Computational investigation of structural, electronic, and optical properties of $(In_xGa_{1-x})_2O_3$ alloys as candidates for emitter layer application in solar cells

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Supplementary Material

Table S1: Average value of bond lengths in Å for the first nearest neighbors around an element in the $(In_xGa_{1-x})_2O_3$ alloy system.

Material	Element		
	In	Ga	O
Ga_2O_3	-	1.90	1.90
$(In_{0.25}Ga_{0.75})_2O_3$	2.24	1.99	1.99
$(In_{0.50}Ga_{0.50})_2O_3$	2.20	2.01	2.01
$(In_{0.75}Ga_{0.25})_2O_3$	2.20	2.06	2.06
In_2O_3	2.20	-	2.20

Table S2: Elastic constants of $(In_xGa_{1-x})_2O_3$ alloys in GPa computed using GGA functional.

Parameters	Materials				
	Ga_2O_3	$(In_{0.25}Ga_{0.75})_2O_3$	$(In_{0.50}Ga_{0.50})_2O_3$	$(In_{0.75}Ga_{0.25})_2O_3$	In_2O_3
C_{11}	384.46	294.32	315.41	318.41	284.10
C_{12}	169.51	107.20	149.02	162.79	143.51
C_{13}	124.34	66.02	112.39	120.70	106.34
C_{14}	0.00	5.33501	0.90258	-0.12053	0
C_{15}	15.55	15.07	12.74	12.20	7.40
C_{22}	$= C_{11}$	289.77	303.96	311.55	$= C_{11}$
C_{23}	124.36	63.88	106.60	117.00	$= C_{13}$
C_{24}	0.00	5.51	1.34	0.21	0
C_{25}	$= - C_{15}$	-16.47	-9.60	-10.38	-7.40
C_{26}	0.00	1.14	2.33	0.86	0
C_{33}	351.47	255.70	271.75	244.80	214.71
C_{34}	0.00	5.27	0.91	-0.20	0
C_{35}	0.00	0.72	1.54	0.84	0
C_{36}	0.00	-3.93	-1.08	1.62	0
C_{44}	107.47	92.25	80.28	76.24	70.30
C_{45}	0.00	5.04	3.40	-0.87	0
C_{55}	86.33	75.97	73.23	68.16	64.29
C_{56}	0.00	-0.05	-0.13	-0.12	0
C_{66}	$= C_{55}$	76.17	73.58	68.89	$= C_{55}$

Bulk Modulus (B_V)	217.43	146.00	180.80	159.73	166.14
Bulk Modulus (B_R))	215.23	143.24	178.25	180.18	160.26
Bulk Modulus (B)	216.33	144.61	179.2	169.96	163.20
Shear Modulus (G_V)	102.83	89.06	80.28	82.21	68.22
Shear Modulus (G_R)	98.43	84.30	77.93	7.05	66.96
Shear Modulus(G)	100.63	86.68	79.10	77.13	67.59
Pugh's Ratio(k)	0.465	0.60	0.44	0.45	0.41
Vickers hardness (H_V)	10.09	12.10	8.00	8.12	6.66
Young's modulus (Y)	261.76	217.30	206.91	200.98	178.17
Poisson's ratio (v)	0.30	0.25	0.31	0.30	0.31

Table S3: Charge Transfer in units of elementary charge e form In, Ga to O in $(In_xGa_{1-x})_2O_3$ alloys calculated using Bader charge analysis method using GGA functional.

Material	Ga to O	In to O
Ga_2O_3	1.88	-
$(In_{0.25}Ga_{0.75})_2O_3$	1.87	1.85
$(In_{0.50}Ga_{0.50})_2O_3$	1.87	1.85
$(In_{0.75}Ga_{0.25})_2O_3$	1.84	1.85
In_2O_3	-	1.82

Table S4: Effective masses (m^*) and charge carrier mobility of $(In_xGa_{1-x})_2O_3$ alloys. Electron and hole effective masses are given in units of electron mass (m_0), and mobilities are reported in cm^2/Vs.

Material	Electron effective mass m_e^*/m_0	Hole effective mass m_h^*/m_0	Electron mobility cm^2/Vs	Hole mobility cm^2/Vs
Ga_2O_3	0.23	2.40	76.37	7.31
$(In_{0.25}Ga_{0.75})_2O_3$	0.20	2.83	87.91	6.20
$(In_{0.50}Ga_{0.50})_2O_3$	0.18	3.39	98.15	5.18
$(In_{0.75}Ga_{0.25})_2O_3$	0.17	6.51	103.89	2.69
In_2O_3	0.16	8.54	110.34	2.05

Table S5: SQS-generated structures for $(In_xGa_{1-x})_2O_3$ alloy system.

Material	POSCAR
Ga_2O_3	Ga12 O18 1.00000000000000 5.0546553702803463 -0.0000000000000000 -0.0000000000000000 -2.5273276851401731 4.3774603738286793 0.0000000000000000 -0.0000000000000000 -0.0000000000000000 13.6064963566653017 Ga O 12 18 Direct -0.0000000000000000 -0.0000000000000000 0.1441114408251677 0.3333330000000032 0.6666669999999968 0.0225555591748362 0.6666669999999968 0.3333330000000032 0.1892215591748355 0.3333330000000032 0.6666669999999968 0.3107784408251645 0.6666669999999968 0.3333330000000032 0.4774444408251638 -0.0000000000000000 -0.0000000000000000 0.3558885591748323 0.3333330000000032 0.6666669999999968 0.5225555591748361 -0.0000000000000000 -0.0000000000000000 0.6441114408251678 0.3333330000000032 0.6666669999999968 0.8107784408251646 0.6666669999999968 0.3333330000000032 0.6892215591748354 -0.0000000000000000 -0.0000000000000000 0.8558885591748322 0.6666669999999968 0.3333330000000032 0.9774444408251639 0.0000000000000111 0.3030475356657972 0.2500000000000000 0.3030475356657750 -0.0000000000000000 0.2500000000000000 0.6969524643342140 0.6969524643342028 0.2500000000000000 0.6666669999999857 0.0302854643341989 0.0833330000000032 0.9697145356657899 0.6363805356658004 0.0833330000000032 0.3636194643342218 0.3333330000000032 0.0833330000000032 0.6666670000000079 0.6363805356658004 0.5833330000000032 0.9697145356657788 0.3333330000000032 0.5833330000000032 0.3636194643342107 0.0302854643341989 0.5833330000000032 0.3333329999999921 0.3636194643341996 0.4166669999999968 0.6363805356657892 0.9697145356658011 0.4166669999999968 0.0302854643342211 0.6666669999999968 0.4166669999999968 0.3333330000000143 0.9697145356658011 0.9166669999999968 0.6363805356657781 0.6666669999999968 0.9166669999999968 0.0302854643342100 0.3636194643341996 0.9166669999999968 -0.0000000000000111 0.6969524643342028 0.7500000000000000 0.3030475356657861 0.3030475356657972 0.7500000000000000 0.6969524643342251 -0.0000000000000000 0.7500000000000000

Material	POSCAR
$(In_{0.25}Ga_{0.75})_2O_3$	from sqs 1.00000000000000 5.1779830701160927 0.0000007450303821 -0.0000000000000000 -2.5889921802733484 4.4842649518700242 0.0000000000000000 -0.0000000000000000 0.0000000000000000 13.8384369521802402 Ga In O 9 3 18 Direct -0.0000000000000000 -0.0000000000000000 0.1461031712762620 -0.0000000000000000 -0.0000000000000000 0.3493479336957159 0.6666669999999968 0.3333330000000032 0.1867944022005774 0.6666669999999968 0.3333330000000032 0.9731506918765294 0.6666669999999968 0.3333330000000032 0.6940798496236847 0.3333330000000032 0.6666669999999968 0.5216868273946516 0.3333330000000032 0.6666669999999968 0.3104442059761559 0.3333330000000032 0.6666669999999968 0.8124934819218541 -0.0000000000000000 -0.0000000000000000 0.8564475693938126 0.6666669999999968 0.3333330000000032 0.4693460075208832 0.3333330000000032 0.6666669999999968 0.0296078564876003 -0.0000000000000000 -0.0000000000000000 0.6408456748299648 0.0001954015442635 0.3069873822393994 0.2488924876319540 0.3067919806944125 -0.0001954015432885 0.2488924876319540 0.6930126177613239 0.6932080193038892 0.2488924876319540 0.6964286336560132 0.0588643829560869 0.0854482348076347 0.9411356172022353 0.6375632507705844 0.0854482348076347 0.3624367491417492 0.3035713662733311 0.0854482348076347 0.6334870091018865 0.6123527722593174 0.5855578764157482 0.9788667632825264 0.3665129910040114 0.5855578764157482 0.3876472276155847 0.0211332367366736 0.5855578764157482 0.3006096031557518 0.3596724902928199 0.4129298784281598 0.6403275096334010 0.9409381127026668 0.4129298784281598 0.0590618872108496 0.6993903970045108 0.4129298784281598 0.3340508133028669 0.9772205220340233 0.9149448725242839 0.6431687087007274 0.6659491867340093 0.9149448725242839 0.0227794779964079 0.3568312912319647 0.9149448725242839 -0.0027624381719857 0.6878637401909242 0.7554440927929887 0.3121362597767137 0.3093738216728754 0.7554440927929887 0.6906261783952716 0.0027624381362002 0.7554440927929887

Material	POSCAR
$(In_{0.50}Ga_{0.50})_2O_3$	from sqs 1.00000000000000 5.2885329804384646 0.0000013773307796 0.0000000000000000 -2.6442676830227994 4.5800036933381794 0.0000000000000000 -0.0000000000000000 0.0000000000000000 14.1121263936287242 Ga In O 6 6 18 Direct -0.0000000000000000 0.0000000000000000 0.1485007551106182 -0.0000000000000000 0.0000000000000000 0.3535022914048418 0.6666669999999968 0.3333330000000032 0.4735187092182574 0.3333330000000032 0.6666669999999968 0.3112035795947764 0.3333330000000032 0.6666669999999968 0.8175385188023656 -0.0000000000000000 0.0000000000000000 0.8529860501958817 0.6666669999999968 0.3333330000000032 0.2008006673618108 0.6666669999999968 0.3333330000000032 0.9740328412317627 0.6666669999999968 0.3333330000000032 0.6947846372629630 0.3333330000000032 0.6666669999999968 0.5171892492166850 0.3333330000000032 0.6666669999999968 0.0312602335545487 -0.0000000000000000 0.0000000000000000 0.6402516467388749 0.0314738592755706 0.3062453376344540 0.2530107237676172 0.2747714781944854 -0.0314738596270353 0.2530107237676172 0.6937546625299440 0.7252285219925814 0.2530107237676172 0.6948463455537857 0.0439777651535909 0.0885195651428456 0.9560222350532157 0.6508675807083932 0.0885195651428456 0.3491324193929964 0.3051536541380184 0.0885195651428456 0.6707069286546629 0.6201443330019990 0.5760035784982224 0.9494384044675294 0.3292930712234630 0.5760035784982224 0.3798556668778056 0.0505615957745407 0.5760035784982224 0.3398506715942095 0.3542137954443458 0.4092478120260174 0.6457862044782270 0.9856378762243918 0.4092478120260174 0.0143621239275656 0.6601493283312599 0.4092478120260174 0.3110965964156865 0.9543967077725831 0.9129791892474395 0.6432991116296145 0.6889034038165694 0.9129791892474395 0.0456032919547015 0.3567008884108447 0.9129791892474395 0.0252012984140016 0.7127012739519277 0.7550494047533957 0.2872987263284416 0.3125000247020827 0.7550494047533957 0.6874999752575566 -0.0252012986540106 0.7550494047533957

Material	POSCAR
$(In_{0.75}Ga_{0.25})_2O_3$	from sqs 1.00000000000000 5.4063431343426132 0.0000016909830937 -0.0000000000000000 -2.7031730316057794 4.6820301523783563 -0.0000000000000000 -0.0000000000000000 -0.0000000000000000 14.3004266445831583 In Ga O 9 3 18 Direct 0.0000000000000000 0.0000000000000000 0.1376745412080821 0.0000000000000000 0.0000000000000000 0.3560581172625490 0.6666669999999968 0.3333330000000032 0.9804455768511189 0.6666669999999968 0.3333330000000032 0.4736751925242719 0.6666669999999968 0.3333330000000032 0.6886771507851396 0.3333330000000032 0.6666669999999968 0.5266431337595550 0.3333330000000032 0.6666669999999968 0.3004927892659473 0.3333330000000032 0.6666669999999968 0.8099415600238377 0.0000000000000000 0.0000000000000000 0.8599693072382233 0.6666669999999968 0.3333330000000032 0.1886869808837911 0.3333330000000032 0.6666669999999968 0.0243739986106423 0.0000000000000000 0.0000000000000000 0.6464381764512108 -0.0301942652852370 0.2906242559841891 0.2457454959260242 0.3208185215681307 0.0301942657343528 0.2457454959260242 0.7093757437171062 0.6791814782814583 0.2457454959260242 0.6350371602765088 0.0154711328574911 0.0864015681789958 0.9845288668073938 0.6195650270297208 0.0864015681789958 0.3804349729160950 0.3649628401127908 0.0864015681789958 0.6946457503403531 0.6568785088939412 0.5847858570238956 0.9622337581095984 0.3053542493687758 0.5847858570238956 0.3431214915500458 0.0377662417372858 0.5847858570238956 0.3343015194404844 0.3757985630923287 0.4144175817306511 0.6242014369733974 0.9585039562823554 0.4144175817306511 0.0414960435861208 0.6656984806253134 0.4144175817306511 0.3277507852243390 0.9512812771615202 0.9235217057193867 0.6235294921078519 0.6722492146056496 0.9235217057193867 0.0487187226678113 0.3764705082328273 0.9235217057193867 0.0030308714469902 0.7134952616841691 0.7474356164662570 0.2865047384809241 0.2895356095901611 0.7474356164662570 0.7104643900720859 -0.0030308712743300 0.7474356164662570

Material	POSCAR
In_2O_3	In12 O18 1.00000000000000 5.5723384259617497 0.0000000000000000 -0.0000000000000000 -2.7861692129808748 4.8257864808439939 0.0000000000000000 0.0000000000000000 0.0000000000000000 14.7234443562011759 In O 12 18 Direct 0.6666669999999968 0.3333330000000032 0.1905387300023887 0.3333330000000032 0.6666669999999968 0.3094612699976113 0.3333330000000032 0.6666669999999968 0.0238727300023895 0.0000000000000000 -0.0000000000000000 0.1427942699976145 0.3333330000000032 0.6666669999999968 0.5238727300023895 0.0000000000000000 -0.0000000000000000 0.6427942699976144 0.0000000000000000 -0.0000000000000000 0.3572057300023855 0.6666669999999968 0.3333330000000032 0.4761272699976106 0.0000000000000000 -0.0000000000000000 0.8572057300023856 0.6666669999999968 0.3333330000000032 0.9761272699976105 0.6666669999999968 0.3333330000000032 0.6905387300023889 0.3333330000000032 0.6666669999999968 0.8094612699976111 0.3701722112697763 0.0368382112697905 0.0833330000000032 0.7035052112697647 -0.0000000000000000 0.2500000000000000 0.0000000000000148 0.7035052112697944 0.2500000000000000 0.6666669999999819 0.6298277887302088 0.0833330000000032 0.2964947887302204 0.2964947887302056 0.2500000000000000 0.9631617887302392 0.3333330000000032 0.0833330000000032 0.0368382112697756 0.3701722112697912 0.4166669999999968 0.3701722112697615 0.3333330000000032 0.5833330000000032 0.6666670000000117 0.0368382112697905 0.5833330000000032 0.3333329999999884 0.9631617887302095 0.4166669999999968 0.9631617887302243 0.6298277887302088 0.5833330000000032 0.6298277887302385 0.6666669999999968 0.4166669999999968 0.7035052112697796 0.7035052112697944 0.7500000000000000 0.0368382112697608 0.6666669999999968 0.9166669999999968 0.3333330000000180 0.3701722112697912 0.9166669999999968 -0.0000000000000148 0.2964947887302056 0.7500000000000000 0.6298277887302236 0.9631617887302095 0.9166669999999968 0.2964947887302353 -0.0000000000000000 0.7500000000000000

Table S6: Lattice constants of $(In_xGa_{1-x})_2O_3$ alloys (x = 0.25, 0.50, and 0.75) obtained from three SQS-generated POSCAR structures.

Materials	Sample A		Sample B		Sample C	
	a (Å)	c (Å)	a (Å)	c (Å)	a (Å)	c (Å)
$(In_{0.25}Ga_{0.75})_2O_3$	5.18	13.84	5.17	13.82	5.17	13.83
$(In_{0.50}Ga_{0.50})_2O_3$	5.29	14.11	5.29	14.08	5.28	14.11
$(In_{0.75}Ga_{0.25})_2O_3$	5.41	14.30	5.40	14.28	5.40	14.30

Table S7: Electronic bandgap of $(In_xGa_{1-x})_2O_3$ alloys (x = 0.25, 0.50, and 0.75) obtained from three SQS-generated POSCAR structures computed using both GGA and hybrid HSE06 functionals.

Materials	Sample A (eV)		Sample B (eV)		Sample C (eV)	
	GGA	HSE06	GGA	HSE06	GGA	HSE06
$(In_{0.25}Ga_{0.75})_2O_3$	1.88	3.70	1.87	3.65	1.88	3.67
$(In_{0.50}Ga_{0.50})_2O_3$	1.56	3.29	1.52	3.25	1.55	3.28
$(In_{0.75}Ga_{0.25})_2O_3$	1.31	3.02	1.31	3.01	1.31	3.02

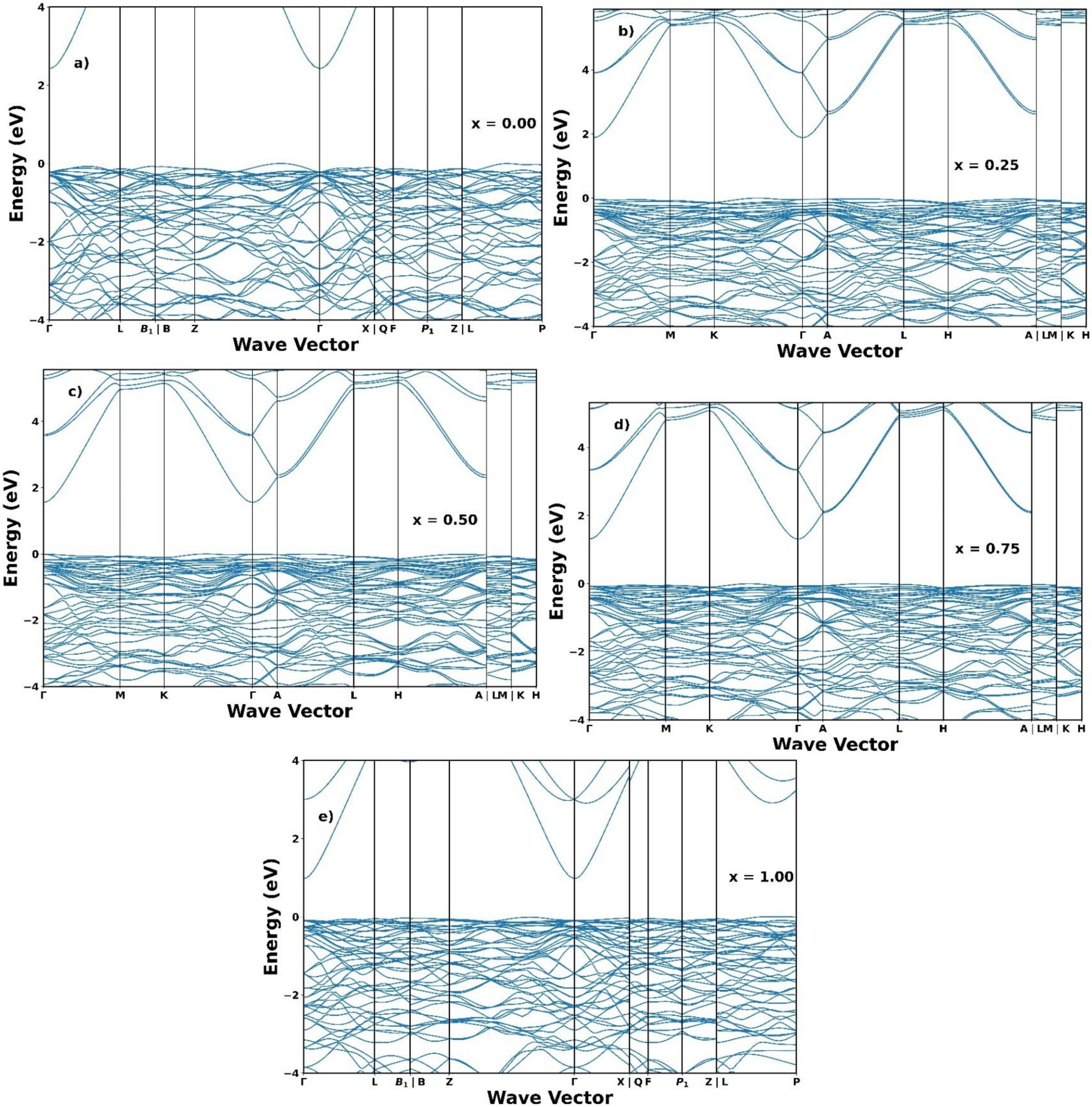


Figure S1: Electronic band-structure of $(In_xGa_{1-x})_2O_3$ alloys computed using GGA functional. Fermi energy is set at 0 eV.

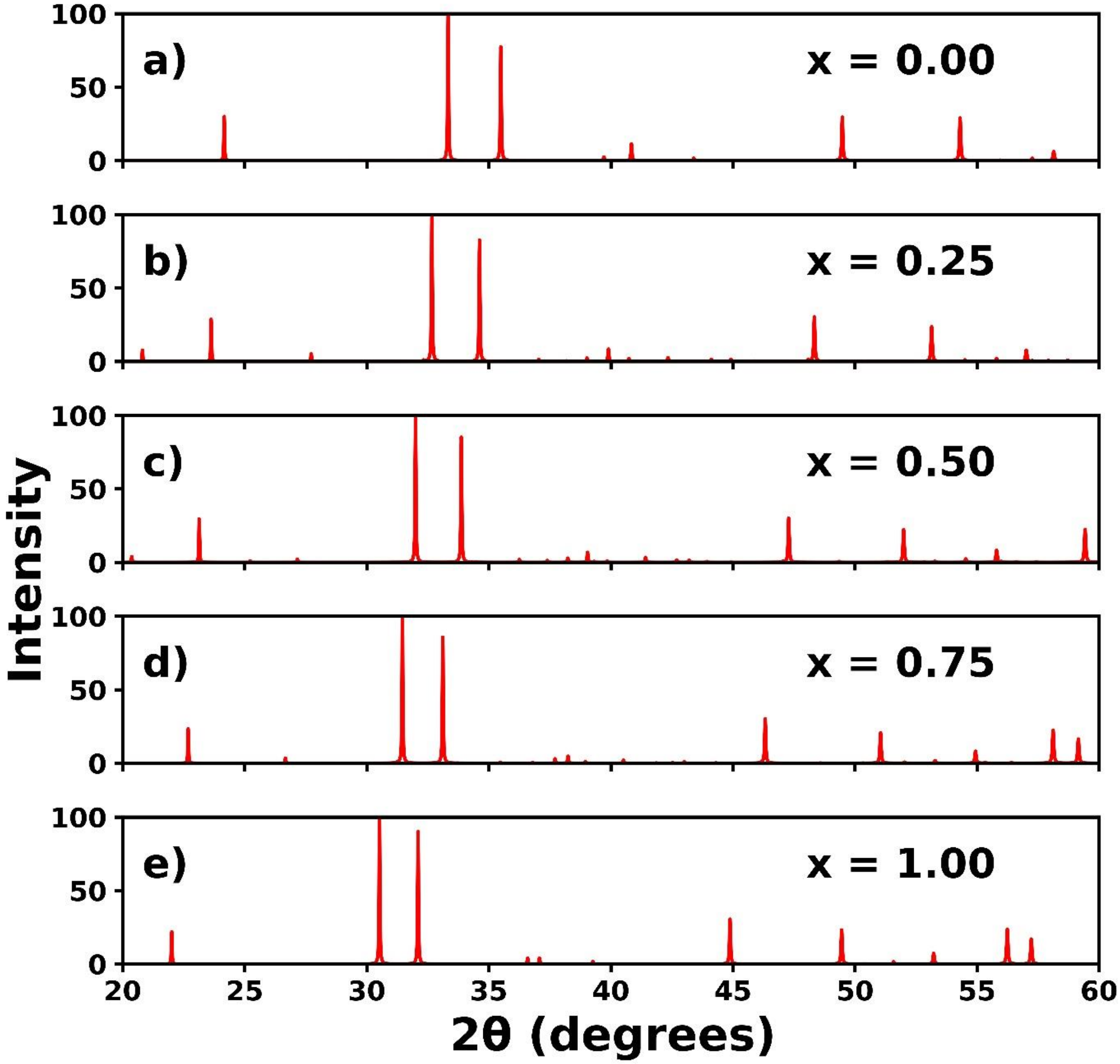
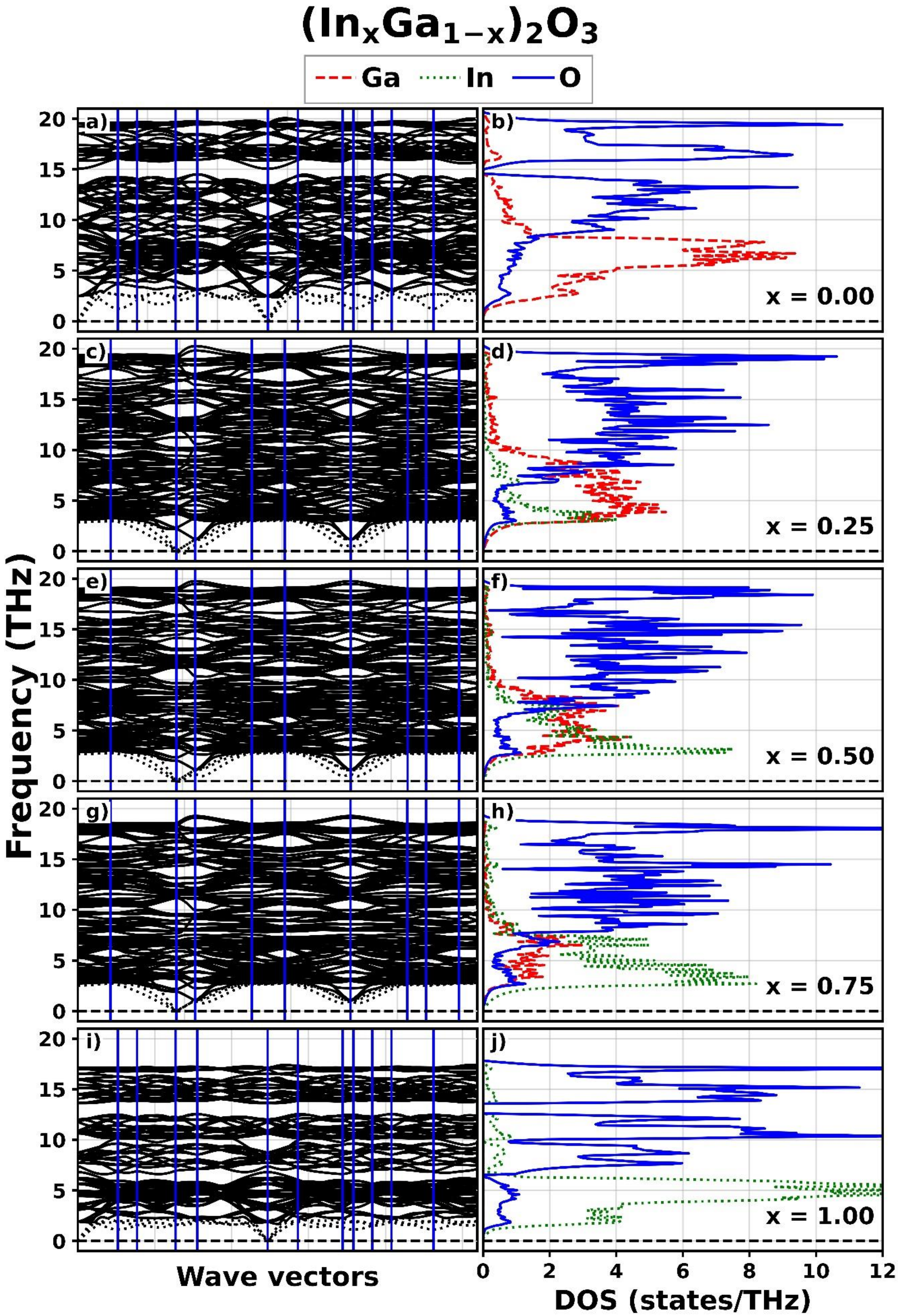


Figure S2: X-ray diffraction (XRD) for $(In_xGa_{1-x})_2O_3$ generated using the VESTA program with a wavelength (λ) of 1.54 Å.



$(In_xGa_{1-x})_2O_3$
Ga
In
O
a)
b)
c)
d)
e)
f)
g)
h)
i)
j)
x = 0.00
x = 0.25
x = 0.50
x = 0.75
x = 1.00
Frequency (THz)
Wave vectors
DOS (states/THz)

Figure S3: Phonon band structure and densities of states (DOS) for different compositions computed using GGA functional. For x = 0 and 1.0, the path is Γ-L-B_1-B-Z-Γ-X-Q-F-P_1-Z-L-P and for x = 0.25, 0.50, and 0.75, the path is M-K-Γ-A-L-H-H-A-L-M-K. The dashed lines in phonon dispersion represent the transitional modes.