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SUPPORTING INFORMATION (ESI)

Structural evolution, optical gap and thermoelectric properties of $RbPb_2Br_5$ layered halide, prepared by mechanochemistry.

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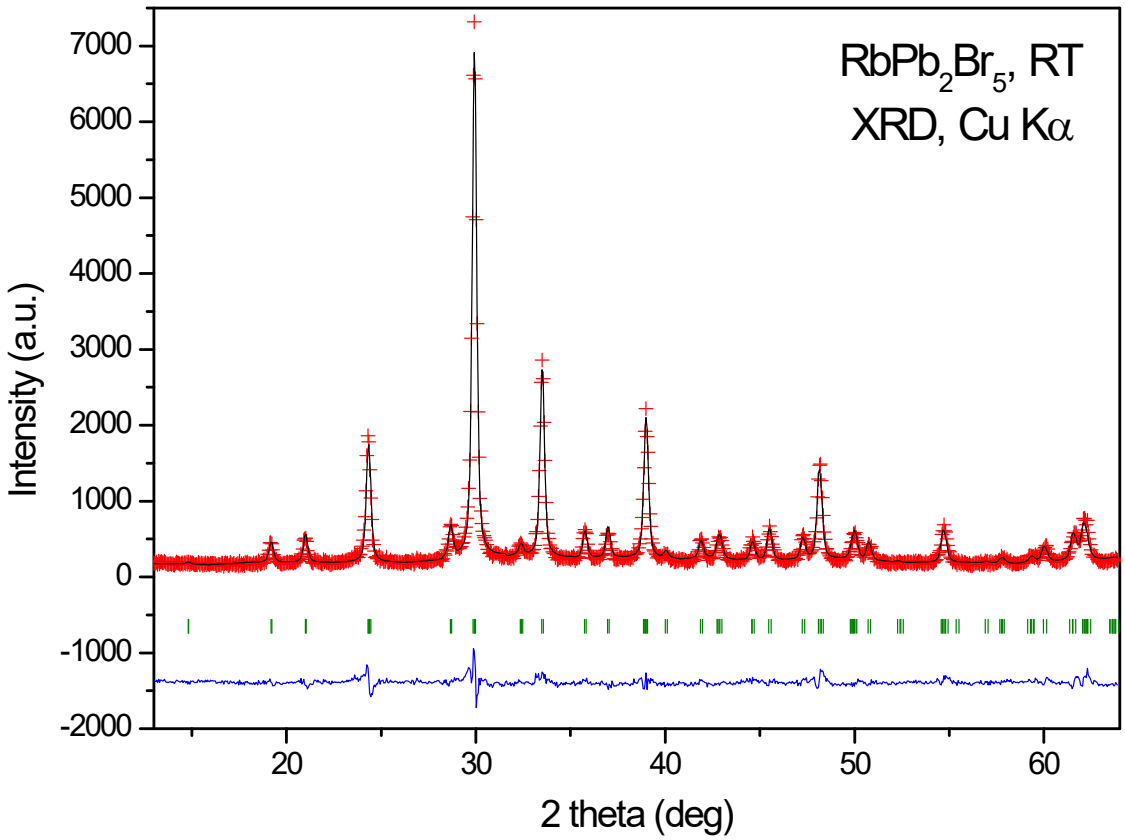


Figure S1. Preliminary refinement of the crystal structure of $RbPb_2Br_5$, prepared by ball milling, in the $(NH_4)Pb_2Br_5$ structural model, from laboratory XRD data, with Cu Kα radiation.

Table S1: Crystallographic data for $RbPb_2Br_5$ refined from NPD data at 15 K.

System: Tetragonal, Space group: *I4/mcm*, Z = 4. Unit-cell parameters: *a* = 8.35800(18) Å, c= 14.3910(4) Å and V = 1005.30(4) Å^3.						
Atom		**x**	**y**	**z**	**U_{iso}**	**Occ**
Rb	4*a*	0	0	0.25	0.0052(12)	1
Pb	8*h*	0.16763(15)	0.66763(15)	0	0.0025 (7)	1
Br1	4*c*	0	0	0	0.0051(13)	1
Br2	16*l*	0.15573(12)	0.65573(12)	0.36318(8)	0.0039(7)	1
R_p: 7.57%; R_{wp}: 8.22%; R_{exp}: 5.35%; χ^2: 2.36; R_{Bragg}: 2.06%						

Table S2: Crystallographic data for $RbPb_2Br_5$ refined from NPD data at room temperature

System: Tetragonal, Space group: *I4/mcm*, Z = 4. Unit-cell parameters: *a* = 8.4365(4) Å, c= 14.5686(7) Å and V = 1036.90(8) Å^3.						
Atom		**x**	**y**	**z**	**U_{iso}**	**Occ**
Rb	4*a*	0	0	0.25	0.0389(15)	1
Pb	8*h*	0.1680(2)	0.6680(2)	0	0.0296(6)	1
Br1	4*c*	0	0	0	0.0277(14)	1
Br2	16*l*	0.15596(19)	0.65596(19)	0.36389(11)	0.0317(7)	1
R_p: 13.09%; R_{wp}: 11.47%; R_{exp}: 8.24%; χ^2: 1.94; R_{Bragg}: 2.06%						

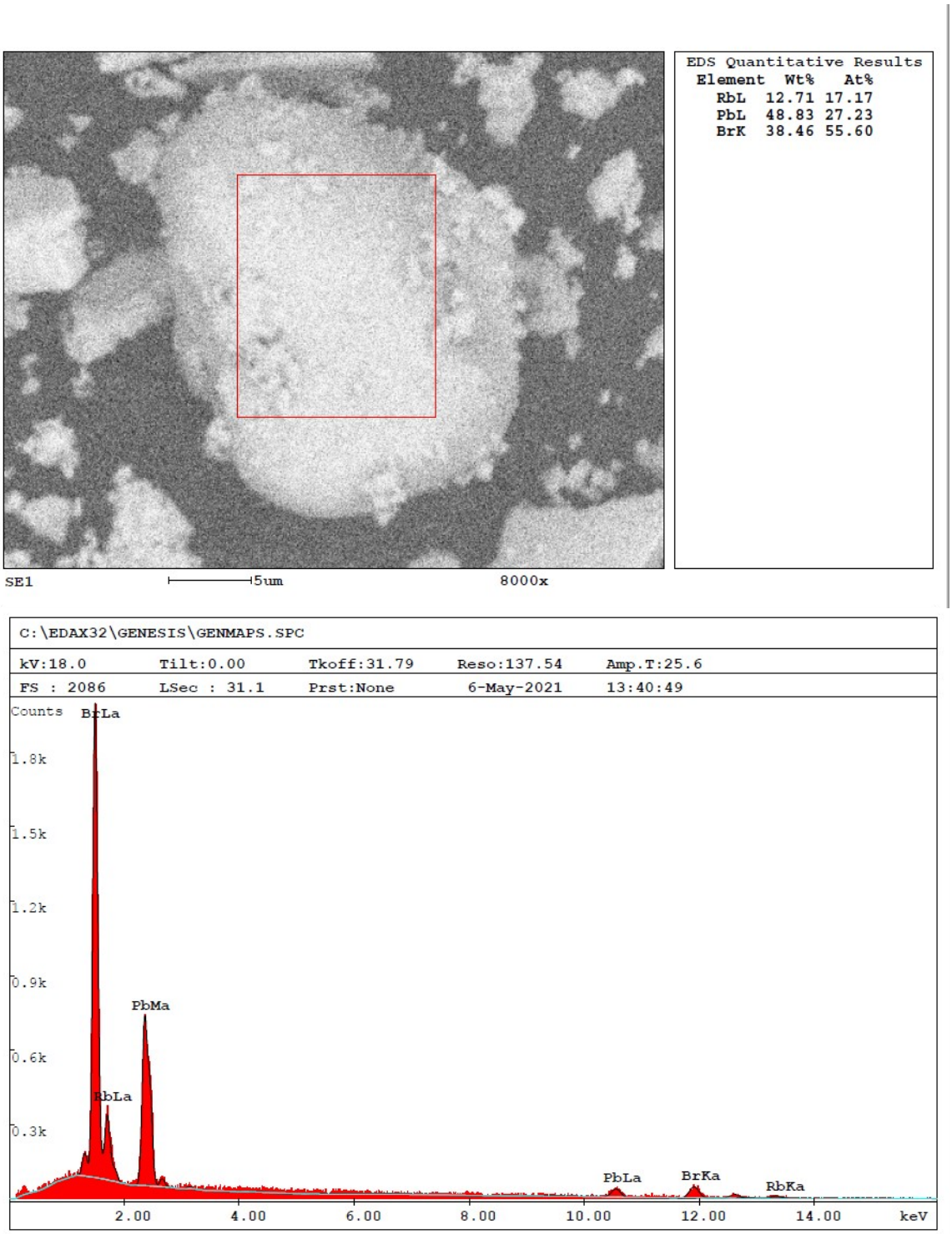
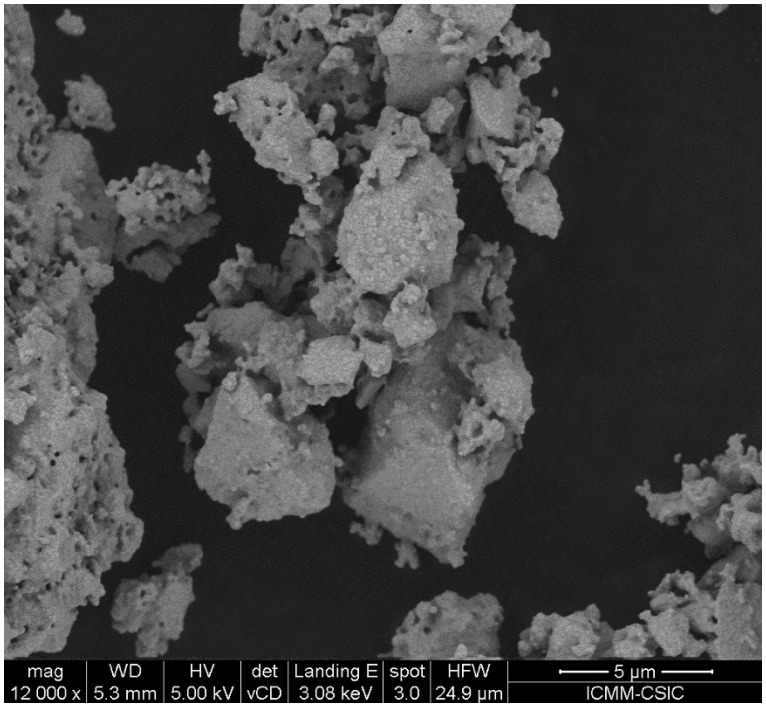


Figure S2. a) SEM image where the EDX spectrum was collected, and relative contents of Rb, Pb and Br, and b) typical EDX spectrum.



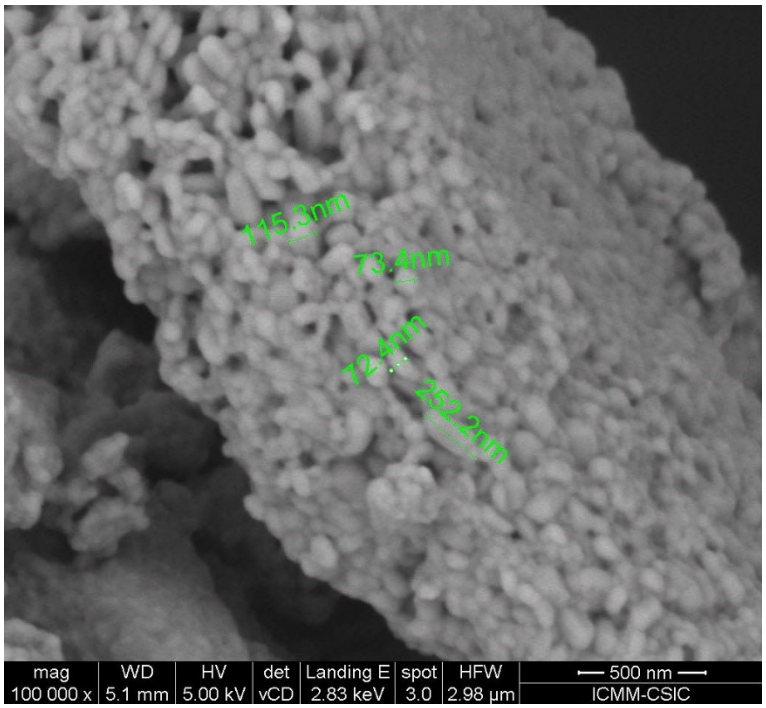


Figure S3. SEM images of $RbPb_2Br_5$ with different magnifications

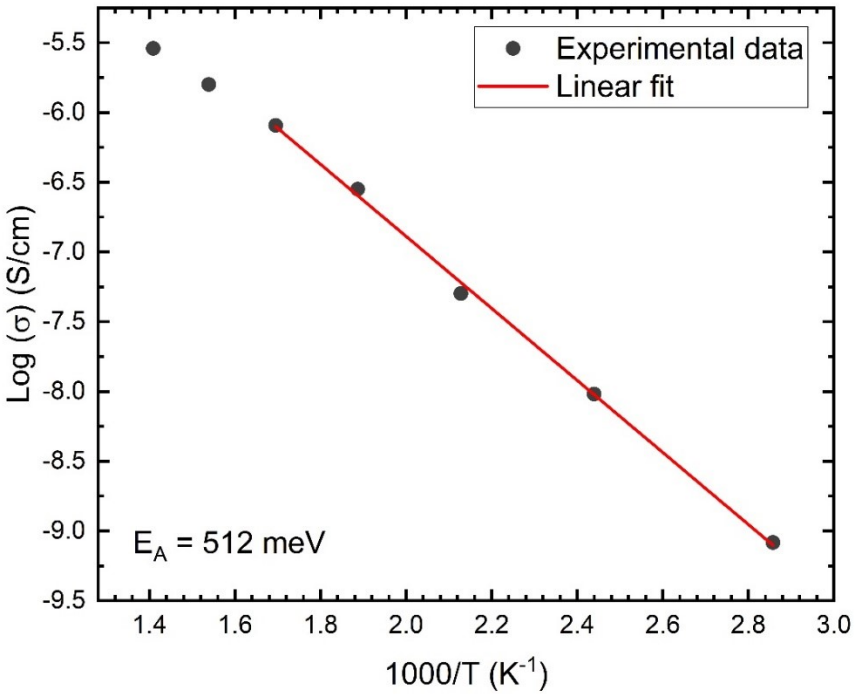


Figure S4. Activation energy for the carriers of the $RbPb_2Br_5$ perovskite calculated from the measured electrical conductivity.

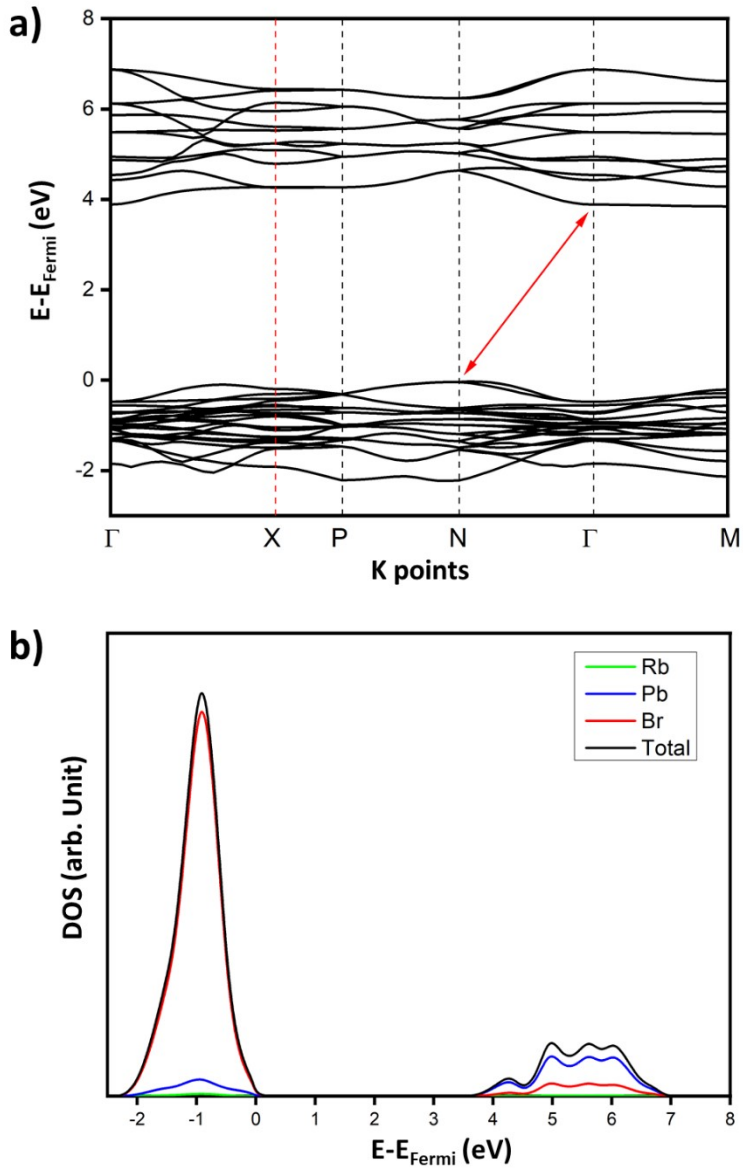


Figure S5. **a)** Band structure and **b)** density of states (DOS) of $RbPb_2Br_5$ halide as determined from DFT-based calculations.