.3872098265714648 0.8714748003249631 0.8844436429467486 0.3768200940677902 0.1190841077633218 0.6217298289852140 0.6365708409262838 0.8795045449543561 0.6374748367280137 0.1227049114588231 0.1223854151309796 0.8754890603487450 0.8636023540186729 0.8822268446418983 0.8659411256680236 0.8712376575279638 0.1097306199862926 0.6121767641389071 0.6273197260628398 0.3724144955783572 0.6279119435577885 0.6283577039933579 0.1086484970475142 0.8732575853351607 0.8709040935959846 0.3696892269462696 0.8722949934310519 0.3771975965850868 0.6430463535995652 0.1236580753062207 0.6227928400736428 0.3782417335216241 0.1217397413929572 0.1228607204861302 0.6246217014110378 0.3750655977213709 0.8768423224550367 0.3605091035919684 0.3799826713884117 0.8736907105821703 0.6310312667579908 0.1276162188619032 0.6149262953635716 0.8717654344449689 0.1124089518918443 0.6270718907790782 0.6278890274654406 0.3744300162157512 0.8682542221781434 0.8858314079054848 0.3849567127228998

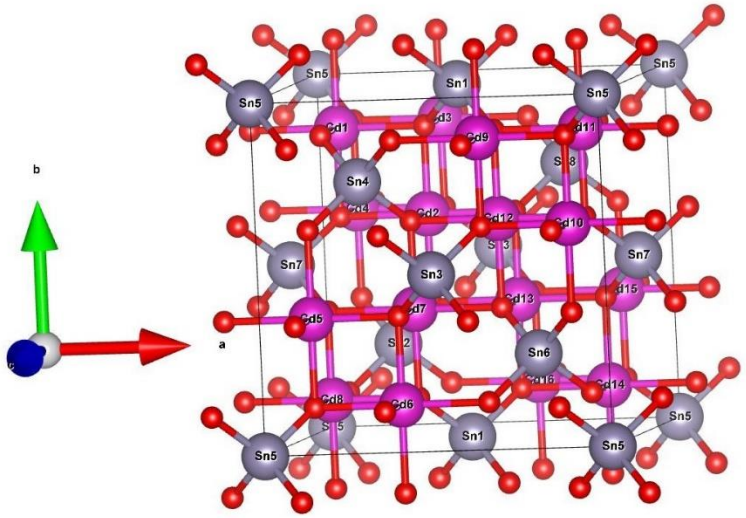
Table S8: SQS-generated structures of orthorhombic (o-) $(Cd_xZn_{1-x})_2SnO_4$ alloy system.

Material	POSCAR
$(Cd_{0.25}Zn_{0.75})_2SnO_4$	from sqs 1.00000000000000 6.1795191360516730 0.0000000000000000 -0.0391769194006659 0.0000000000000000 6.3865183252535287 0.0000000000000000 -0.0560354931497790 0.0000000000000000 8.9423843276440902 Cd Zn Sn O 2 6 4 16 Direct 0.5019072431839623 0.2500000000000000 0.6461252180776126 0.2451529687735967 0.2500000000000000 0.2445845227419958 0.0006974785538337 0.7500000000000000 0.1396422609041571 0.0015135292552565 0.2500000000000000 0.8555197097093195 0.5014589839157304 0.7500000000000000 0.3600034654061278 0.7518185359645625 0.2500000000000000 0.2483887792546475 0.7536053180756542 0.7500000000000000 0.7535346872254801 0.2444242903521229 0.7500000000000000 0.7552149311064141 0.5072975671656981 -0.0039530264033800 0.0011210013654859 -0.0056672184285713 -0.0034526390631597 0.4994443242620371 -0.0056672184285713 0.5034526390631596 0.4994443242620371 0.5072975671656981 0.5039530264033799 0.0011210013654859 0.5153221211999339 0.0080014949287940 0.2312708113110479 -0.0020581320415583 0.9830932806434620 0.7324465277966766 -0.0163153745486144 0.0040097383762702 0.2682234236678257 0.4999510366423734 0.9631346833076063 0.7741551433612810 -0.0020581320415583 0.5169067193565380 0.7324465277966766 0.5153221211999339 0.4919985050712060 0.2312708113110479 0.4999510366423734 0.5368653166923937 0.7741551433612810 -0.0163153745486144 0.4959902616237298 0.2682234236678257 0.7620277743898820 0.7500000000000000 0.5059689638108901 0.2297762684459285 0.7500000000000000 0.5003764704373068 0.2795556192131317 0.2500000000000000 -0.0147614595426618 0.7360134777290395 0.2500000000000000 -0.0013050772785355 0.2694469504878935 0.7500000000000000 0.0048217305093355 0.7400699941754028 0.7500000000000000 -0.0011113857678687 0.7732409193691941 0.2500000000000000 0.4879828315770998 0.2122306481362859 0.2500000000000000 0.5016918882999718

Material	POSCAR
$(Cd_{0.50}Zn_{0.50})_2SnO_4$	from sqs 1.00000000000000 6.2584904678501072 0.0000000000000000 0.0000000000000000 0.0000000000000000 6.4563049975090658 0.0000000000000000 0.0000000000000000 0.0000000000000000 9.0941929923016467 Zn Cd Sn O 4 4 4 16 Direct 0.5000000000000000 0.2500000000000000 0.6368012899845095 0.5000000000000000 0.7500000000000000 0.3530775469385947 0.2577946283753515 0.2500000000000000 0.2572101962490157 0.7422053716246485 0.2500000000000000 0.2572101962490157 0.0000000000000000 0.7500000000000000 0.1489180325738537 0.0000000000000000 0.2500000000000000 0.8650241117107443 0.7398562541764273 0.7500000000000000 0.7415848348173883 0.2601437458235726 0.7500000000000000 0.7415848348173883 0.5000000000000000 0.0025215265118580 0.0081424496686369 0.0000000000000000 0.0032356391133688 0.4918368847052215 0.0000000000000000 0.4967643608866311 0.4918368847052215 0.5000000000000000 0.4974784734881419 0.0081424496686369 0.5000000000000000 0.0152443993151573 0.2367836672953798 0.0000000000000000 0.9875562018381022 0.7147009537725595 0.0000000000000000 0.0394924766237476 0.2701975948877146 0.5000000000000000 0.0119952344906320 0.7788708155675954 0.0000000000000000 0.5124437981618978 0.7147009537725595 0.5000000000000000 0.4847556006848427 0.2367836672953798 0.5000000000000000 0.4880047655093679 0.7788708155675954 0.0000000000000000 0.4605075233762524 0.2701975948877146 0.7737490643836740 0.7500000000000000 0.4806111474441601 0.2262509356163264 0.7500000000000000 0.4806111474441601 0.2767927319936602 0.2500000000000000 0.0195049183183865 0.7232072680063399 0.2500000000000000 0.0195049183183865 0.2826621962610478 0.7500000000000000 0.0007321262340629 0.7173378037389522 0.7500000000000000 0.0007321262340629 0.7647769708359474 0.2500000000000000 0.4979139204360274 0.2352230291640527 0.2500000000000000 0.4979139204360274

Material	POSCAR
$(Cd_{0.75}Zn_{0.25})_2SnO_4$	from sqs 1.00000000000000 6.3659620987277084 0.0000000000000000 0.0493629202773121 0.0000000000000000 6.4928397238694755 0.0000000000000000 0.0695454213440516 0.0000000000000000 9.2655464377898671 Cd Zn Sn O 6 2 4 16 Direct 0.4990631715358091 0.2500000000000000 0.6361814429326237 0.0010700832092102 0.2500000000000000 0.8641579513800070 0.5056262137542533 0.7500000000000000 0.3558574526951742 0.7571733851004845 0.2500000000000000 0.2449458111244867 0.7532148853595527 0.7500000000000000 0.7543529838365860 0.2461077847640893 0.7500000000000000 0.7531536903816248 0.0028687852021653 0.7500000000000000 0.1458717286629776 0.2475510066217089 0.2500000000000000 0.2470911982331352 0.4924531272900404 -0.0004202331751990 0.0082649703423040 0.0067105569706863 -0.0010227992788885 0.4910001809169451 0.0067105569706863 0.5010227992788884 0.4910001809169451 0.4924531272900404 0.5004202331751992 0.0082649703423040 0.4827957966160562 0.0266776084311336 0.2269605634869862 0.0009652398265694 0.9936307925143706 0.7124661070439462 0.0153247288100184 0.0058734037008524 0.2671244748662411 0.4977574848948763 0.9890844680833910 0.7874194113407542 0.0009652398265694 0.5063692074856294 0.7124661070439462 0.4827957966160562 0.4733223915688665 0.2269605634869862 0.4977574848948763 0.5109155319166090 0.7874194113407542 0.0153247288100184 0.4941265962991476 0.2671244748662411 0.7868125098889756 0.7500000000000000 0.4951883260887970 0.2227918369914410 0.7500000000000000 0.4985448658287845 0.2714700905470586 0.2500000000000000 0.0127952710543711 0.7108502308710676 0.2500000000000000 -0.0005588857584859 0.2674032242810718 0.7500000000000000 0.0120672079639611 0.7219796387506623 0.7500000000000000 0.0180896464481664 0.7879312514627523 0.2500000000000000 0.4939027002620026 0.2260720328432032 0.2500000000000000 0.4818871928714338

a)



b)

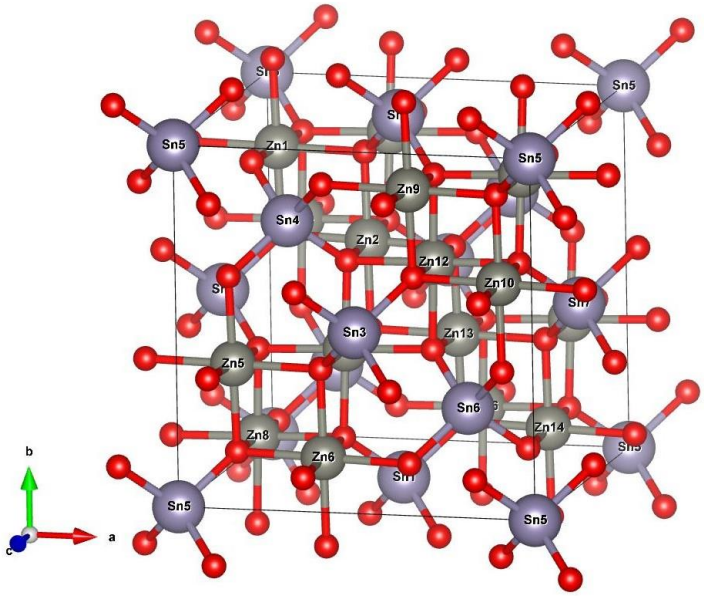
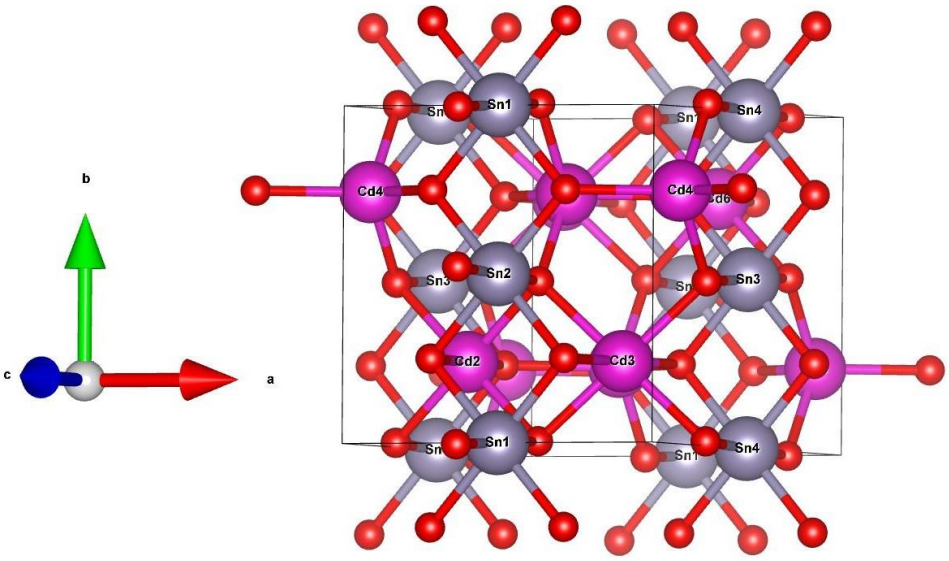


Figure S1: Crystal structure of cubic phase Cd_2SnO_4 **(a)** and Zn_2SnO_4 **(b)** generated using VESTA software [1]. Red spheres denote the oxygen atoms.

a)



b)

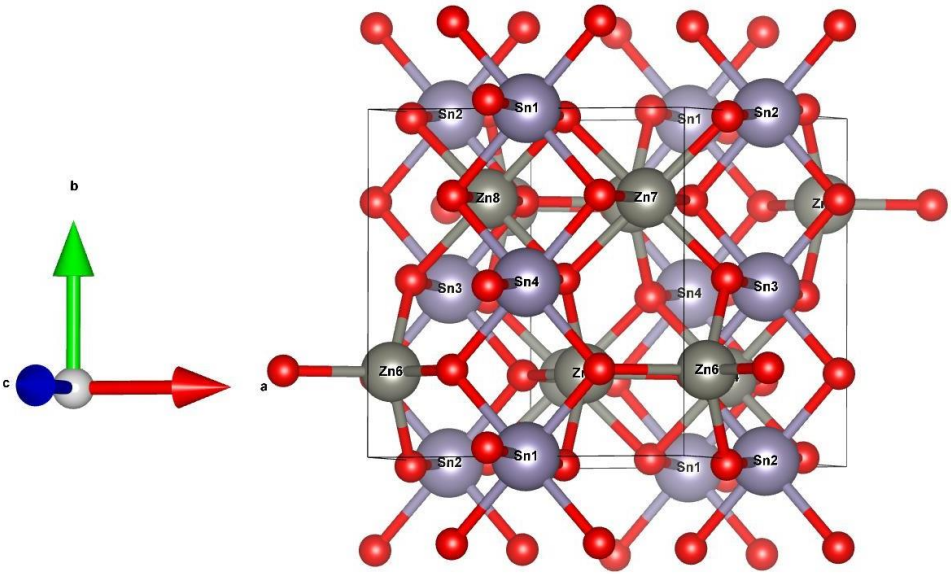


Figure S2: Crystal structure of orthorhombic phase Cd_2SnO_4 **(a)** and Zn_2SnO_4 **(b)** generated using VESTA software [1]. Red spheres denote the oxygen atoms.

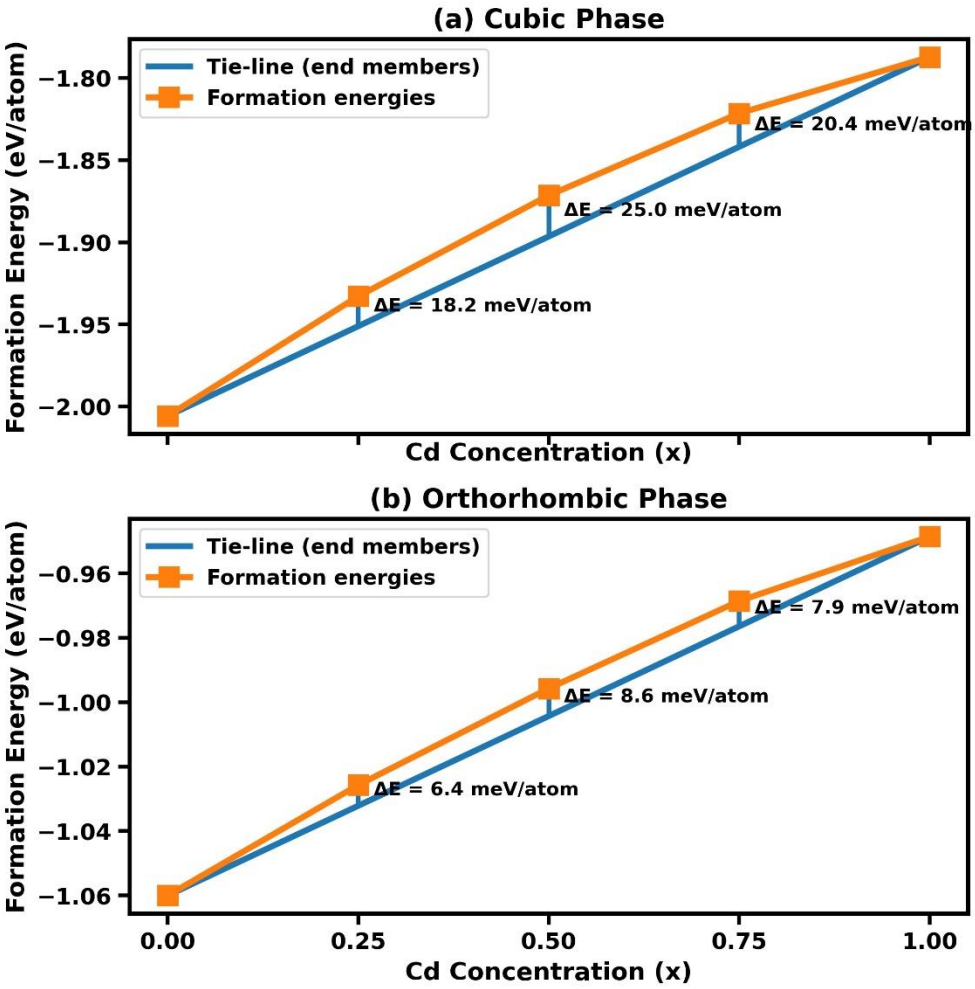


Figure S3: Convex hull diagram for the $(Cd_xZn_{1-x})_2SnO_4$ alloys in the a) cubic and b) orthorhombic phases. The straight line represents the tie line connecting end members Zn_2SnO_4 and Cd_2SnO_4. The vertical distance ΔE indicates the energy difference between the formation energies and the reference line.

Fig S4.a)

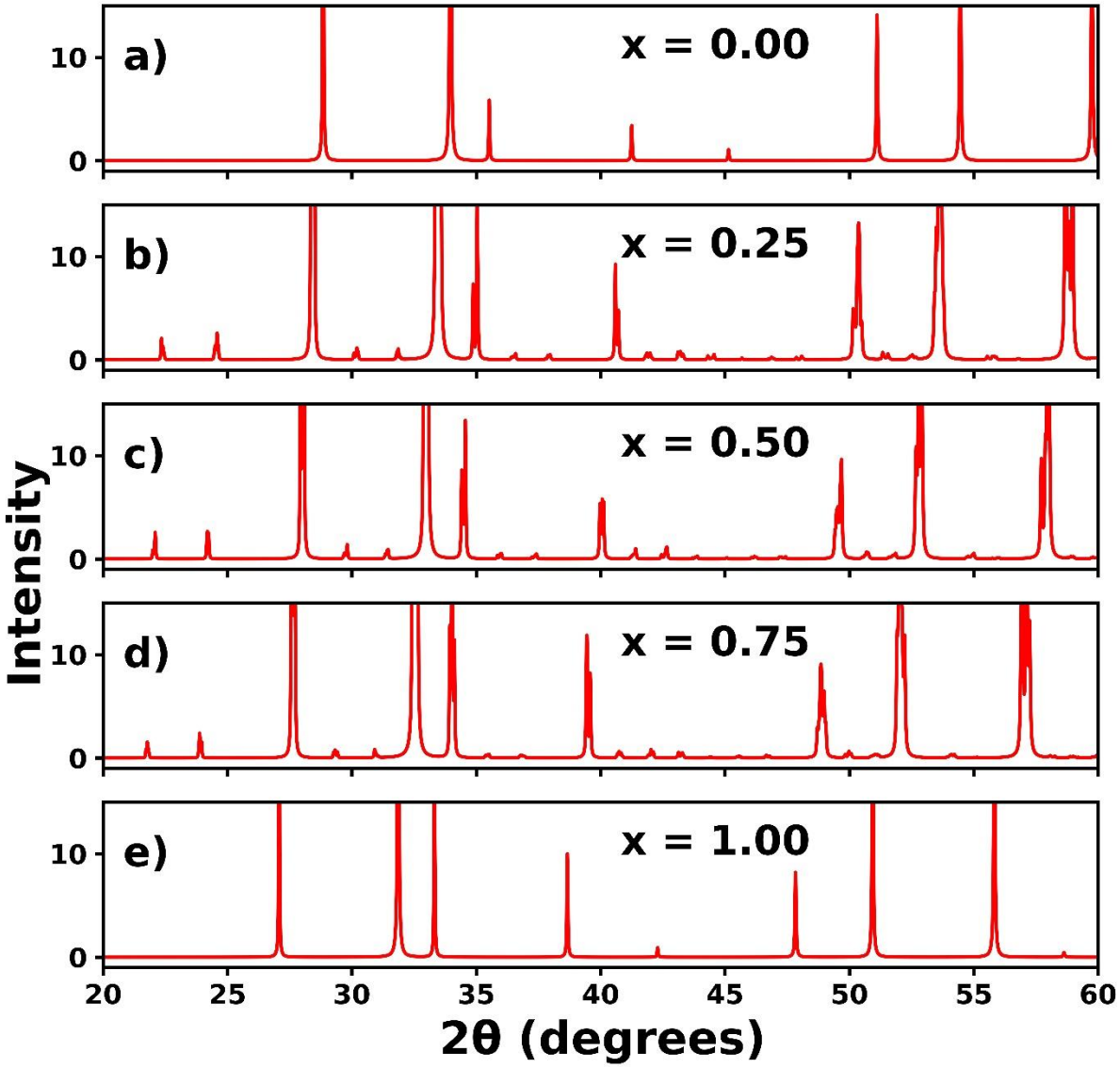


Figure S4 (a, b): Powder diffraction patterns of cubic and orthorhombic $(Cd_xZn_{1-x})_2SnO_4$, generated using the VESTA program [1] with a wavelength (λ) of 1.54 Å. **(S4.a)** for cubic $(Cd_xZn_{1-x})_2SnO_4$ and **(S4.b)** for orthorhombic $(Cd_xZn_{1-x})_2SnO_4$ at compositions x = 0.00, 0.25, 0.50, 0.75, and 1.00.

Fig S4.b)

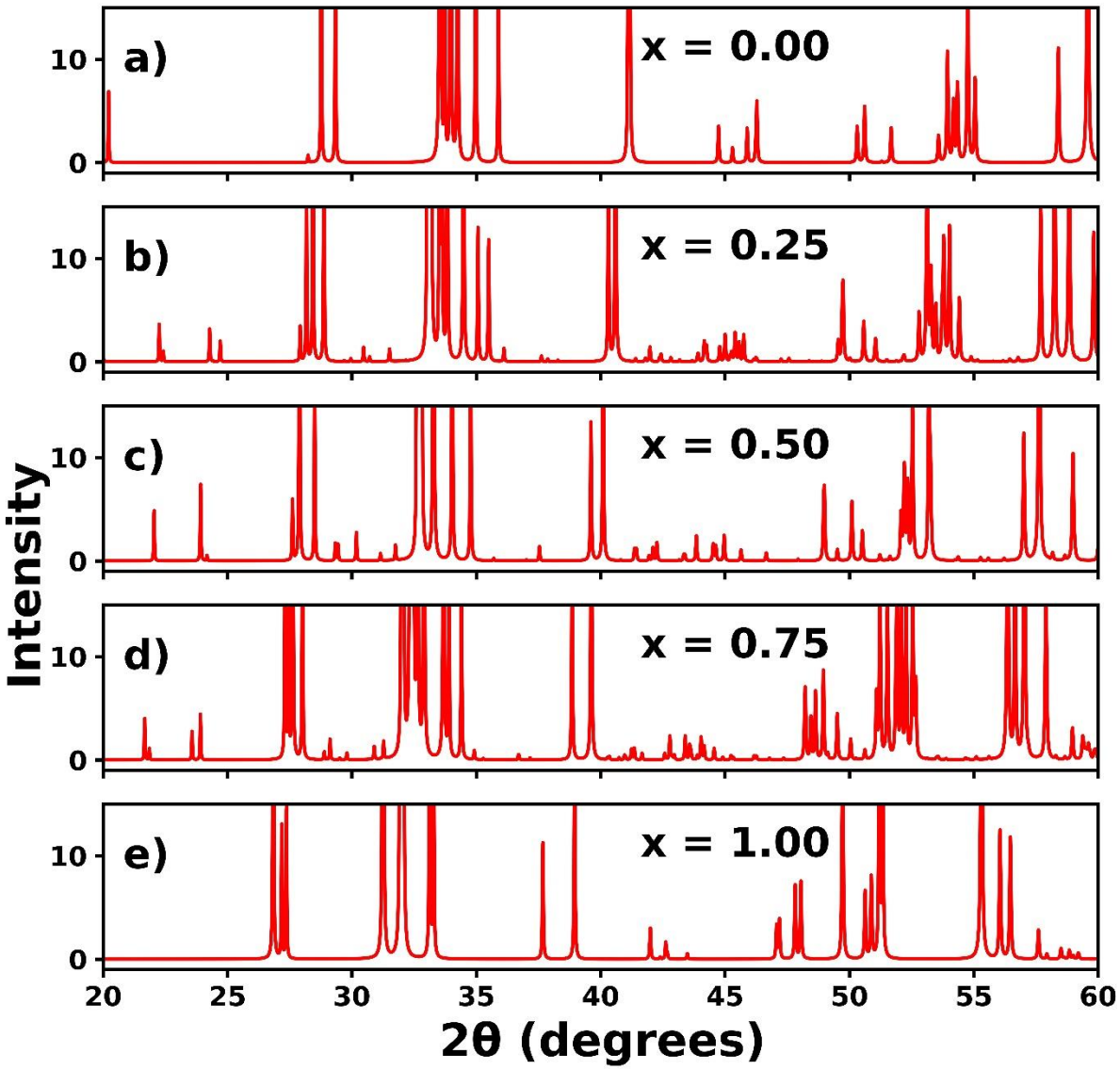

a)
x = 0.00
b)
x = 0.25
c)
x = 0.50
d)
x = 0.75
e)
x = 1.00
Intensity
10
0
20
25
30
35
40
45
50
55
60
2θ (degrees)

Fig S5.a)

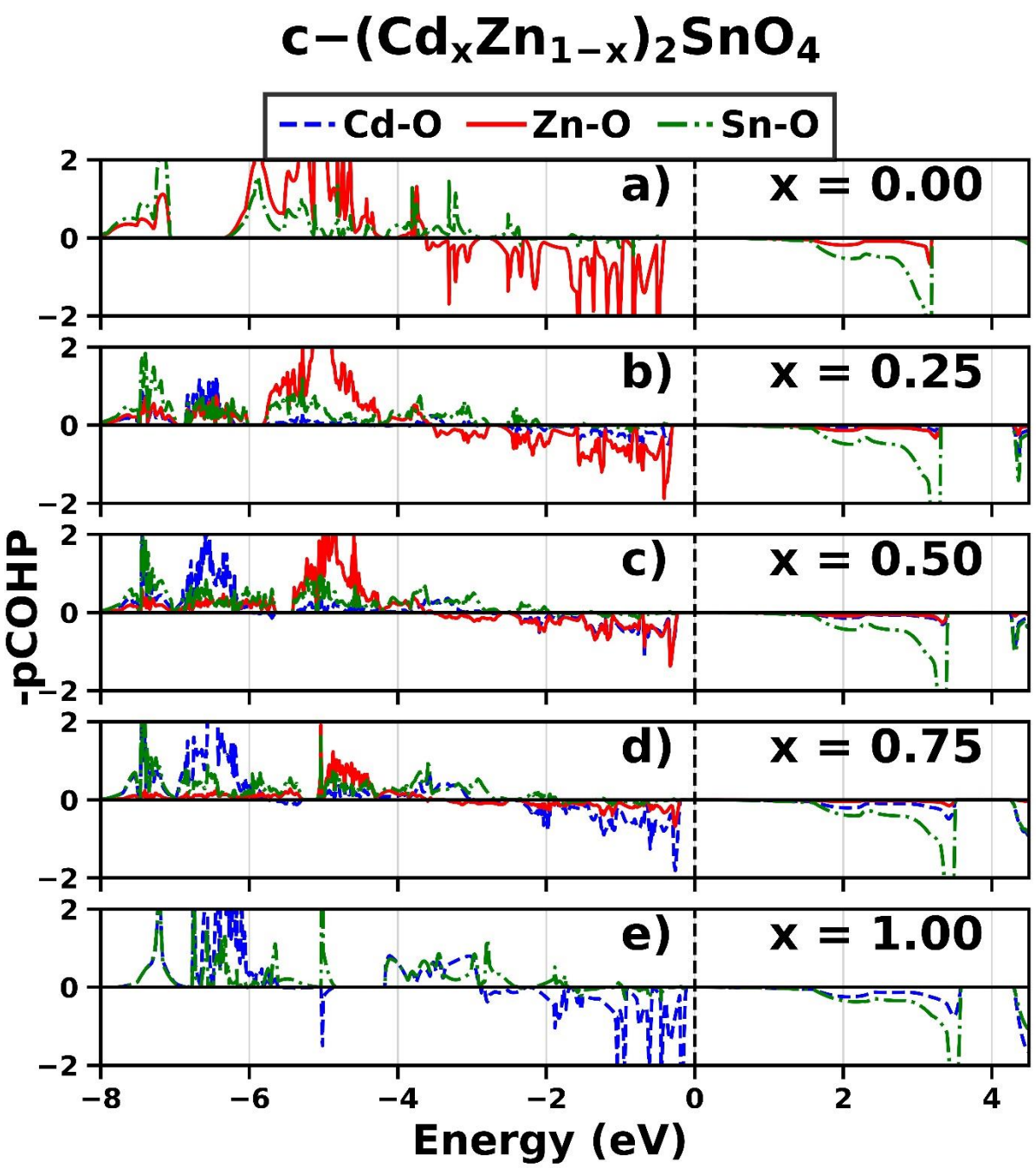


Figure S5 (a, b): Negative Projected Crystal Orbital Hamilton Population (-pCOHP) interaction of Cd-O, Zn-O, and Sn-O of cubic and orthorhombic $(Cd_xZn_{1-x})_2SnO_4$ for the first nearest neighbor interaction. The positive and negative values of -pCOHP represent the bonding and antibonding interactions. The Fermi energy is set at 0 eV, **(S5.a)** for cubic $(Cd_xZn_{1-x})_2SnO_4$ and **(S5.b)** for orthorhombic $(Cd_xZn_{1-x})_2SnO_4$ at compositions x = 0.00, 0.25, 0.50, 0.75 and 1.00.

Fig S5.b)

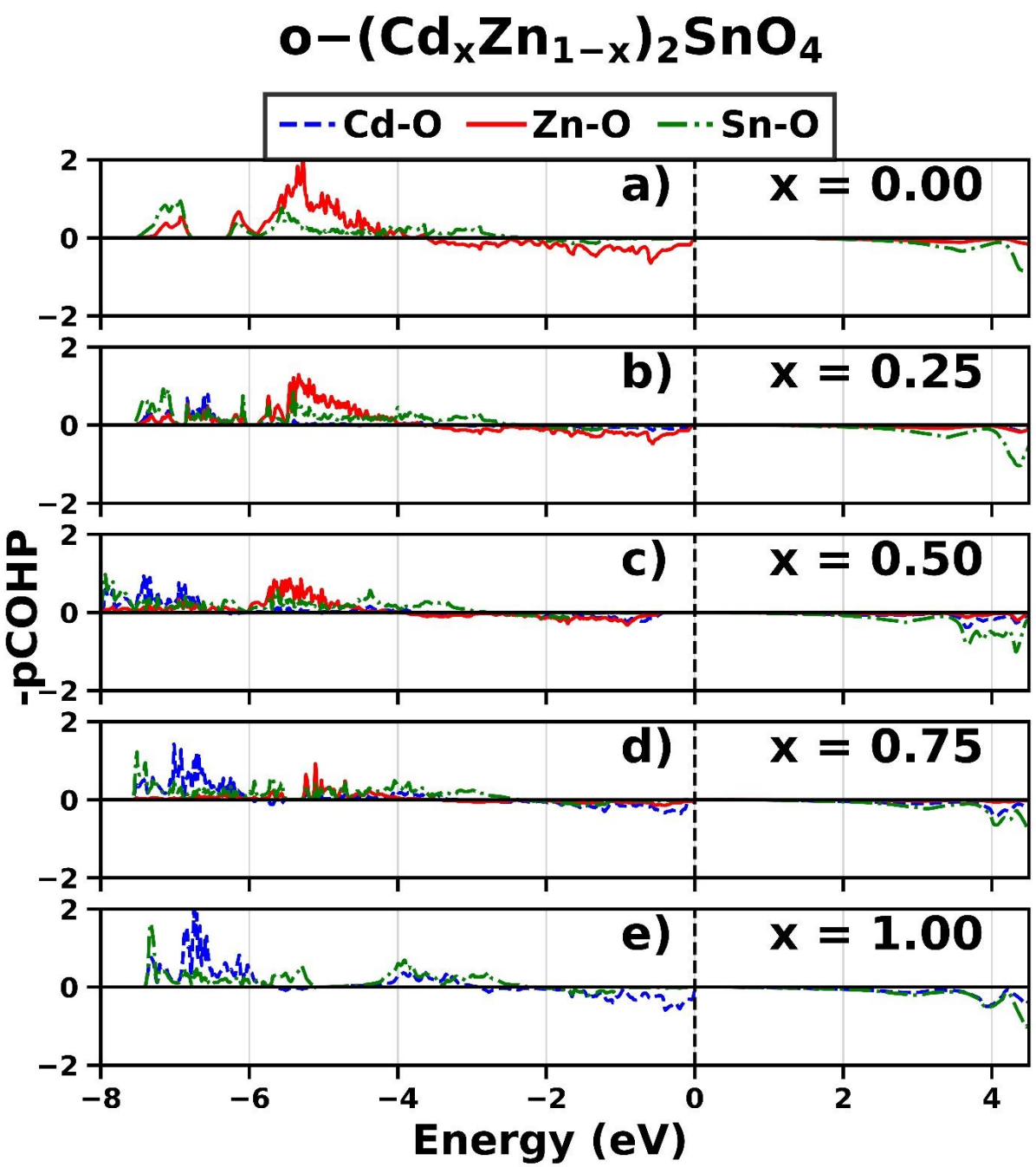

o−(Cd$_x$Zn$_{1-x}$)$_2$SnO$_4$
Cd-O
Zn-O
Sn-O
a) x = 0.00
b) x = 0.25
c) x = 0.50
d) x = 0.75
e) x = 1.00
-pCOHP
Energy (eV)

Fig S6.a)

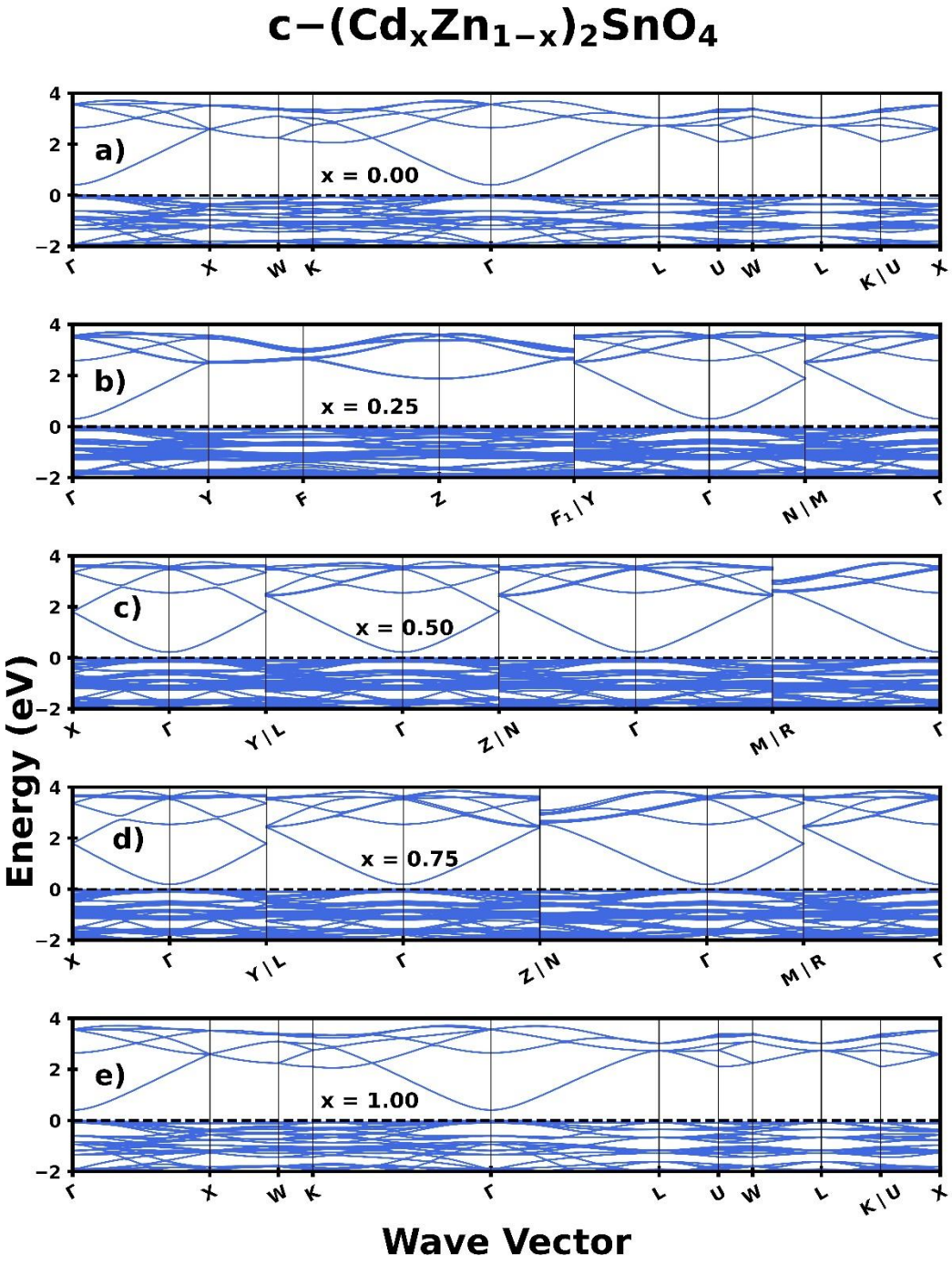
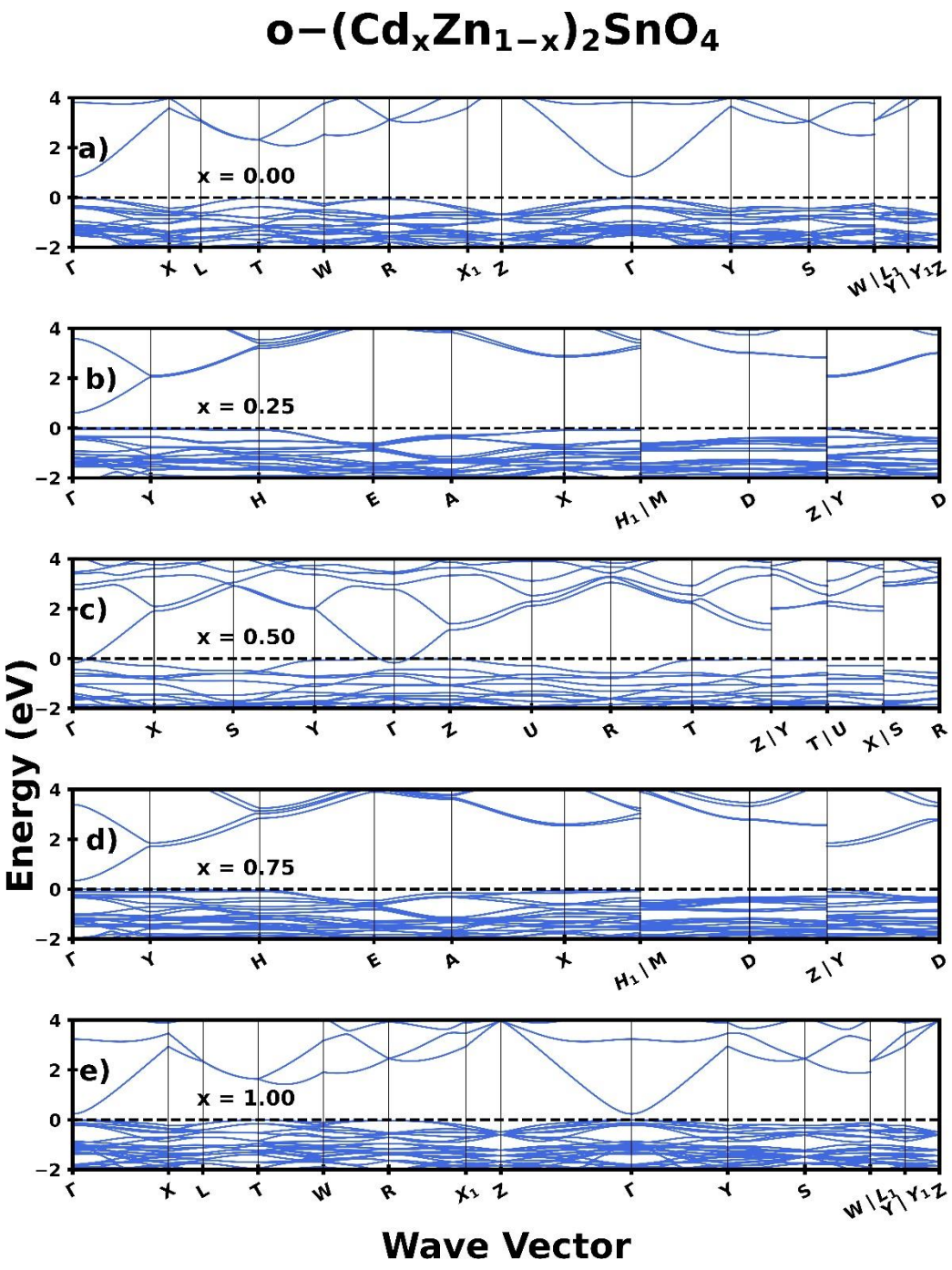


Figure S6 (a, b): Electronic band-structure of **c**ubic and orthorhombic $(Cd_xZn_{1-x})_2SnO_4$, calculated using the GGA functional. Fermi energy is set at 0 eV, **(S6.a)** for cubic $(Cd_xZn_{1-x})_2SnO_4$ and **(S6.b)** for orthorhombic $(Cd_xZn_{1-x})_2SnO_4$ at compositions x = 0.00, 0.25, 0.50, 0.75, and 1.00.

Fig S6.b)


o−(Cd$_x$Zn$_{1-x}$)$_2$SnO$_4$
a)
x = 0.00
b)
x = 0.25
c)
x = 0.50
d)
x = 0.75
e)
x = 1.00
Energy (eV)
Wave Vector

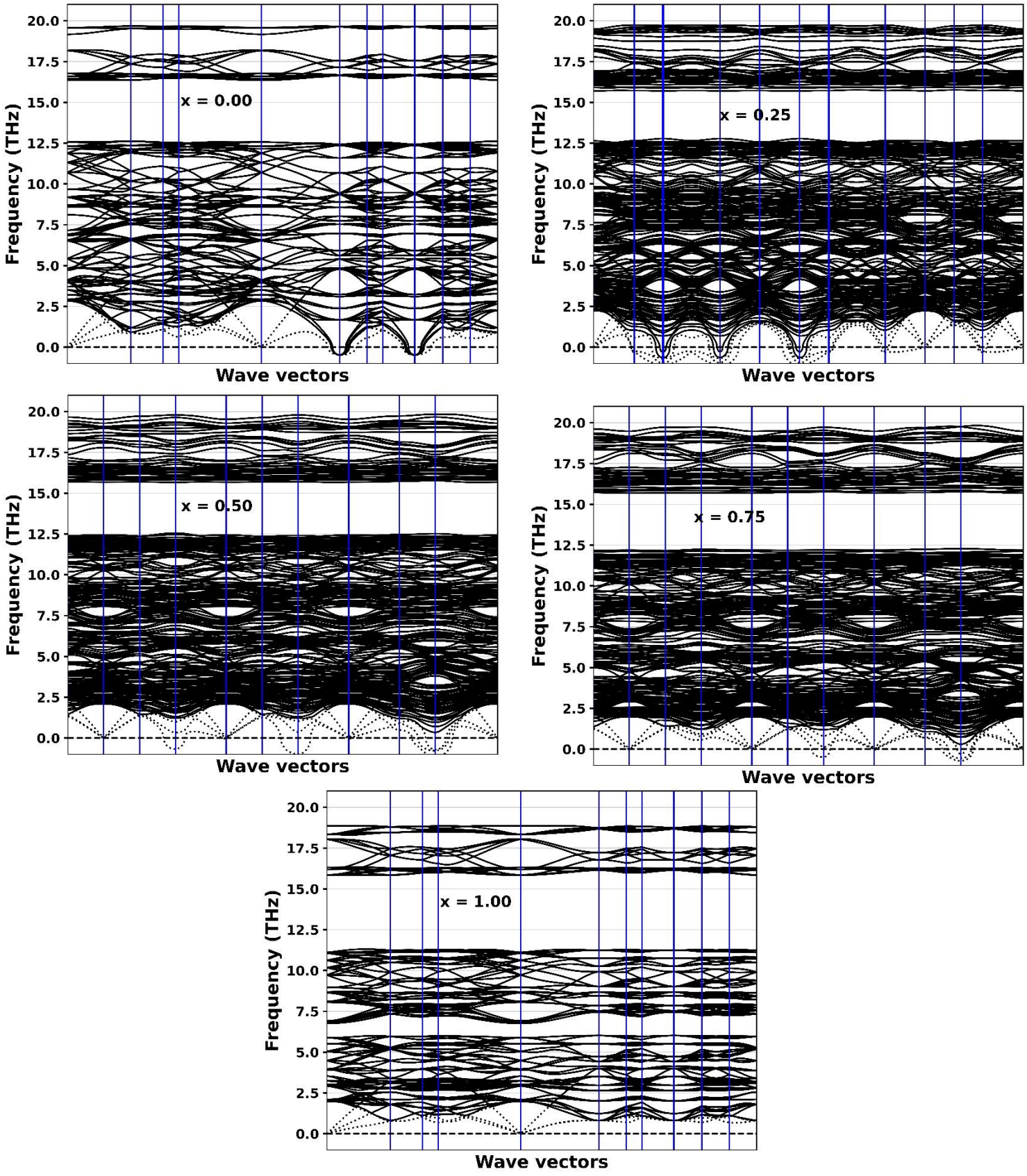


Figure S7 (a): Phonon band structure for different compositions of cubic $(Cd_xZn_{1-x})_2SnO_4$ computed using the GGA functional. The dashed lines in the phonon dispersion represent the transition modes, and the blue lines are high-symmetry paths.

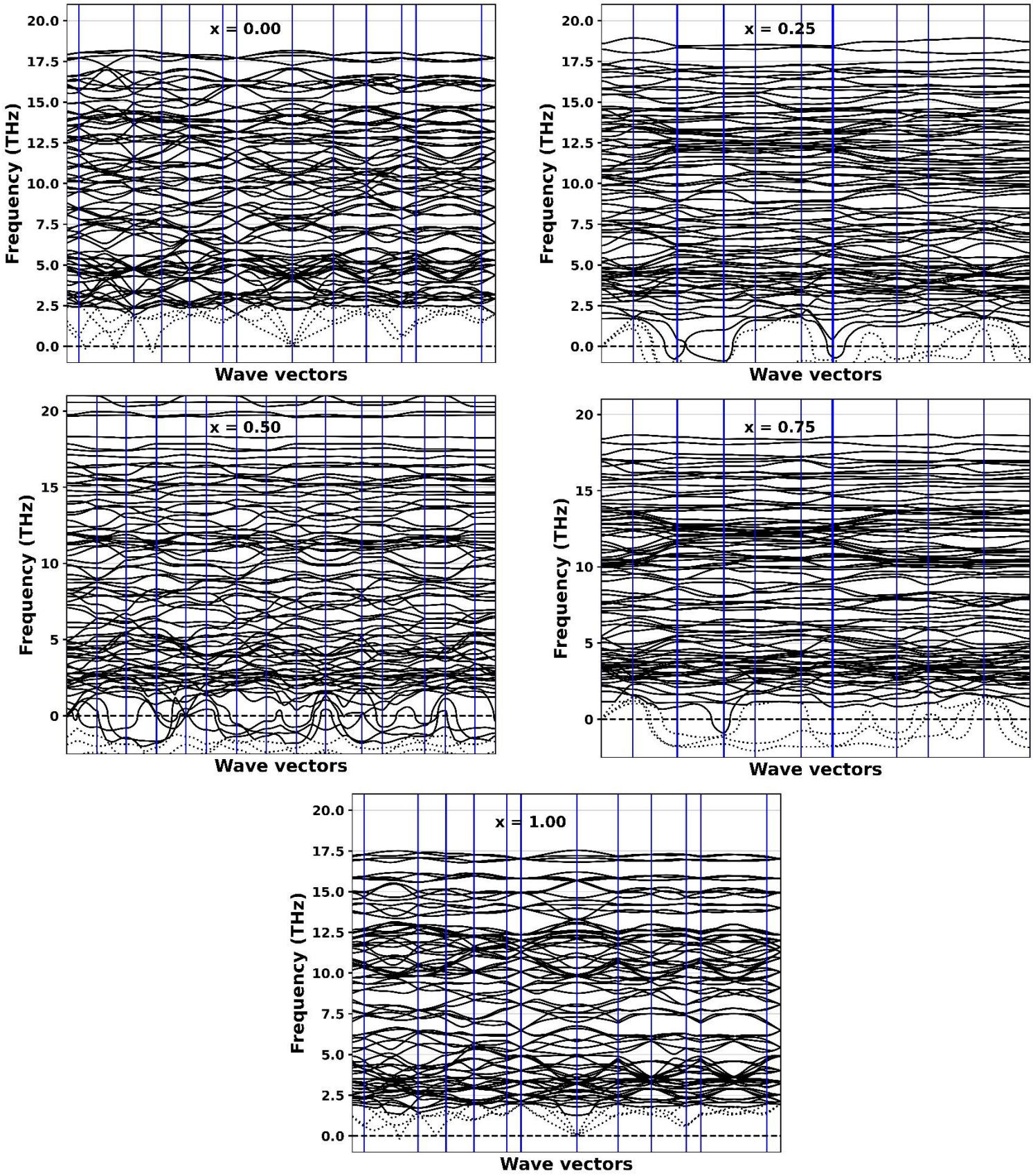


Figure S7 (b): Phonon band structure for different compositions of orthorhombic $(Cd_xZn_{1-x})_2SnO_4$ computed using the GGA functional. The dashed lines in the phonon dispersion represent the transition modes, and the blue lines are high-symmetry paths.

References

[1] K. Momma and F. Izumi, "VESTA 3 for three-dimensional visualization of crystal, volumetric and morphology data," Journal of applied crystallography 44, 1272 (2011).