Supporting Information

Structural stability, optical and thermoelectric properties of the layered $RbSn_2Br_5$ halide synthesized using mechanochemistry

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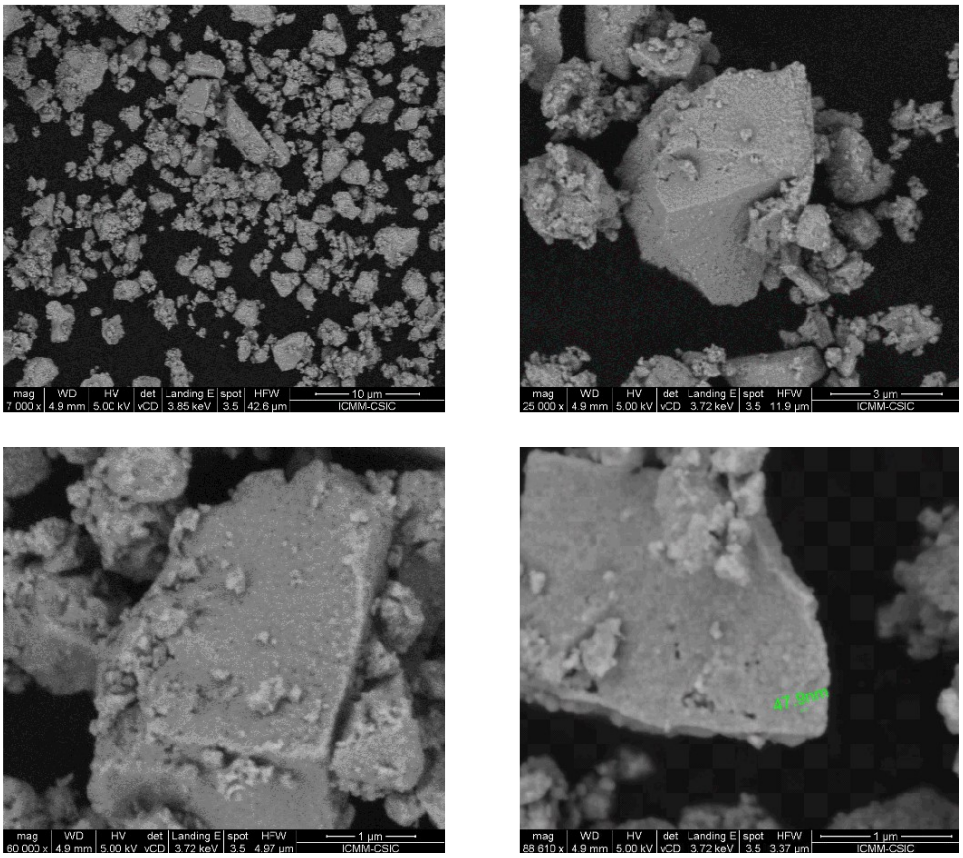

Figure S1: FE-SEM images with **a)** 7,000x, **b)** 25,000x, **c)** 60,000 and **d)** 88,610x magnification.

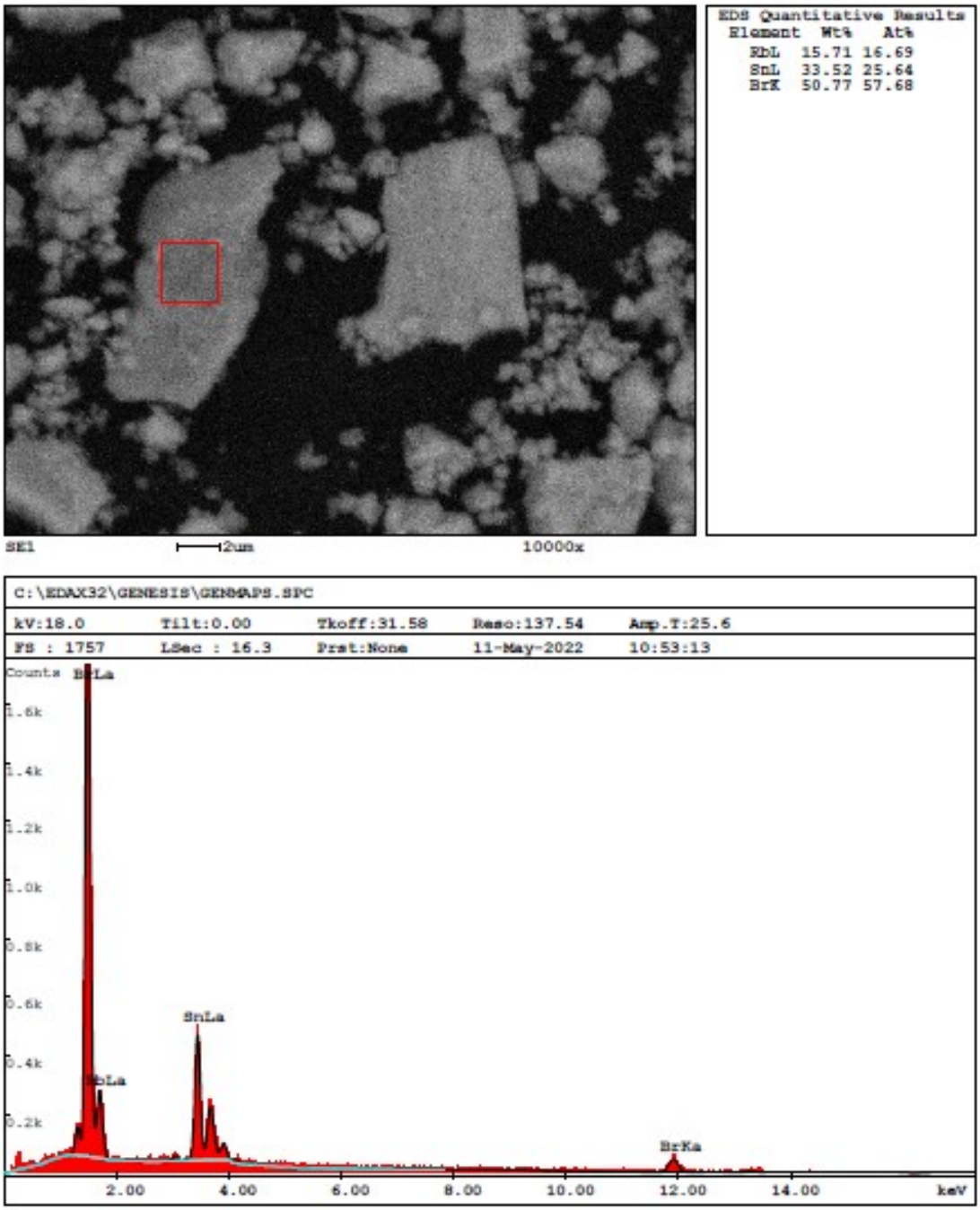

Figure S2. Upper panel: SEM image where the EDX spectrum was collected, and relative contents of Rb, Sn and Br. Lower panel: typical EDX spectrum.

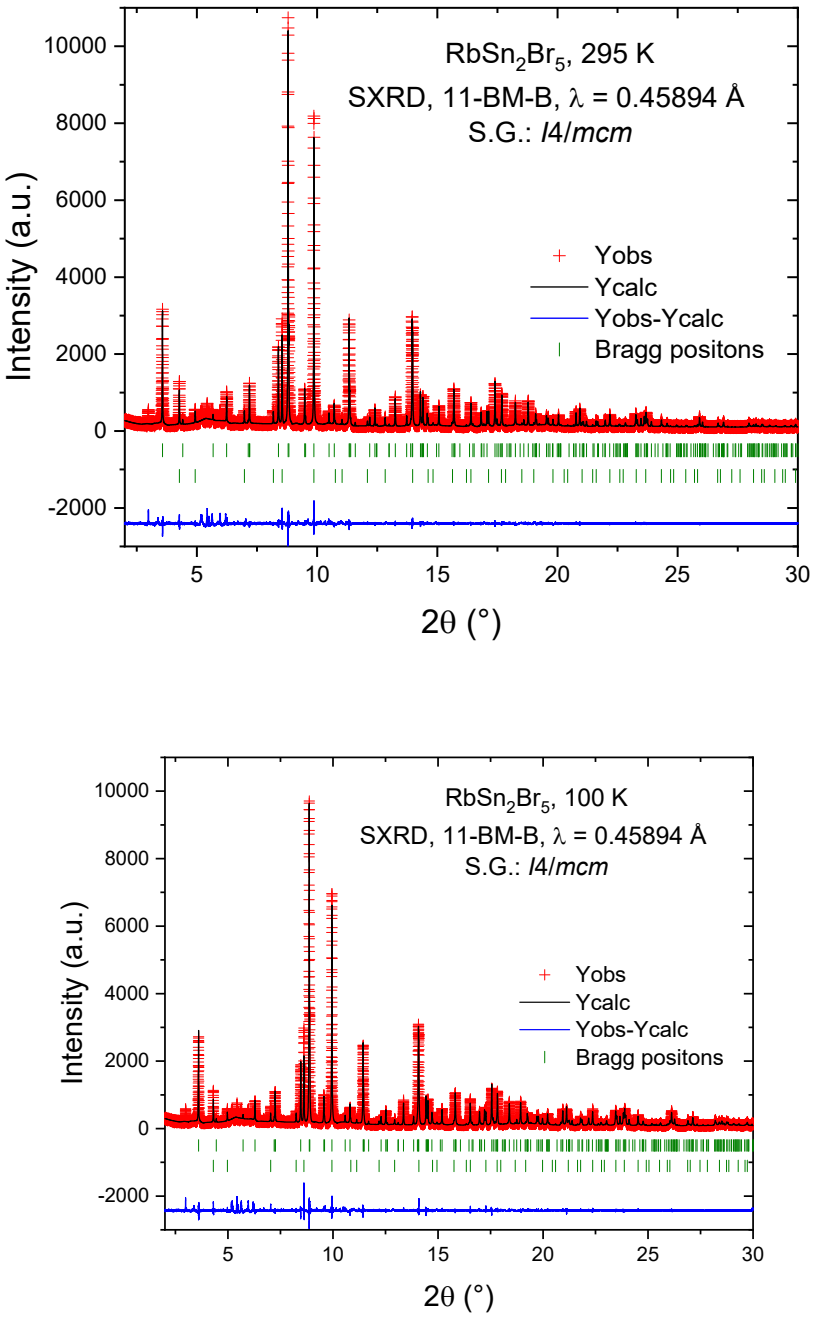

Figure S3. Rietveld refinements from Synchrotron X ray diffractions patterns at 295 and 100 K. The second lines of bars correspond to Rb_2SnBr_6 (Cubic, S.G.: *Fm-3m*) phase, detected and included as impurity in the refinement.

Table S1: Crystallographic parameters for $RbSn_2Br_5$ phase in the tetragonal system (*I4/mcm*) from SXRD data at 295 K. a = 8.43815(3) Å, c = 14.75126(7) Å and V = 1050.33(1) Å^3

	x	y	z	U_{eq}	f_{occ}
Rb	0	0	0.25	0.031(1)	1
Sn	0.17769(9)	0.67769(9)	0	0.0365(6)	1
Br 1	0	0	0	0.023(1)	1
Br 2	0.16161(7)	0.66161(7)	0.36608(5)	0.0239(5)	1
Anisotropic Atomic Displacement Parameters (Å²)					
	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Rb	0.040(1)	0.040(1)	0.032(2)	0	0	0
Sn	0.0329(5)	0.0329(5)	0.0438(9)	−0.0042(8)	0	0
Br 1	0.0131(9)	0.0131(9)	0.043(2)	0	0	0
Br 2	0.0245(4)	0.0245(4)	0.0227(6)	0.0013(7)	−0.0033(4)	−0.0033(4)
R_p = 6.38%, R_{wp} = 8.35%, χ^2 = 1.71, R_{Bragg} = 3.55% Impurity: Rb_2SnBr_6						

Table S2: Crystallographic parameters for $RbSn_2Br_5$ phase in the tetragonal system (*I4/mcm*) from SXRD data at 100 K. a = 8.37171(4) Å, c = 14.61783(8) Å and V = 1024.36(1) Å^3

	x	y	z	U_{eq}	f_{occ}
Rb	0	0	0.25	0.0137(9)	1
Sn	0.17793(9)	0.67793(9)	0	0.0152(5)	1
Br 1	0	0	0	0.0056(9)	1
Br 2	0.16104(7)	0.66104(7)	0.36451(5)	0.0099(4)	1
Anisotropic Atomic Displacement Parameters (Å²)					
	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Rb	0.0168(8)	0.0168(8)	0.007(1)	0.00000	0.00000	0.00000
Sn	0.0124(4)	0.0124(4)	0.0209(7)	0.0005(7)	0.00000	0.00000
Br 1	0.0042(8)	0.0042(8)	0.009(1)	0.00000	0.00000	0.00000
Br 2	0.0095(4)	0.0095(4)	0.0106(5)	0.0015(6)	−0.0001(3)	−0.0001(3)
R_p = 6.80%, R_{wp} = 8.89%, χ^2 = 2.05, R_{Bragg} = 1.99% Impurity: Rb_2SnBr_6						

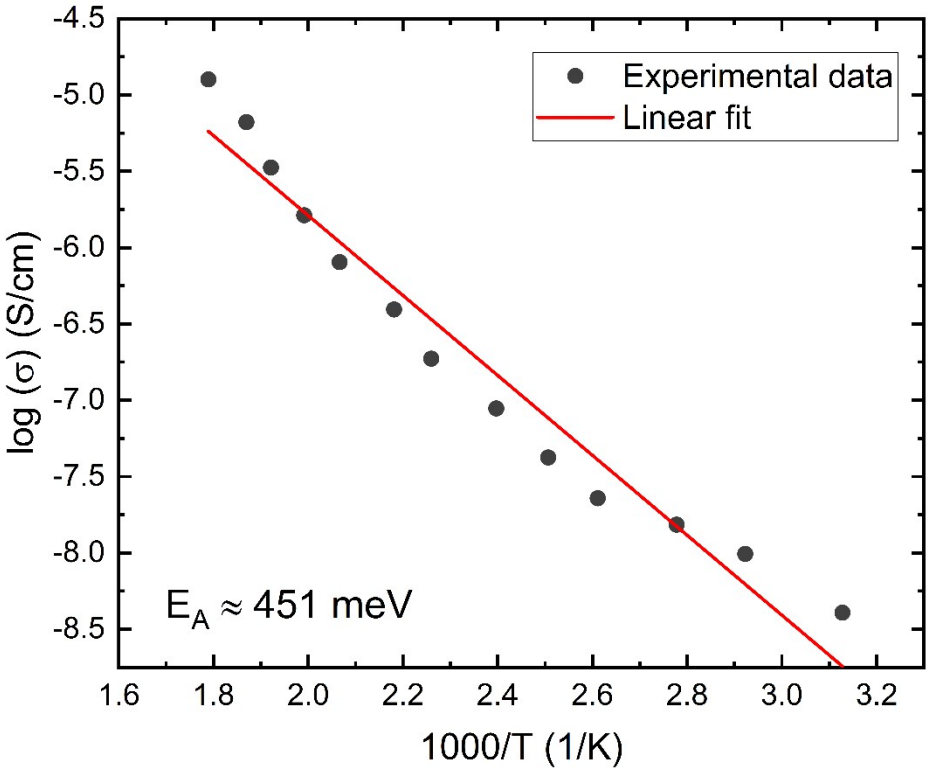

Figure S4. Activation energy for the carriers of the $RbSn_2Br_5$ halide calculated from the measured electrical conductivity.

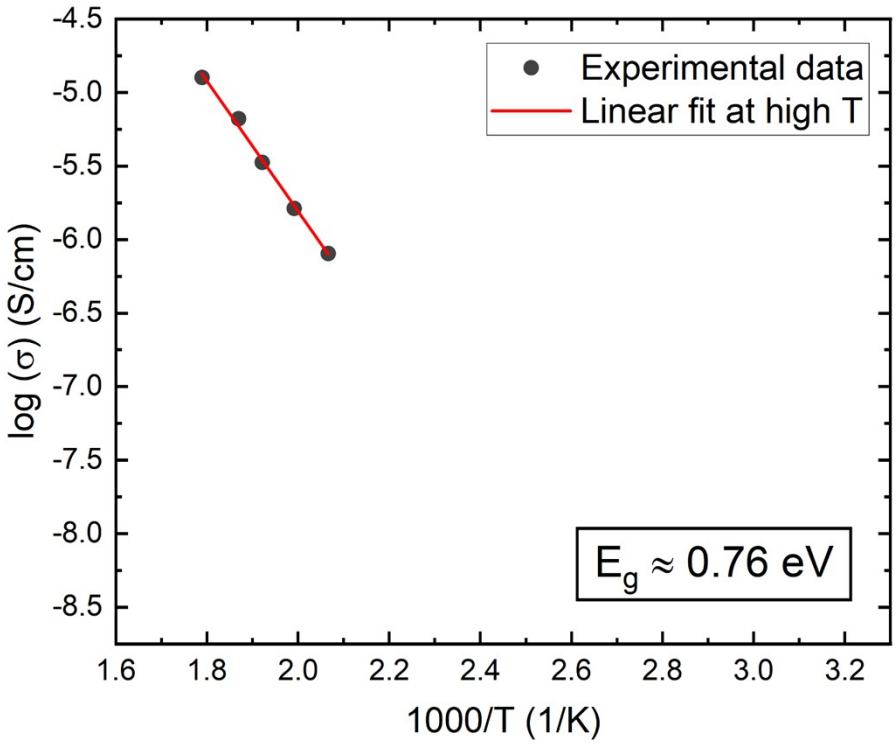

Figure S5. Activation energy for the carriers of the $RbSn_2Br_5$ halide calculated from the measured electrical conductivity at high temperature. The calculated energy band gap is included in the Figure.

Compared with the experimental band gap of ~3 eV obtained from the UV-Vis spectrum, this value is significantly lower, and it is also lower than the one theoretically calculated from the structural model (~2.9 eV). This deviation can be originated by the presence of traps or defects levels in the band gap. For this reason, we can consider the value of ~3 eV offered by the UV-Vis spectrum (which agrees with the calculated one) as the most reliable result.

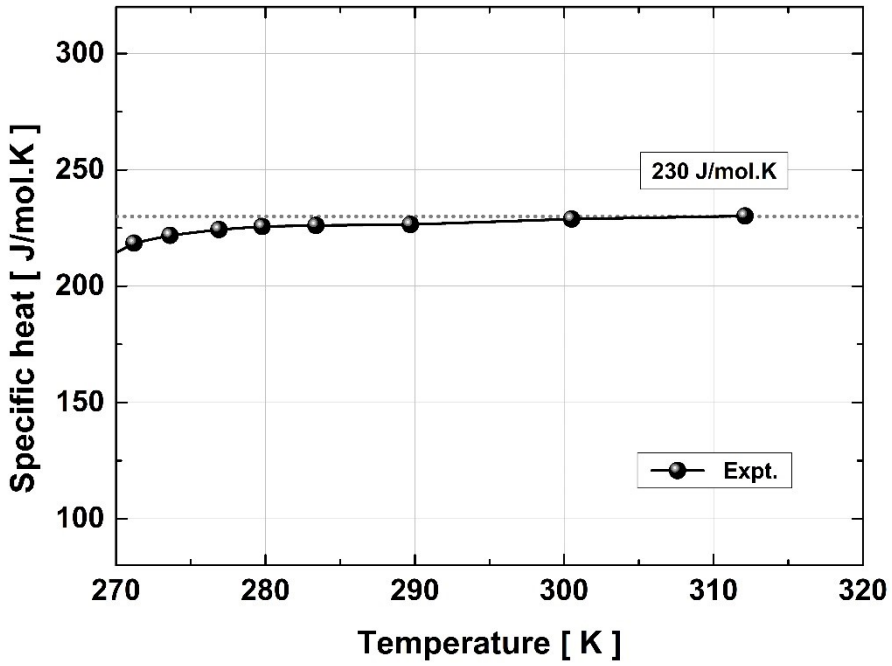

Figure S6. Experimental specific heat of Rb_2SnBr_6 halide (in units of J/mol.K) as derived from heat capacity measurements.

The experimental curve exhibited one plateau in the temperature ranges 270–320 K, converging as $c_p \approx 230$ J/mol.K that is a value estimated from the thermal conductivity using the Dulong-Petit approximation.