Supplementary Materials

Anisotropic Thermal Expansion and Electronic Structure of $LiInSe_2$

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Table S1. Fractional atomic coordinates and isotropic displacement parameters (Å^2) of $LiInSe_2$.

	x	*y*	*z*	B_{iso}
In	0.0774 (2)	0.1259 (9)	0	1.39 (6)
Li	0.077 (5)	0.62 (2)	0.01 (2)	1.7 (9)
Se1	0.0812 (3)	0.127 (2)	-0.3795 (8)	1.13 (6)
Se2	0.4134 (4)	0.122 (2)	0.1275 (8)	1.13 (6)

Table S2. Main bond lengths (Å) of $LiInSe_2$.

In—Se1	2.583 (5)	Li—Se1^{iii}	2.5 (2)
In—Se1^{i}	2.55 (1)	Li—Se1^{iv}	2.58 (5)
In—Se2	2.572 (3)	Li—Se2^{v}	2.6 (1)
In—Se2^{ii}	2.58 (1)	Li—Se2^{ii}	2.5 (2)

Symmetry codes: (i) -*x*, -*y*, *z*+1/2; (ii) *x*-1/2, -*y*+1/2, *z*; (iii) -*x*, -*y*+1, *z*+1/2; (iv) -*x*+1/2, *y*+1/2, *z*+1/2; (v) -*x*+1/2, *y*+1/2, *z*-1/2.

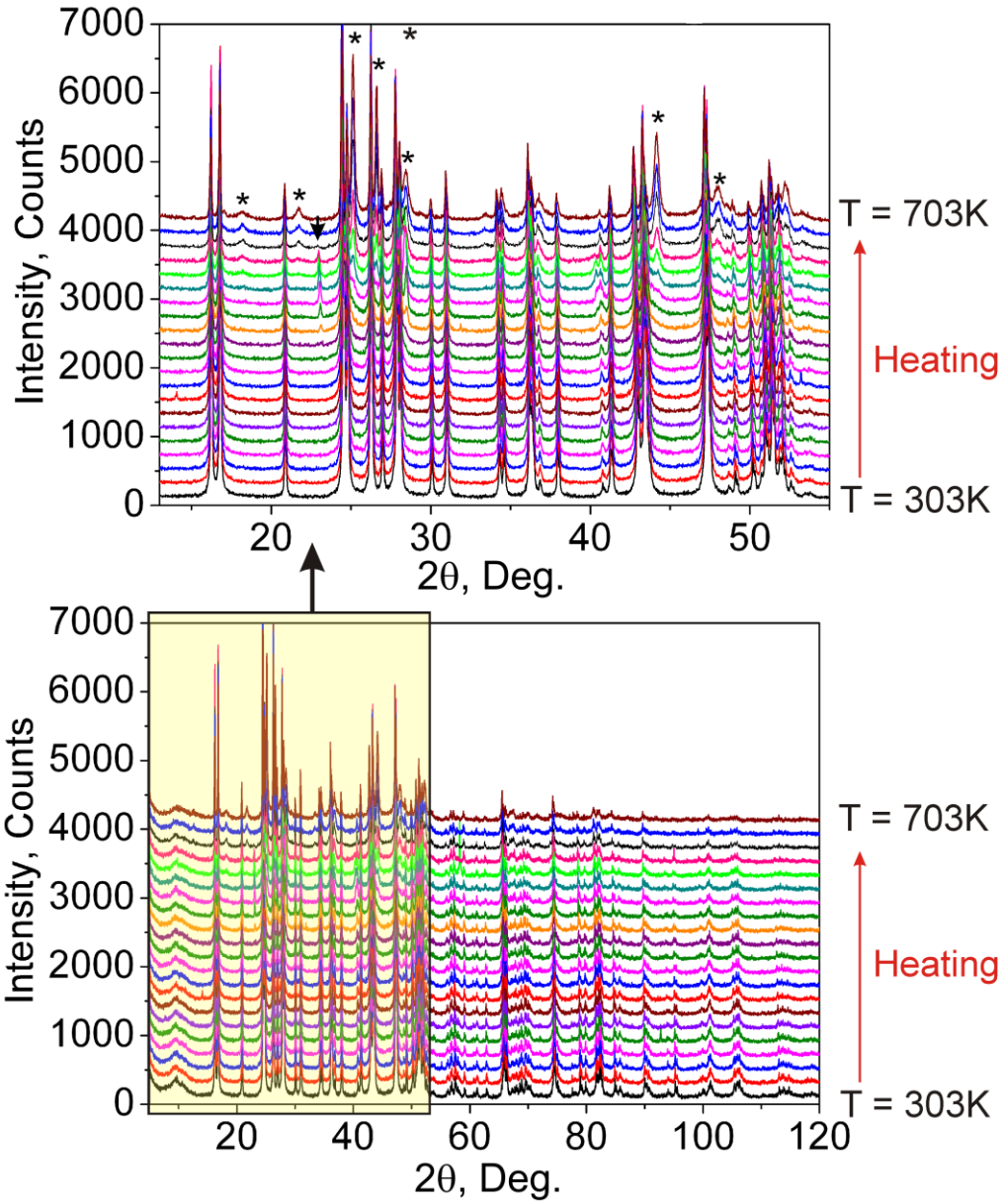


Figure S1. X-ray patterns collected from 303 to 703 K. The major impurity peaks appeared under heating are marked by asterisk and arrow.