

Supporting information for

Structure, Electrical Properties and Conduction Mechanism of New Germanate Mixed Conductors Zn-doped $\text{In}_2\text{Ge}_2\text{O}_7$

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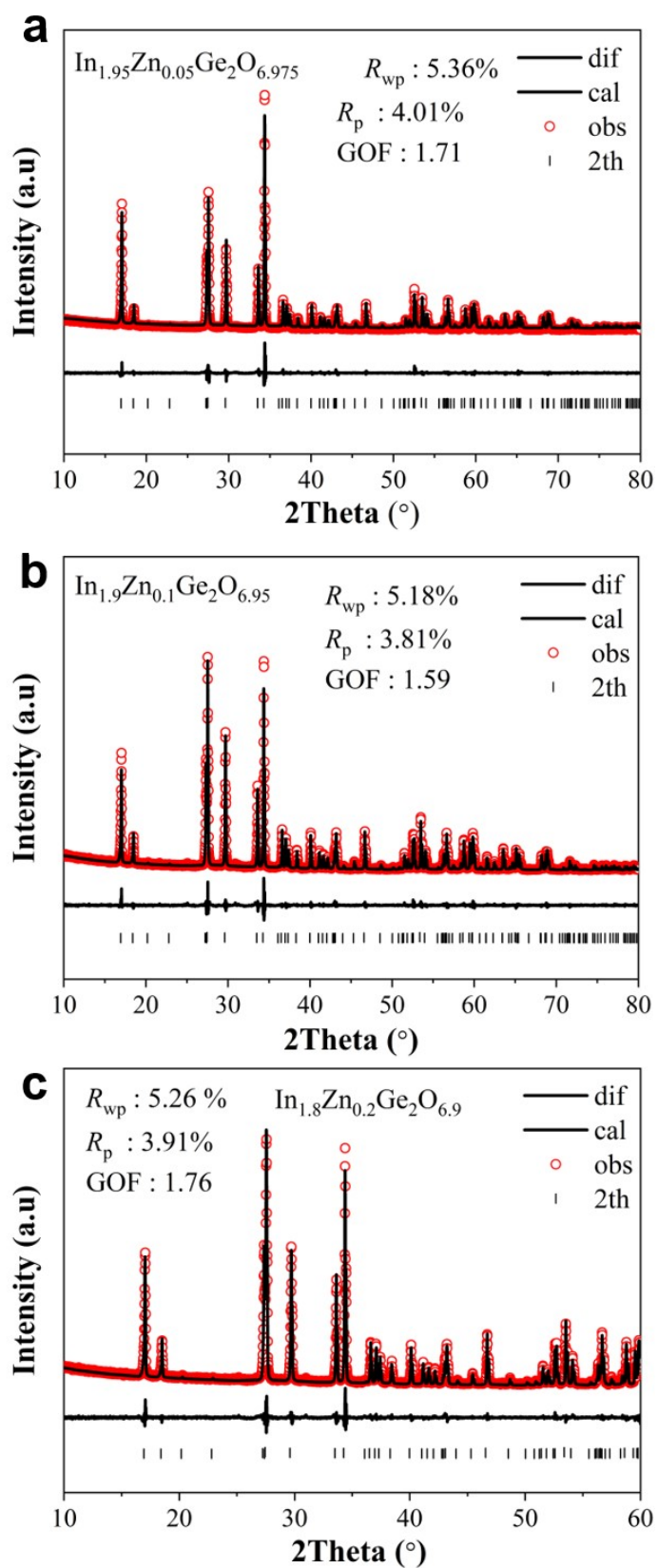


Figure S1. Rietveld refinement plots of $\text{In}_{2-x}\text{Zn}_x\text{Ge}_2\text{O}_{7-0.5x}$ (a) $x = 0.05$; (b) $x = 0.10$; (c)

$x = 0.10$.

Table S1. The final refined structural parameters of $\text{In}_{1.95}\text{Zn}_{0.05}\text{Ge}_2\text{O}_{6.975}$.

Atom	Wyckoff	x	y	z	occ.	B_{iso} (\AA^2)
	site					
In1	4h	0	0.5	0.3070(1)	0.98(2)	2.18
Zn1	4h	0	0.5	0.3070(1)	0.02(2)	2.18
Ge1	4i	0.2328 (2)	0.9105(4)	0	1	2.79
O1	2a	0	0	0	0.98(3)	2.99
O2	4i	0.401(1)	0.231(2)	0	1	0.98
O3	8j	0.2334(6)	0.722(1)	0.1612(7)	1	2.99

Space group: $B2/m$, $a = 6.66002(6)$ \AA , $b = 8.78625(9)$ \AA , $c = 4.92905(5)$ \AA , $\alpha = 90^\circ$, $\beta = 90^\circ$, $\gamma = 102.4899(7)^\circ$, $V = 281.605(5)$ \AA^3 .

Table S2. The final refined structural parameters of $\text{In}_{1.9}\text{Zn}_{0.1}\text{Ge}_2\text{O}_{6.95}$.

Atom	Wyckoff	x	y	z	occ.	B_{iso} (\AA^2)
	site					
In1	4h	0	0.5	0.30714(9)	0.951(8)	1.32
Zn1	4h	0	0.5	0.30714(9)	0.049(8)	1.32
Ge1	4i	0.2336(2)	0.9089(3)	0	1	1.99
O1	2a	0	0	0	0.95(1)	2.98
O2	4i	0.416(1)	0.236(2)	0	1	1.67
O3	8j	0.2355(7)	0.715(1)	0.1614(7)	1	2.98

Space group: $B2/m$, $a = 6.65827(5) \text{ \AA}$, $b = 8.78629(8) \text{ \AA}$, $c = 4.92940(5) \text{ \AA}$, $\alpha = 90^\circ$, $\beta = 90^\circ$, $\gamma = 102.4852(6)^\circ$, $V = 281.558(4) \text{ \AA}^3$.

Table S3. The final refined structural parameters of $\text{In}_{1.85}\text{Zn}_{0.15}\text{Ge}_2\text{O}_{6.925}$.

Atom	Wyckoff site	x	y	z	occ.	$B_{\text{iso}} (\text{\AA}^2)$
In1	4h	0	0.5	0.3073(1)	0.93(1)	1.41
Zn1	4h	0	0.5	0.3073(1)	0.07(1)	1.41
Ge1	4i	0.2336(3)	0.9077(4)	0	1	2.12
O1	2a	0	0	0	0.92(2)	2.99
O2	4i	0.414(1)	0.225(2)	0	1	0.49
O3	8j	0.2372(9)	0.722 (1)	0.1602(8)	1	2.99

Space group: $B2/m$, $a = 6.65969(6) \text{ \AA}$, $b = 8.78586(9) \text{ \AA}$, $c = 4.92856(6) \text{ \AA}$, $\alpha = 90^\circ$, $\beta = 90^\circ$, $\gamma = 102.4897(7)^\circ$, $V = 281.551(5) \text{ \AA}^3$.

Table S4. The final refined structural parameters of $\text{In}_{1.8}\text{Zn}_{0.2}\text{Ge}_2\text{O}_{6.9}$.*

Atom	Wyckoff site	x	y	z	occ	$B_{\text{iso}} (\text{\AA}^2)$
In1	4h	0	0.5	0.3068(1)	0.91(1)	2.05
Zn1	4h	0	0.5	0.3068(1)	0.09(1)	1.64
Ge1	4i	0.2330(3)	0.9092(4)	0	1	3.00
O1	2a	0	0	0	0.91(1)	3.00
O2	4i	0.424(2)	0.222(3)	0	1	3.00

O3	8j	0.2338 (9)	0.714(2)	0.1652(9)	1	3.00
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*Space group: $B2/m$, $a = 6.65986(7)\text{\AA}$, $b = 8.7863(1)\text{\AA}$, $c = 4.92892(6)\text{\AA}$, $\alpha = 90^\circ$, $\beta = 90^\circ$, $\gamma = 102.4929(7)^\circ$, $V = 281.590(5)\text{\AA}^3$.

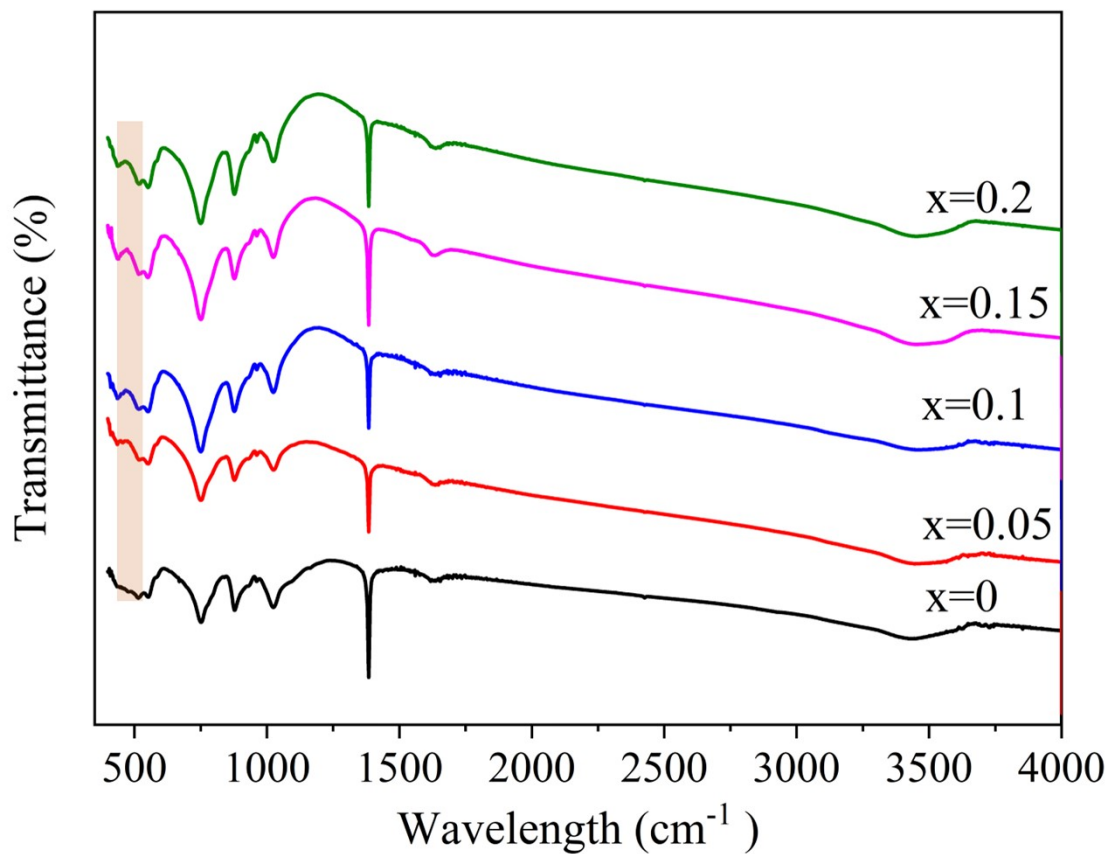


Figure S2. IR spectra of $\text{In}_{2-x}\text{Zn}_x\text{Ge}_2\text{O}_{7-0.5x}$ ($0 \leq x \leq 0.20$).

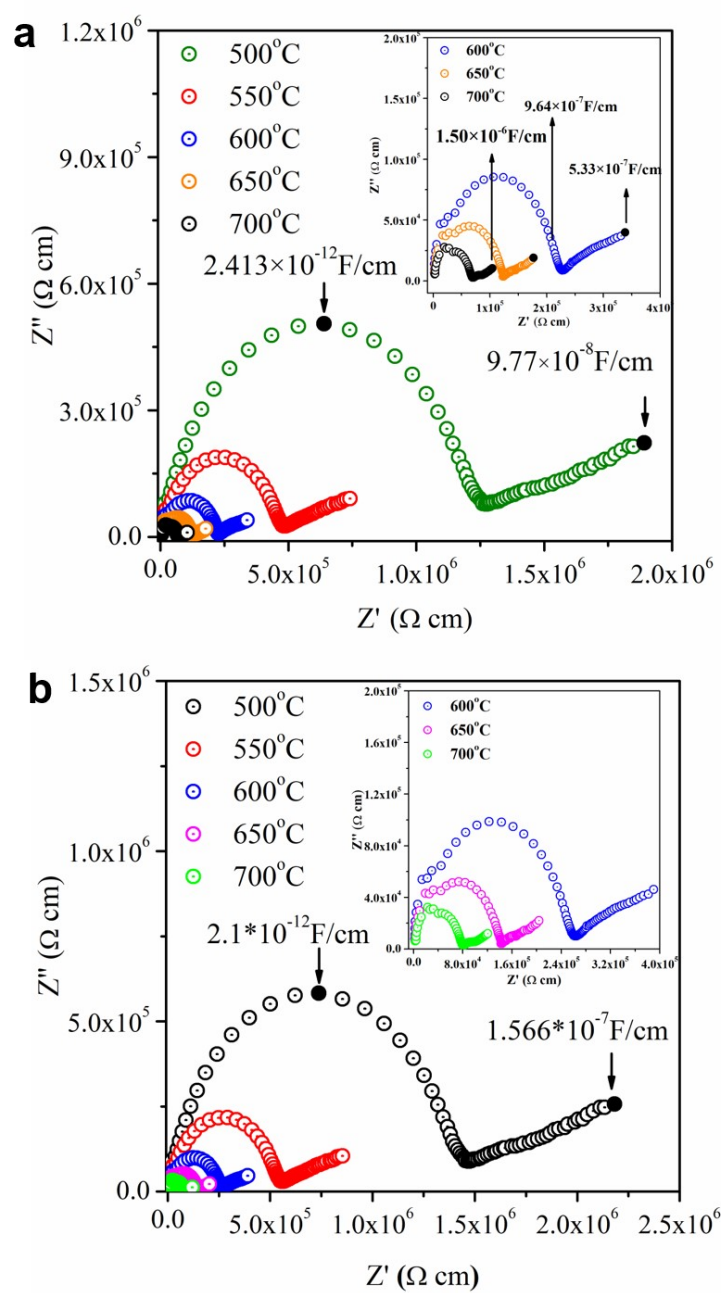


Figure S3. Complex impedance plots of (a) $\text{In}_{2-x}\text{Zn}_x\text{Ge}_2\text{O}_{7-0.5x}$ ($x = 0.05$) and (b) $\text{In}_{2-x}\text{Zn}_x\text{Ge}_2\text{O}_{7-0.5x}$ ($x = 0.10$) in the temperature range from 500 °C to 700 °C.

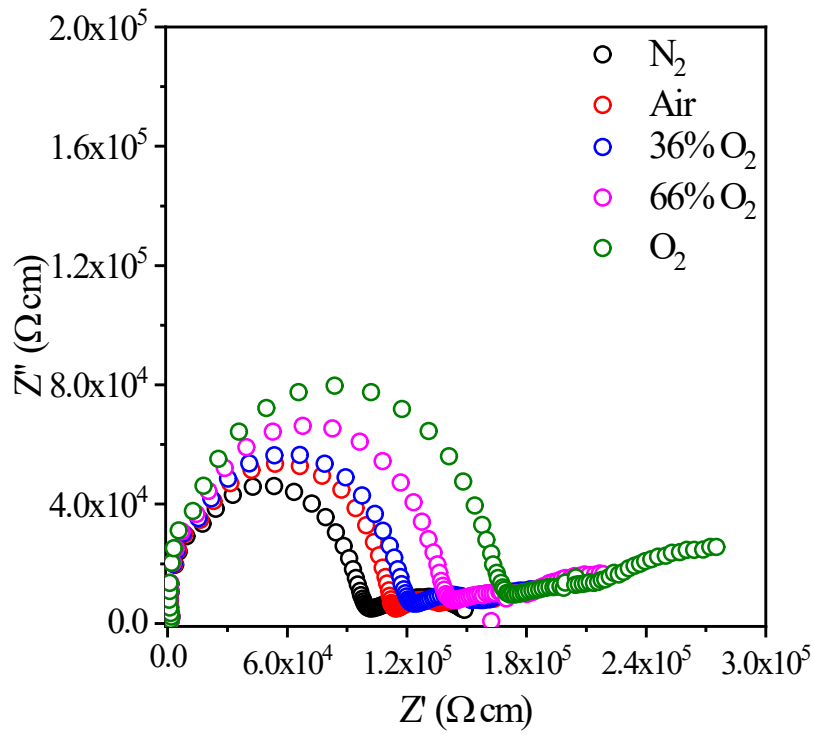


Figure S4. Complex impedance plots of $\text{In}_{2-x}\text{Zn}_x\text{Ge}_2\text{O}_{7-0.5x}$ ($x = 0.10$) at different oxygen partial pressures.

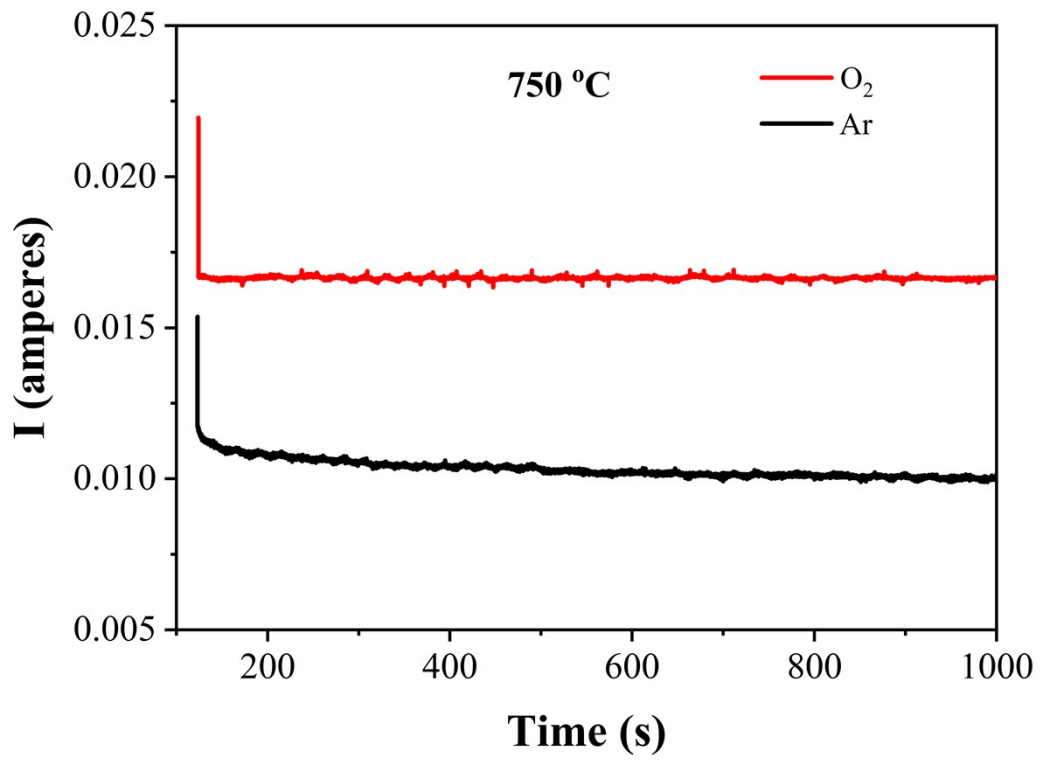


Figure S5. DC chronoamperometry curve of $\text{In}_{2-x}\text{Zn}_x\text{Ge}_2\text{O}_{7-0.5x}$ ($x = 0.2$) at $750\text{ }^\circ\text{C}$.

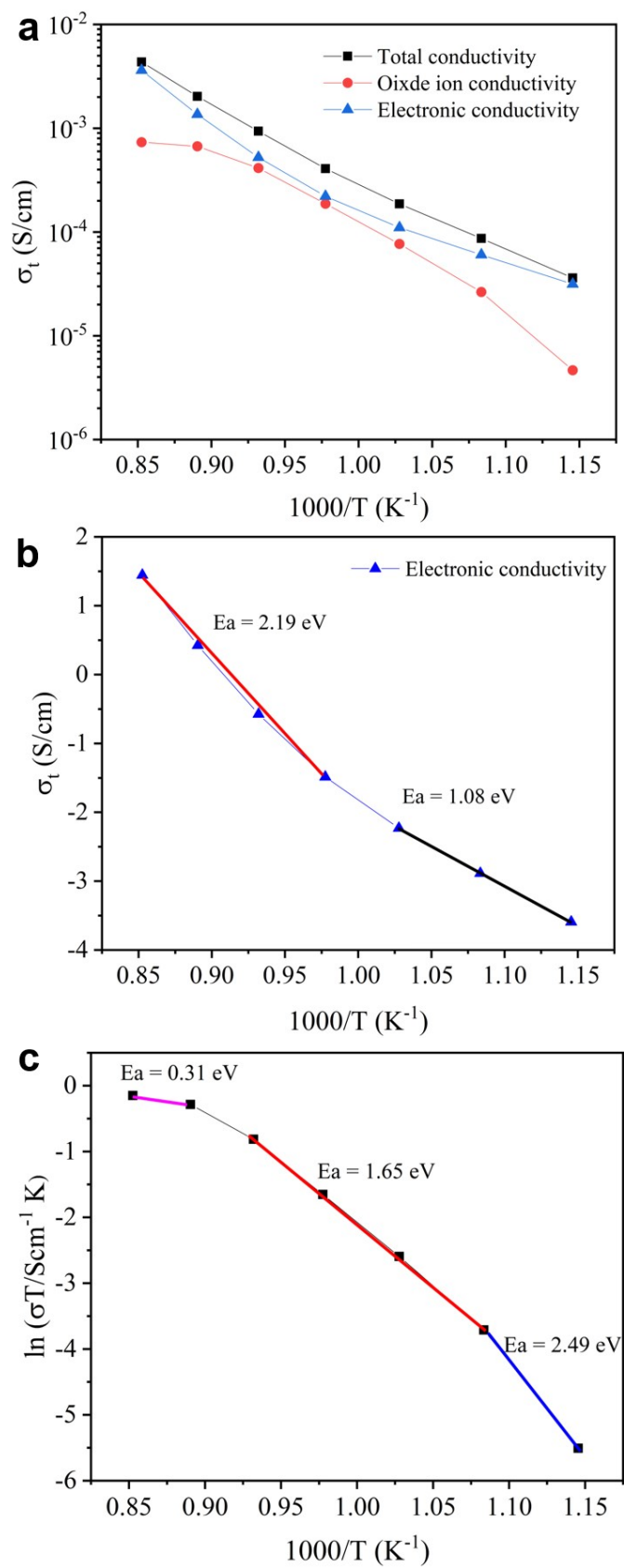


Figure S6. (a) Bulk conductivity, (b) extracted electronic conductivity and (c) oxide ionic conductivity of $\text{In}_{2-x}\text{Zn}_x\text{Ge}_2\text{O}_{7-0.5x}$ ($x = 0.2$).

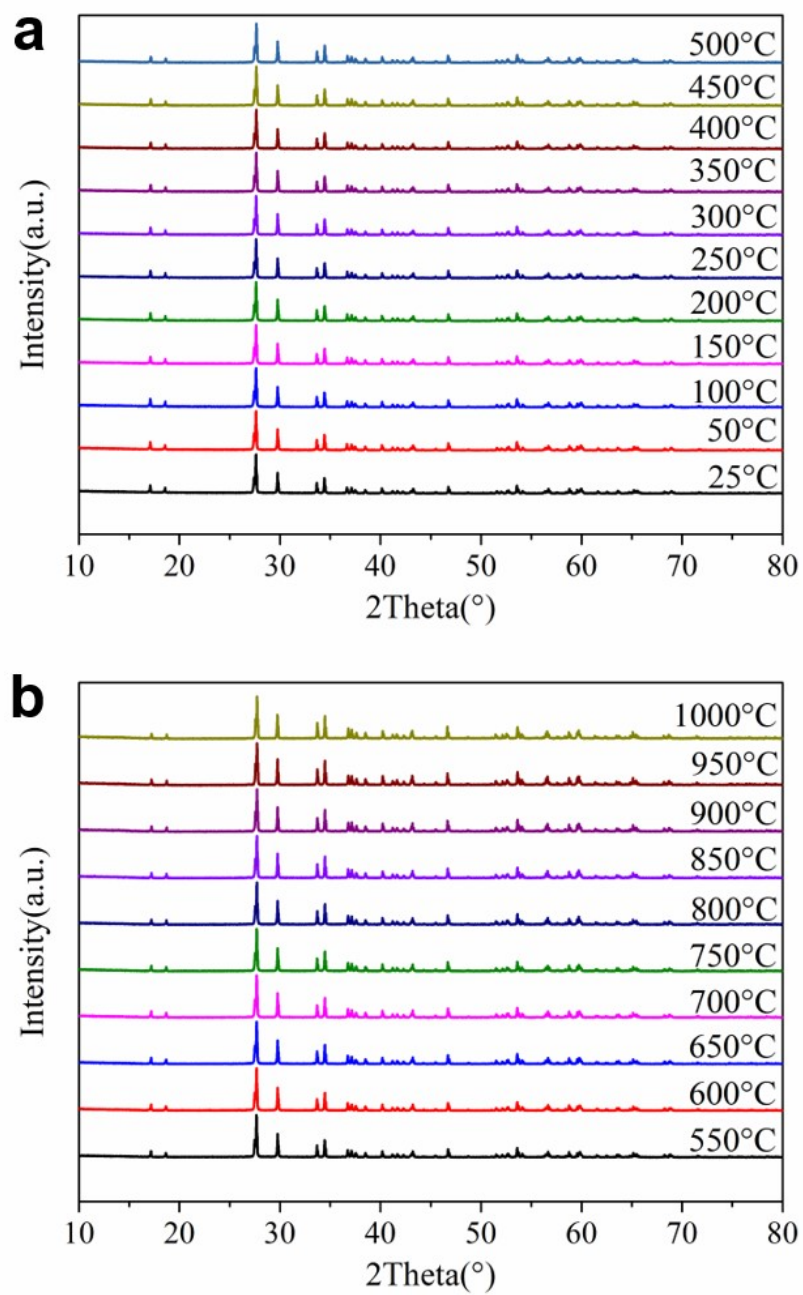


Figure S7. Variable temperature XRD patterns of $\text{In}_{2-x}\text{Zn}_x\text{Ge}_2\text{O}_{7-0.5x}$ ($x = 0.2$) in the temperature region of 25-1000 °C.