

La₁₂Sb₉S₃₈: A New Semiconducting Lanthanum Antimony Polysulfide with a mixed La/Sb site

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SUPPLEMENTARY INFORMATION

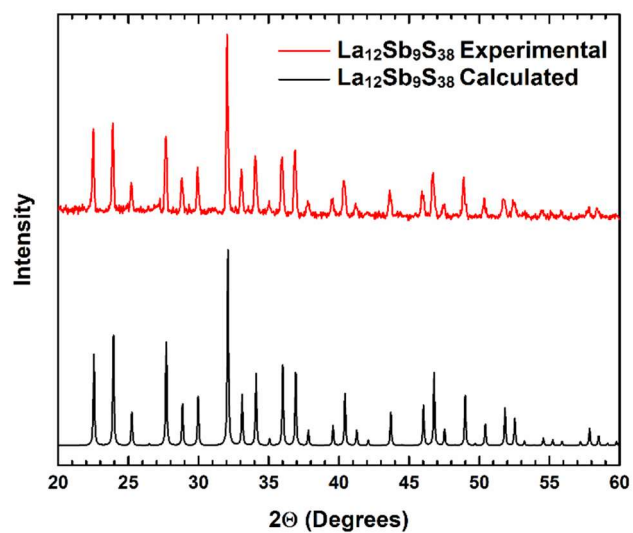


Figure S1. Experimental and calculated X-ray powder patterns of $\text{La}_{12}\text{Sb}_9\text{S}_{38}$.

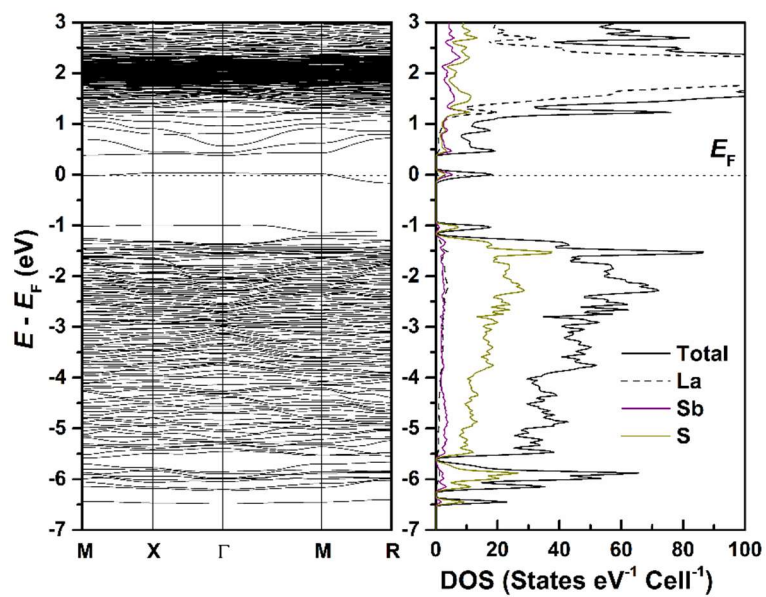


Figure S2. Band structure (left) and density of states (right) of $\text{La}_{12}\text{Sb}_9\text{S}_{38}$.

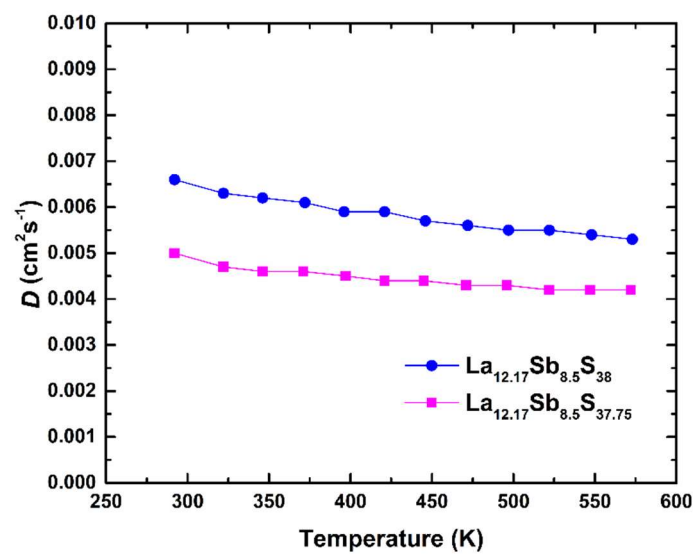


Figure S3. Thermal diffusivity of $\text{La}_{12}\text{Sb}_9\text{S}_{38}$.

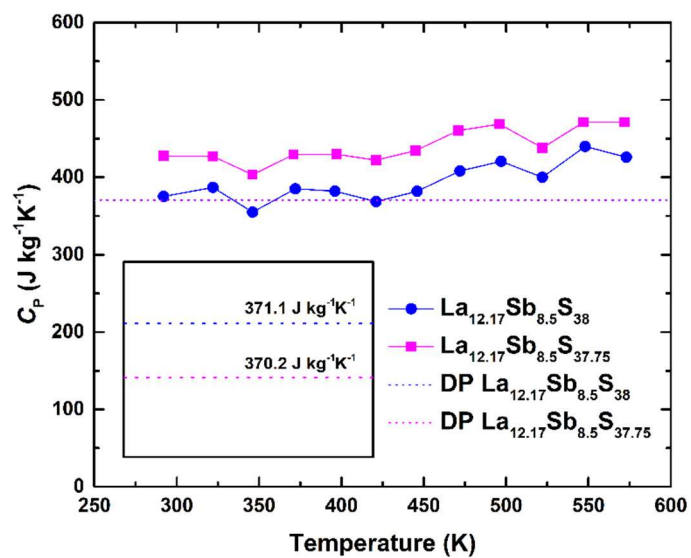


Figure S4. Specific heat of $\text{La}_{12}\text{Sb}_9\text{S}_{38}$ in comparison to the Dulong-Petit (DP) limits.

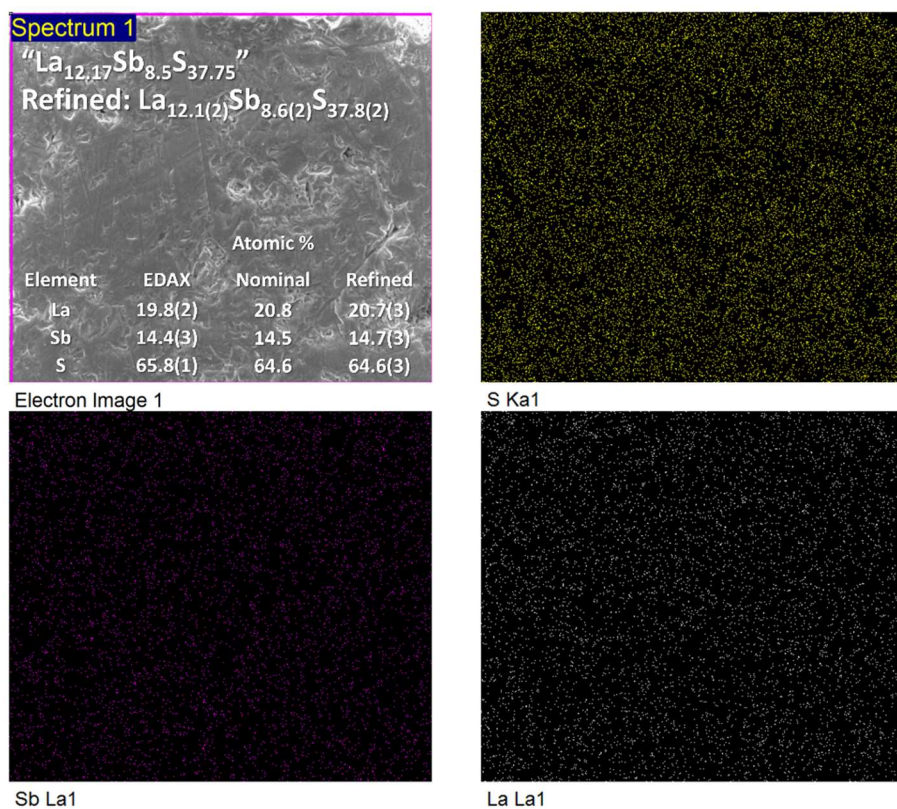


Figure S5. SEM maps and EDX results of the pellet of nominal composition $\text{La}_{12.17}\text{Sb}_{8.5}\text{S}_{37.75}$ in comparison to the formula obtained from the Rietveld refinement.

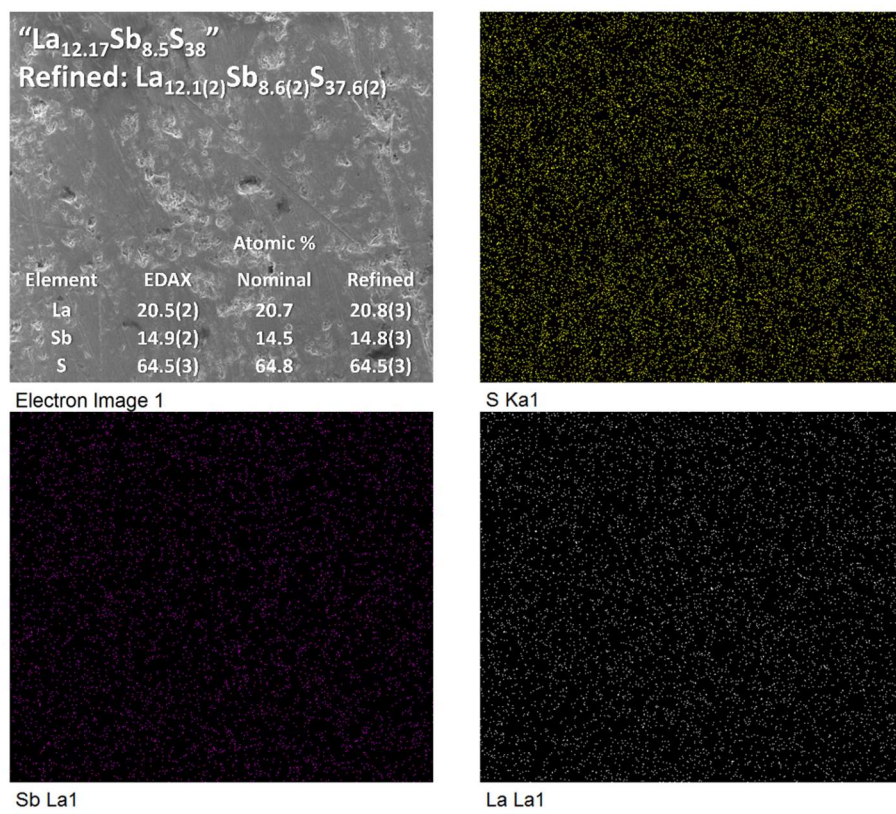


Figure S6. SEM maps and EDX results of the pellet of nominal composition La_{12.17}Sb_{8.5}S₃₈ in comparison to the formula obtained from the Rietveld refinement.

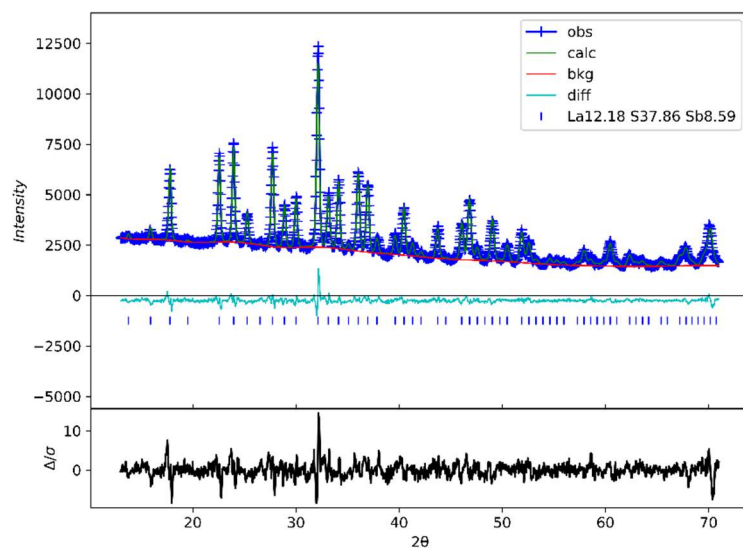


Figure S7. Rietveld refinement of the crushed and ground pellet of nominal composition $\text{La}_{12.17}\text{Sb}_{8.5}\text{S}_{37.75}$.

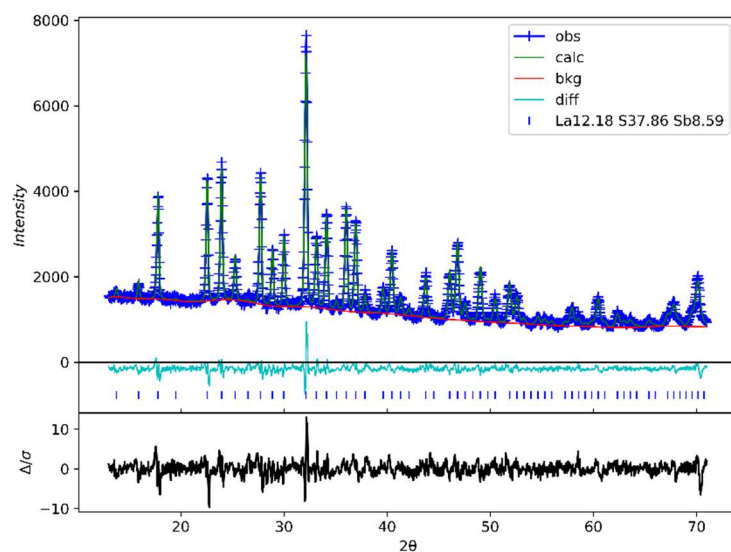


Figure S8. Rietveld refinement of the crushed and ground pellet of nominal composition $\text{La}_{12.17}\text{Sb}_{8.5}\text{S}_{38}$.