Measured and Simulated Thermoelectric Properties of $FeAs_{2-x}Se_x$ (x = 0.30 – 1.0): from Marcasite to Arsenopyrite Structure

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Electronic Supplementary Information

List of Tables and Figures

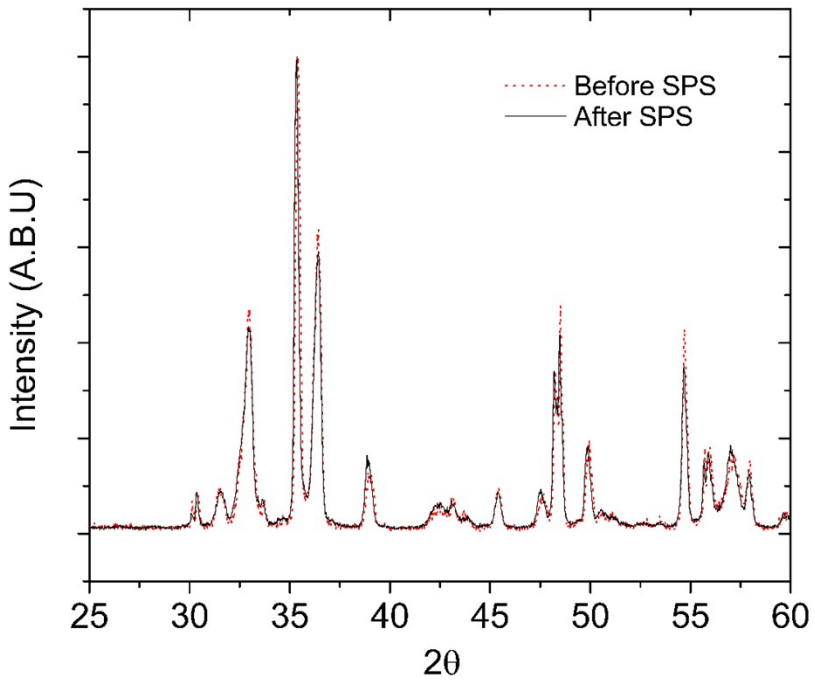

Figure S1: Laboratory (Cu Kα, λ = 1.5406 Å) PXRD patterns before and after SPS.

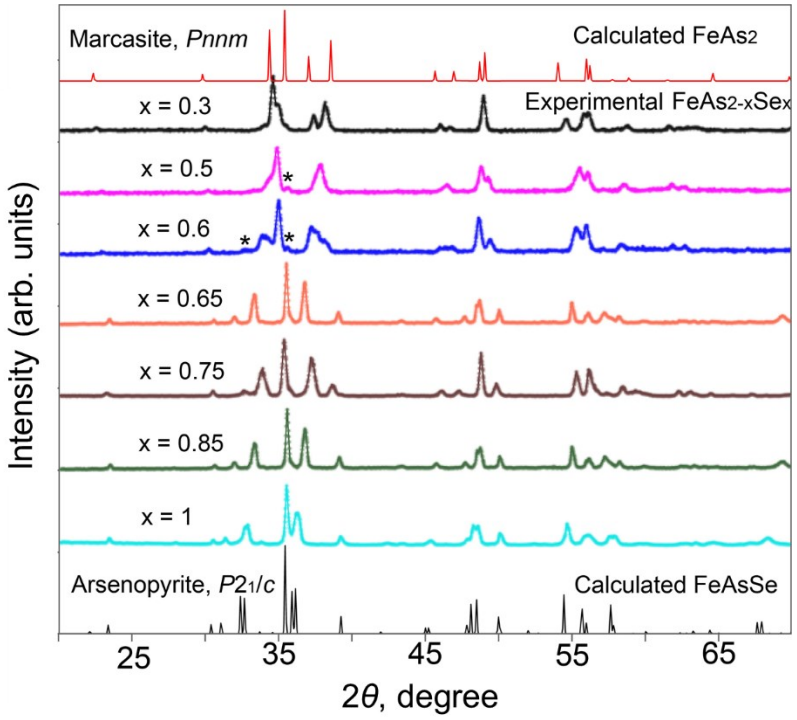

Figure S2: Laboratory PXRD (Cu Kα, λ = 1.5406 Å) patterns of $FeAs_{2-x}Se_x$ (x = 0.30, 0.50, 0.60, 0.65, 0.75, 0.85, 1.0). * represents the peaks of small amount of Arsenopyrite phase.

Table S1. Fractional Positional Coordinates and Anisotropic Thermal Parameters for $FeAs_{1.50}Se_{0.50}$

Label	Wycoff Site	X	Y	Z	Occupancy	U_{11} (Å^2)	U_{22} (Å^2)	U_{33} (Å^2)	U_{23} (Å^2)	U_{13} (Å^2)	U_{12} (Å^2)
Fe1	2a	1/2	1/2	1/2	1.00	0.0039(5)	0.0025(5)	0.0091(5)	0	0	-0.0006(3)
As2	4g	0.31907(9)	0.13693(9)	1/2	0.75	0.0048(3)	0.0031(3)	0.0063(3)	0	0	-0.00047(14)
Se2	4g	0.31907(9)	0.13693(9)	1/2	0.25	0.0048(3)	0.0031(3)	0.0063(3)	0	0	-0.00047(14)

Table S2: Rietveld Refinement Results from Synchrotron PXRD of FeAsSe

Comment	
Nominal formula	FeAsSe
Wavelength (Å)	0.414532
temperature (K)	293 K
Space group	$P2_1/c$
Lattice Parameters *a, b, c, V*	a = 5.95922(6) (Å), b = 5.87517(6) (Å), c = 5.99802(7) (Å), V = 192.499 Å^3, β = 113.5566(5)°
(R_F, GOF)	5.2, 2.1
Site	x, y, z
Fe	0.2720(5), -0.0013(5), 0.2813(4)
As	0.1509(3), 0.6312(3), 0.3666(3)
Se	0.3471(3), 0.3623(3), 0.1713(2)
Fe (Occupancy)	1
As (Occupancy)	1
Se (Occupancy)	0.970(5)

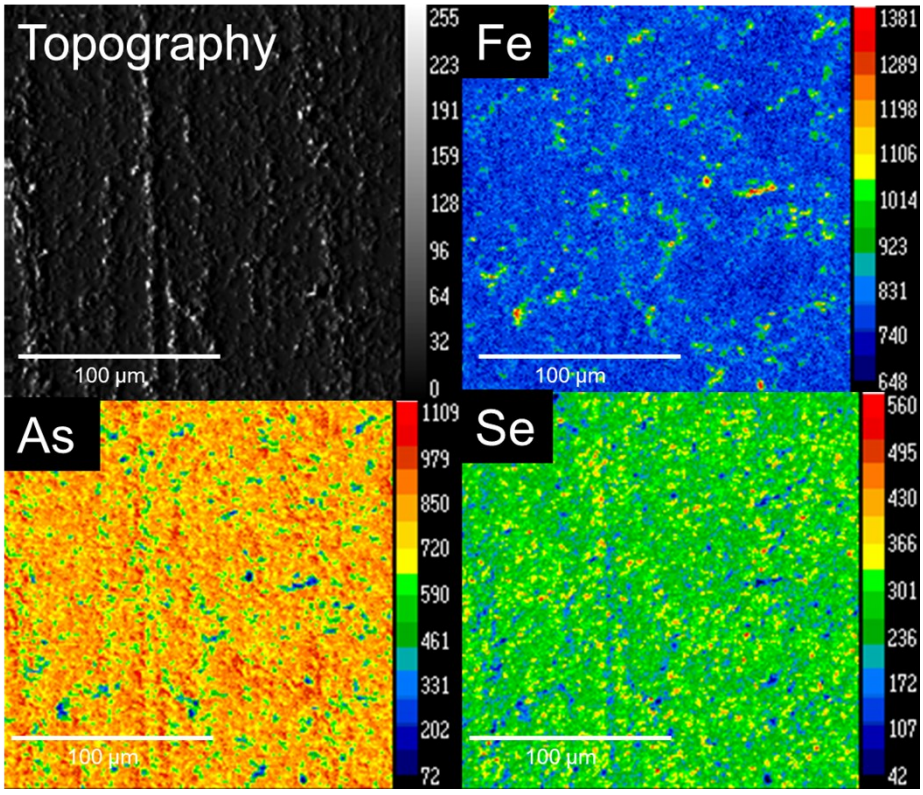

Figure S3: Topological and X-ray elemental maps for polycrystalline FeAsSe.

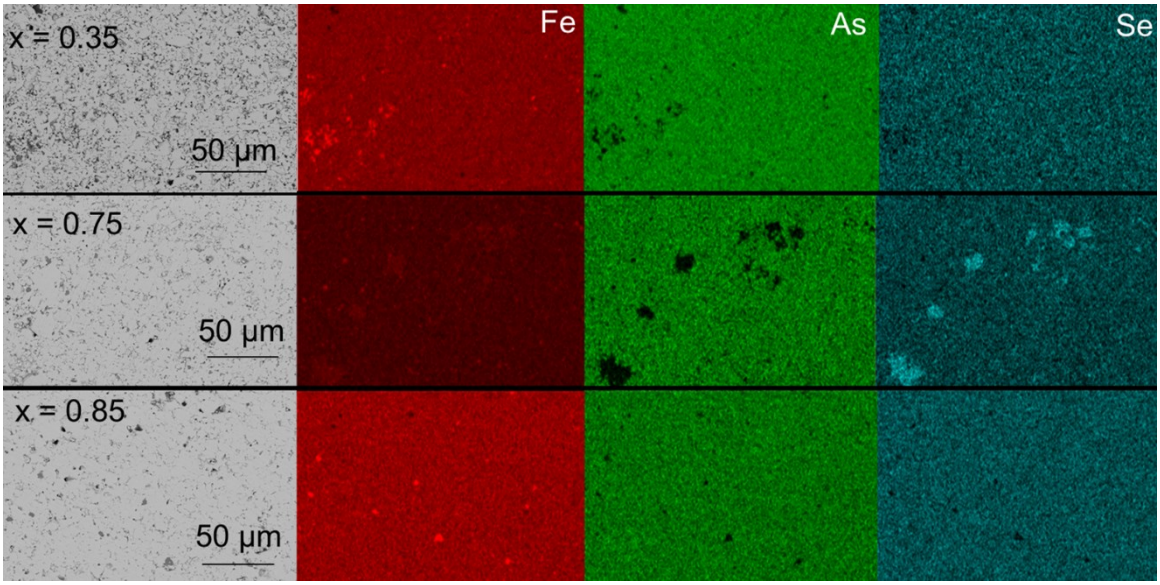

Figure S4: BSE images of $FeAs_{2-x}Se_x$ (x = 0.30, 0.75, 0.85) with Fe, As, and Se X-ray elemental maps.

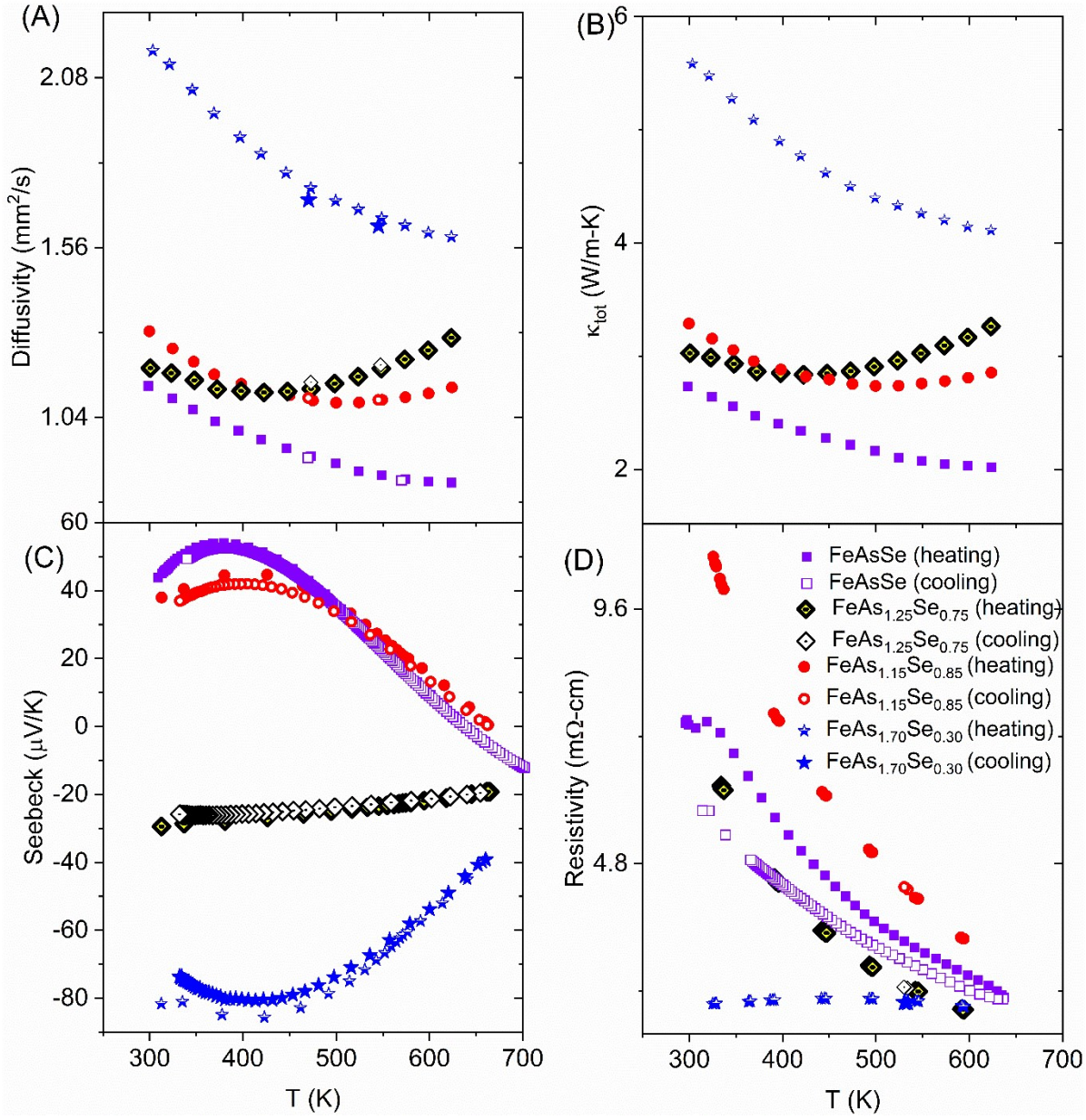

Figure S5: Thermally cycled experimental data showing (A) thermal diffusivity, (B) Thermal conductivity (C), Seebeck, and (D) resistivity for sintered pellets of $FeAs_{2-x}Se_x$ (x = 0.30, 0.75, 0.85).

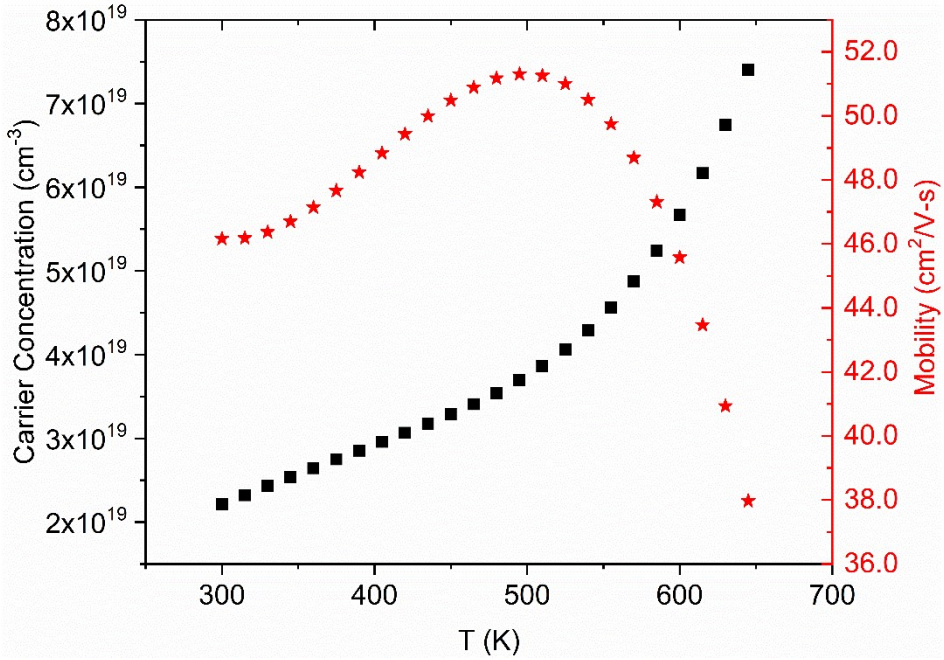

Figure S6: Carrier concentration and carrier mobility of FeAsSe measured on a sintered pellet.

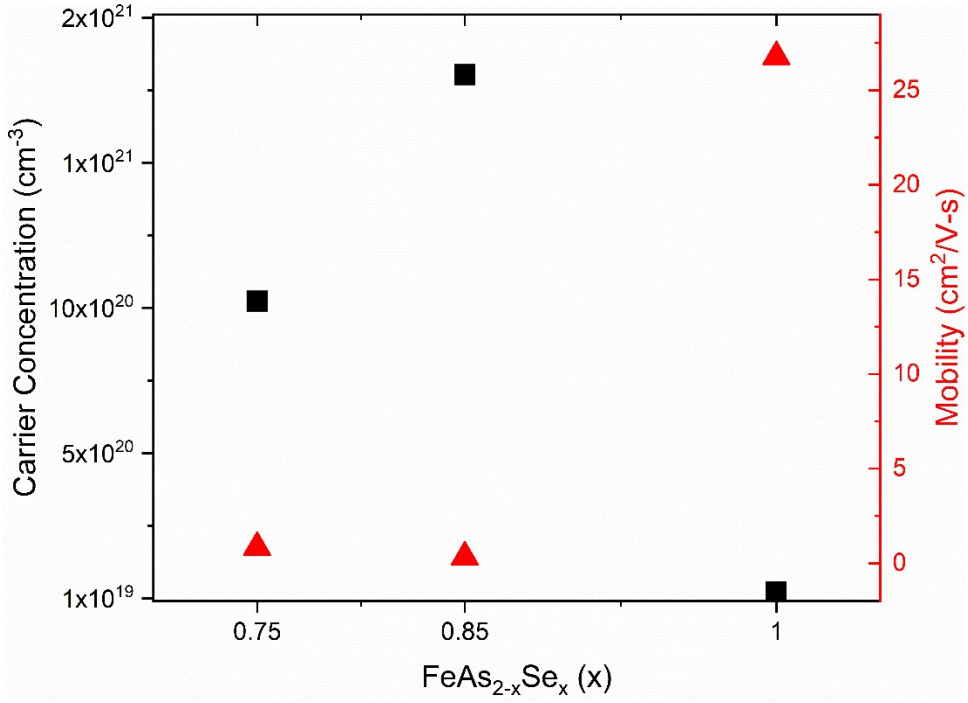

Figure S7: Room temperature carrier concentration and mobility of $FeAs_{2-x}Se_x$ (x = 0.75, 0.85).

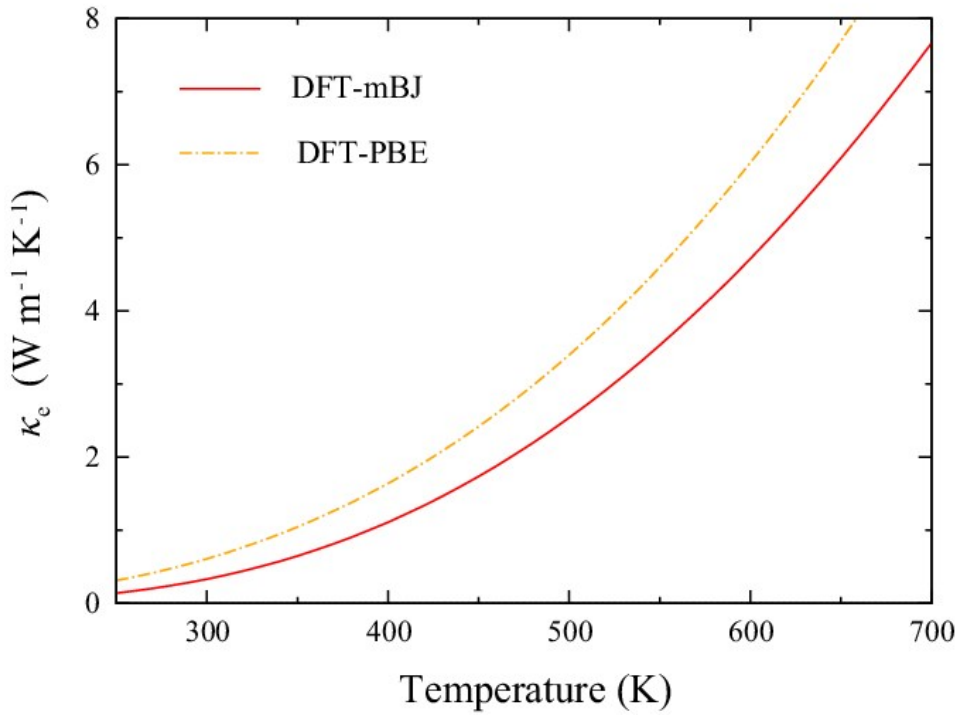

Figure S8: The calculated electronic thermal conductivity of FeAsSe. Two different computational schemes, GGA(PBE) and mBJ, are provided for comparison.