Theoretical Assessment of Multi-Doping Strategies in Amorphous Indium Oxide for Synergistically Enhancing Carrier Mobility and Bias Stability

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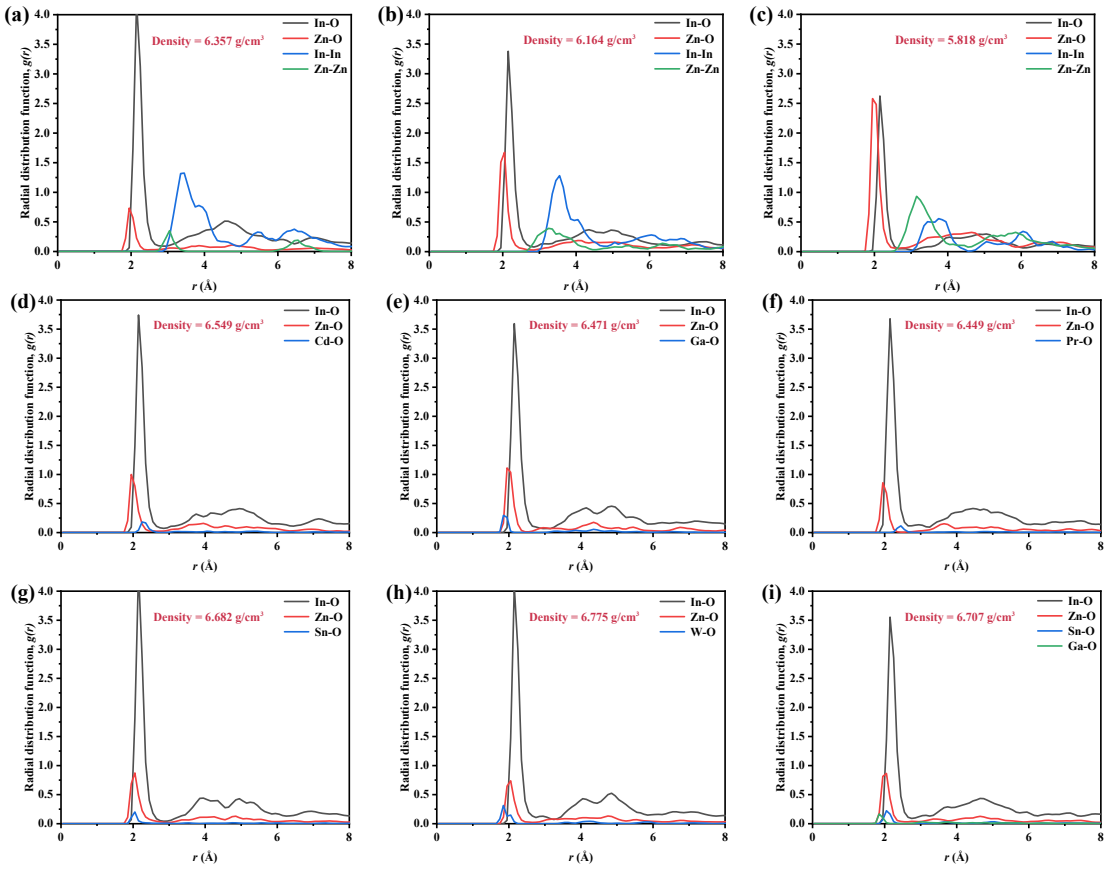
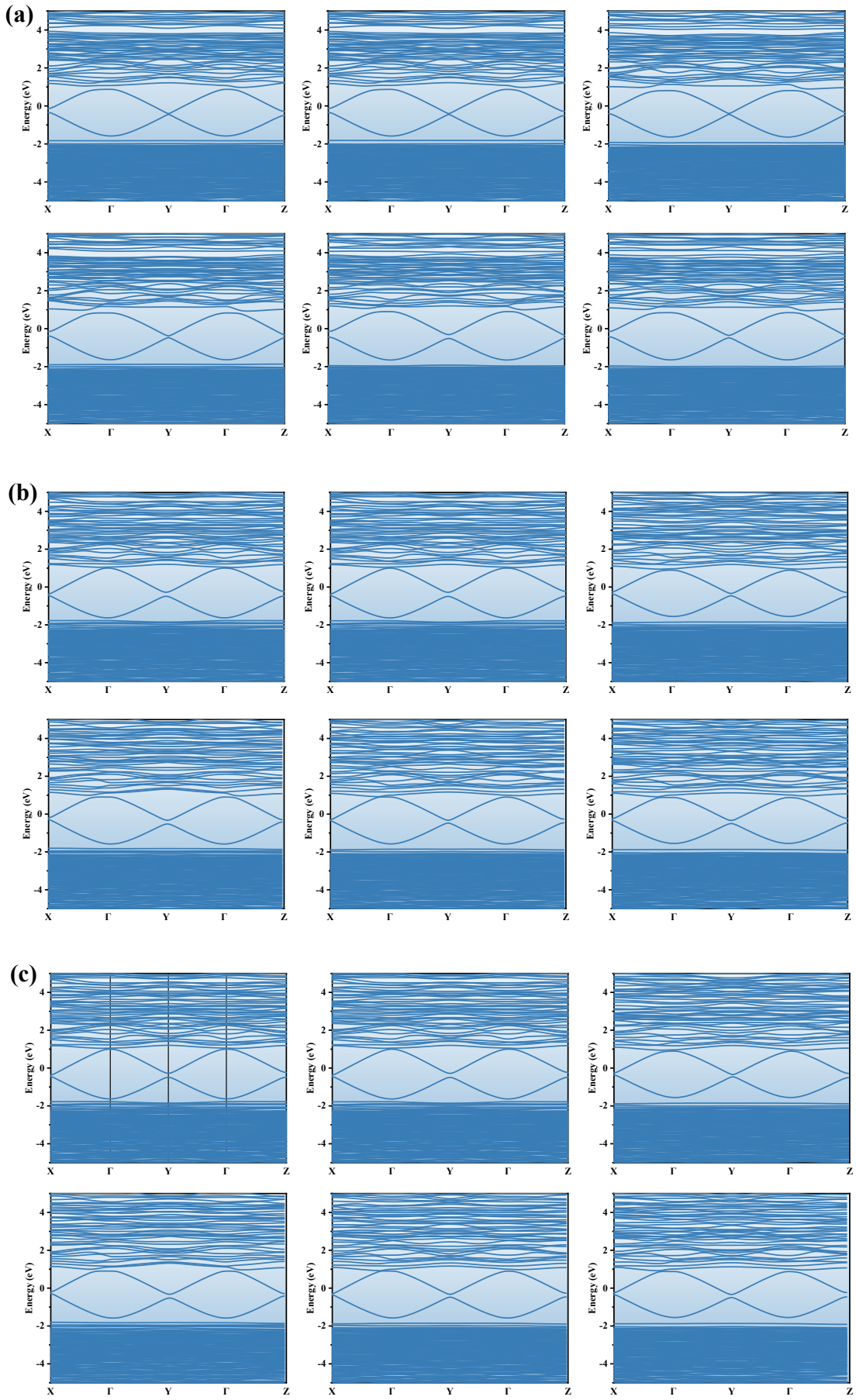
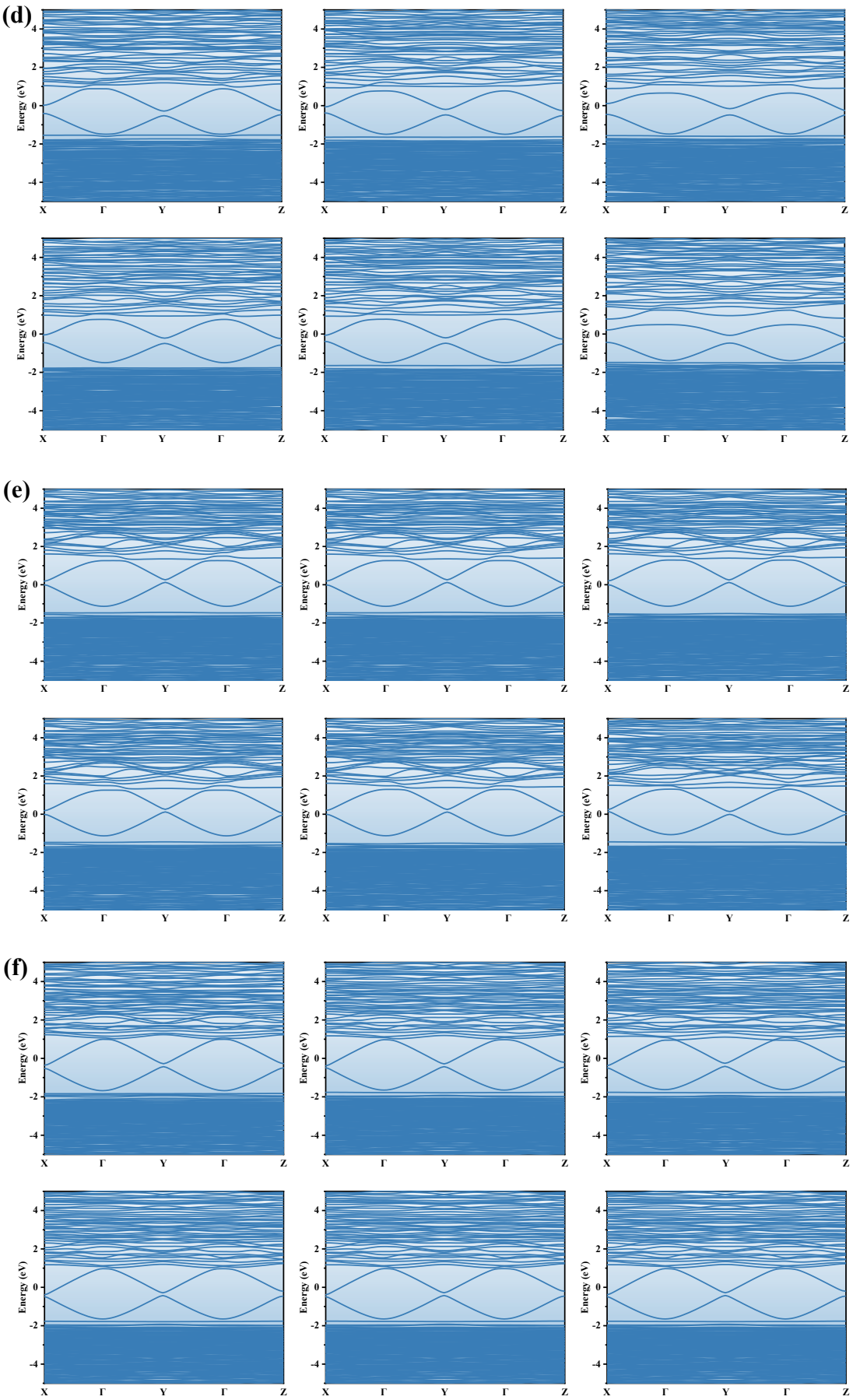
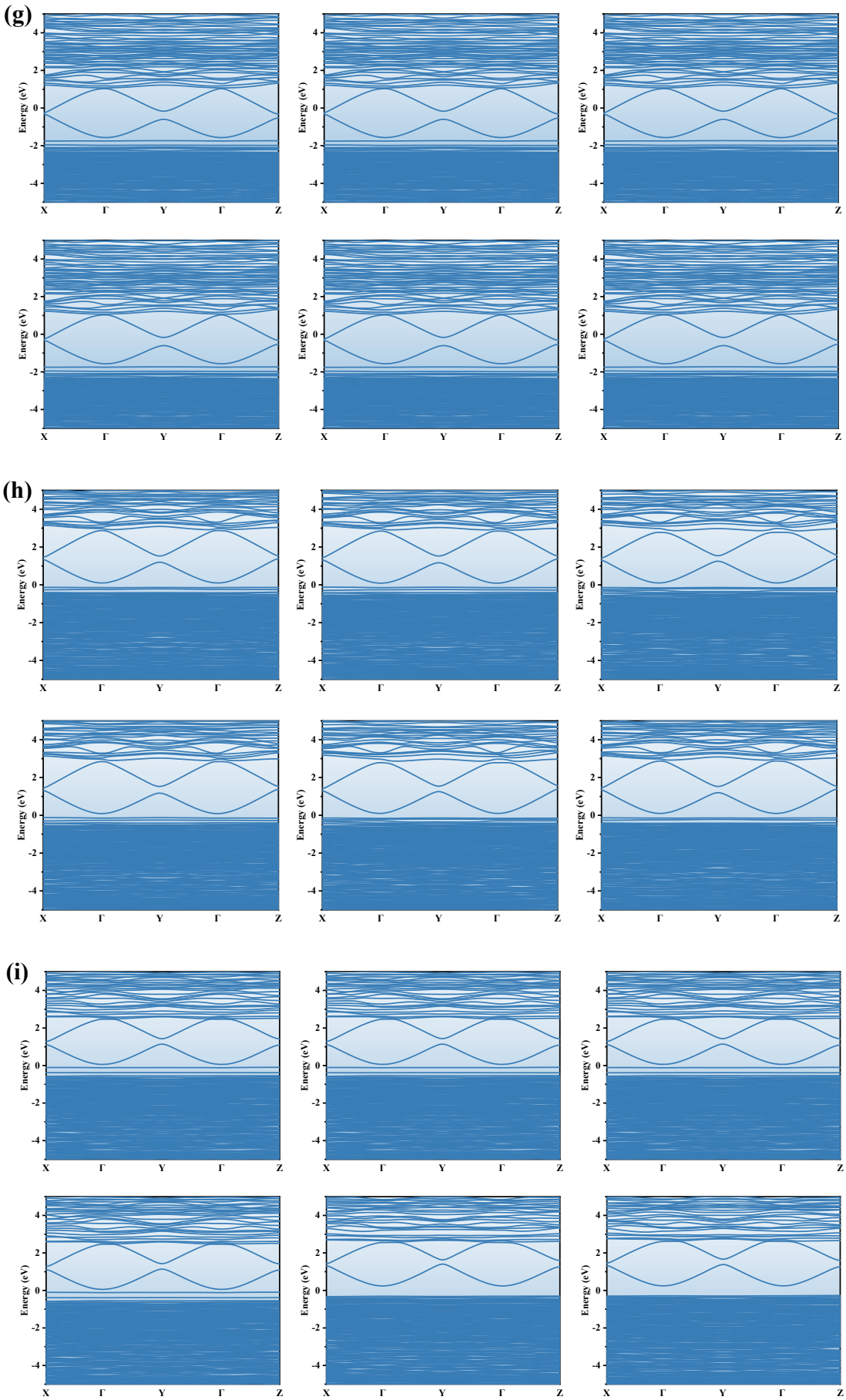


Fig. S1: Radial distribution function plots of **(a)** IZO 18.8%; **(b)** IZO 37.5%; **(c)** IZO 50.0%; **(d)** ICZO; **(e)** IGZO; **(f)** IPZO; **(g)** ITZO; **(h)** IWZO and **(i)** ITGZO.


(a)
(b)
(c)
Energy (eV)
4
2
0
-2
-4
X
Γ
Y
Γ
Z


(d)
(e)
(f)
Energy (eV)
4
2
0
-2
-4
X
Γ
Y
Γ
Z


(g)
(h)
(i)
Energy (eV)
4
2
0
-2
-4
X
Γ
Y
Γ
Z

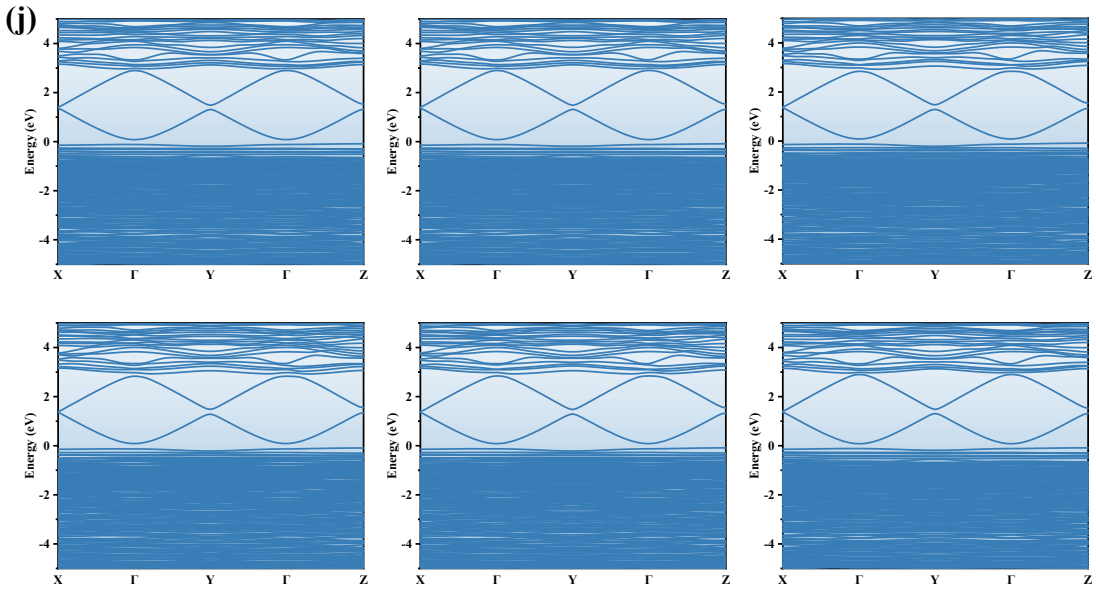
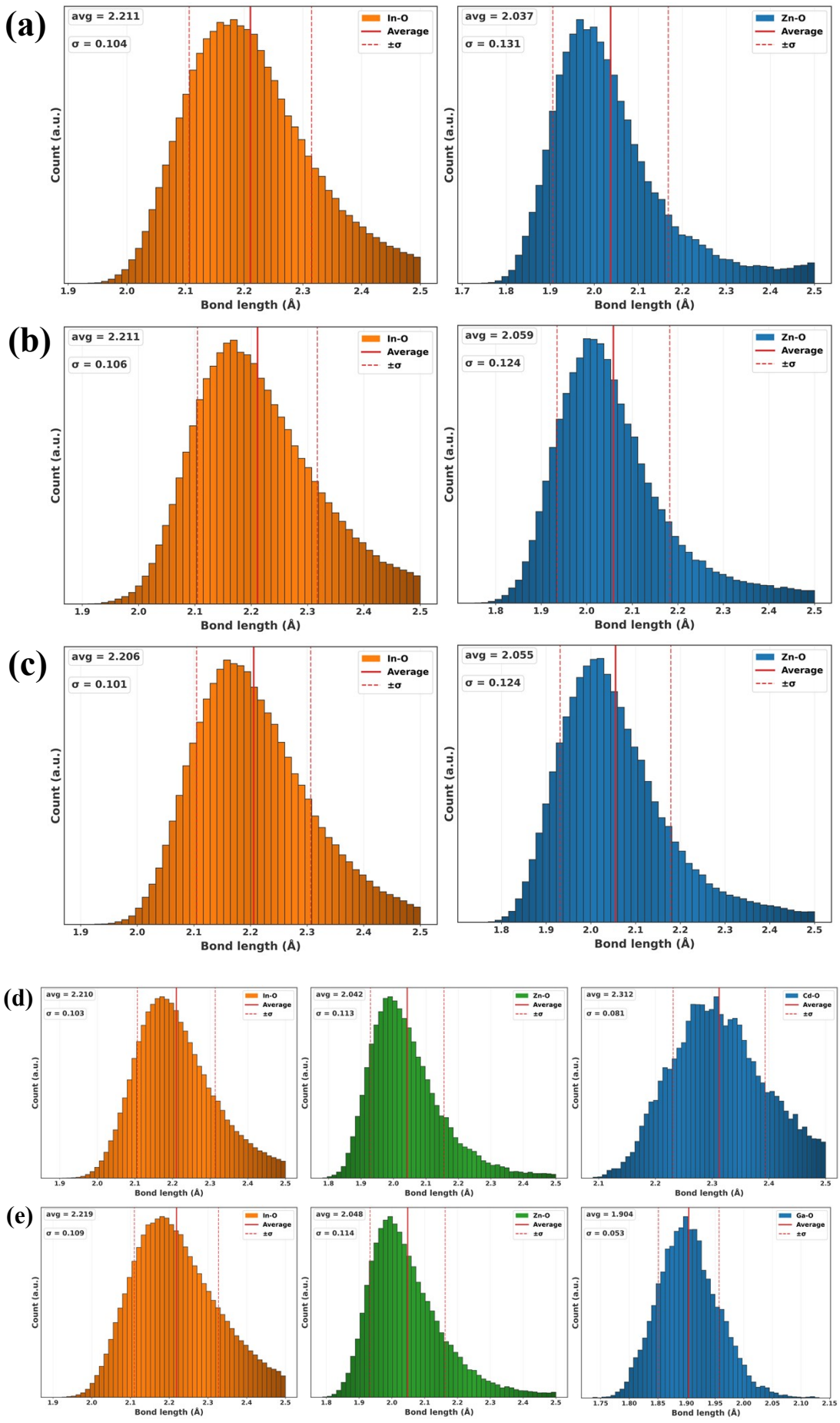


Fig. S2: The pseudo-band structure of **(a)** In_2O_3; **(b)** IZO 18.8%; **(c)** IZO 37.5%; **(d)** IZO 50.0%; **(e)** ICZO; **(f)** IGZO; **(g)** IPZO; **(h)** ITZO; **(i)** IWZO and **(j)** ITGZO.


(a)
avg = 2.211
σ = 0.104
In-O
Average
±σ
Count (a.u.)
Bond length (Å)
avg = 2.037
σ = 0.131
Zn-O
Average
±σ
Count (a.u.)
Bond length (Å)
(b)
avg = 2.211
σ = 0.106
In-O
Average
±σ
Count (a.u.)
Bond length (Å)
avg = 2.059
σ = 0.124
Zn-O
Average
±σ
Count (a.u.)
Bond length (Å)
(c)
avg = 2.206
σ = 0.101
In-O
Average
±σ
Count (a.u.)
Bond length (Å)
avg = 2.055
σ = 0.124
Zn-O
Average
±σ
Count (a.u.)
Bond length (Å)
(d)
avg = 2.210
σ = 0.103
In-O
Average
±σ
Count (a.u.)
Bond length (Å)
avg = 2.042
σ = 0.113
Zn-O
Average
±σ
Count (a.u.)
Bond length (Å)
avg = 2.312
σ = 0.081
Cd-O
Average
±σ
Count (a.u.)
Bond length (Å)
(e)
avg = 2.219
σ = 0.109
In-O
Average
±σ
Count (a.u.)
Bond length (Å)
avg = 2.048
σ = 0.114
Zn-O
Average
±σ
Count (a.u.)
Bond length (Å)
avg = 1.904
σ = 0.053
Ga-O
Average
±σ
Count (a.u.)
Bond length (Å)

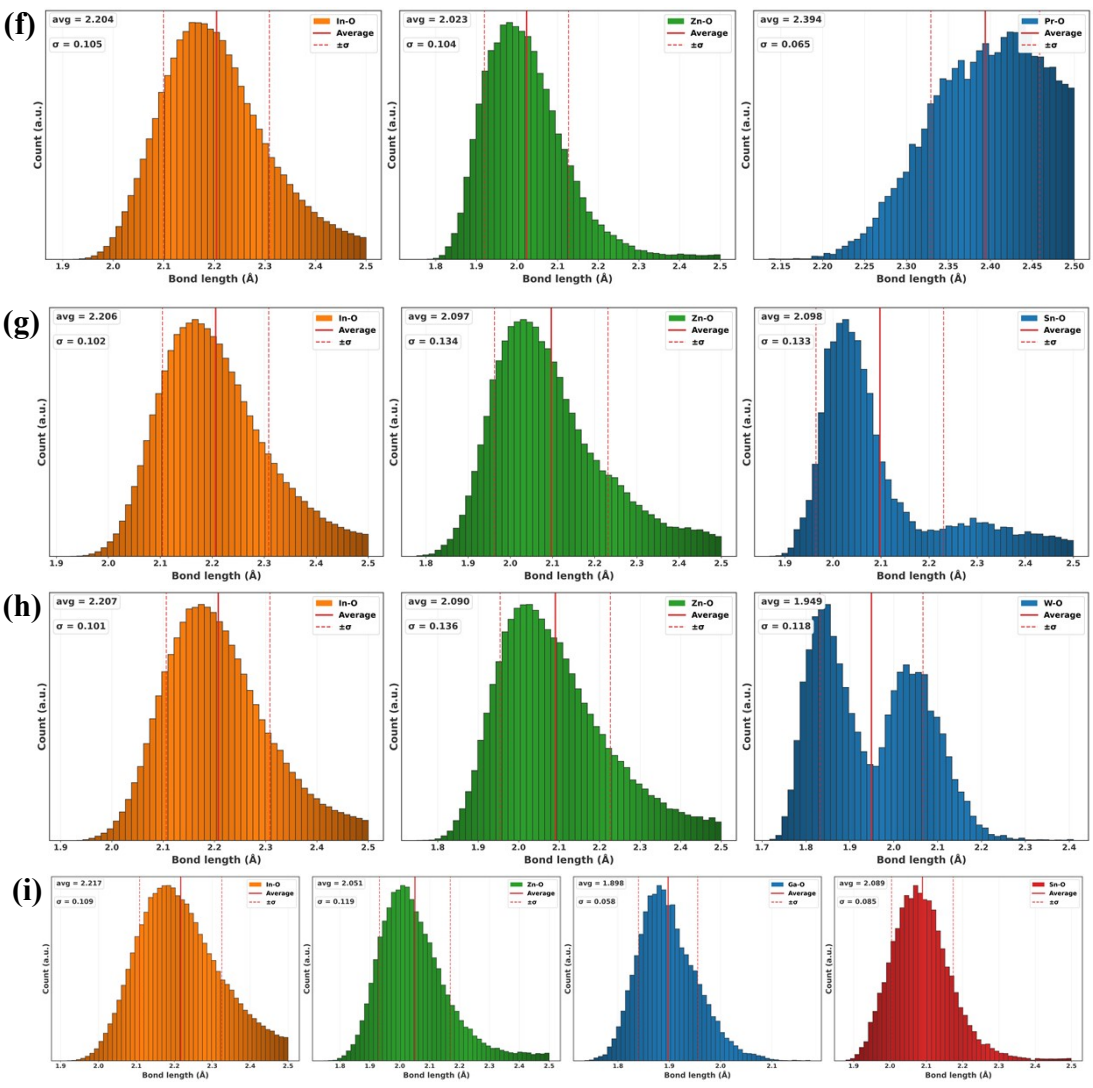


Fig. S3: Statistical histogram of M-O bond lengths for **(a)** IZO 18.8%; **(b)** IZO 37.5%; **(c)** IZO 50.0%; **(d)** ICZO; **(e)** IGZO; **(f)** IPZO; **(g)** ITZO; **(h)** IWZO and **(i)** ITGZO.

Table S1: Amorphous structural information.

Sample	Composition	Oxygen vacancy	Additional compensation charge	Density (g/cm^3)
IO	$In_{32}O_{48}$	0	-	6.845
IZO6	$In_{26}Zn_6O_{45}$	3	-	6.357
IZO12	$In_{20}Zn_{12}O_{42}$	6	-	6.164
IZO16	$In_{16}Zn_{16}O_{40}$	8	-	5.818
ICZO	$In_{25}Zn_6CdO_{45}$	3	hole	6.549
IGZO	$In_{25}Zn_6GaO_{45}$	3	-	6.471
IPZO	$In_{25}Zn_6PrO_{45}$	3	-	6.449
ITZO	$In_{25}Zn_6SnO_{45}$	3	electron	6.682
IWZO	$In_{25}Zn_6WO_{47}$	1	hole	6.775
ITGZO	$In_{24}Zn_6SnGaO_{45}$	3	-	6.707

Table S2: Experimental and theoretical data on M–O bond lengths in *a*-IGZO.

	Bond Length (Å)			**Ref**
	In-O	**Ga-O**	**Zn-O**	
Calculation	2.15	1.79	2.00	[1]
	2.22	2.02	2.05	[2]
	2.14	1.90	2.00	[3]
	2.20	2.00	2.00	[4]
Experiment	2.16	1.87	1.97	[5]
	2.12	1.91	1.92	[6]
This work	2.22	1.90	2.05	-

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