



VIRTUAL SEMINAR

Wednesday, 27.10.2021 at 13:00

Synthetic $\text{CuPbBi}_5\text{S}_9$: a semi- ordered cation deficient aikinite key-matrix for high thermoelectric performances

Krishnendu Maji, CRISMAT, CNRS, Normandie Univ, ENSICAEN, UNICAEN, Caen, France

A highly pure semi-ordered cation deficient aikinite mineral type $\text{CuPbBi}_5\text{S}_9$ has been synthesized by combining mechanical alloying and SPS techniques. This synthetic sulphide, though it exhibits characteristics of a highly resistive degenerate semiconductor ($\rho \sim 5 \cdot 10^3 \Omega \text{ cm}$ and $S \sim 1300 \mu\text{V/K}$ at 400K) and of a poor thermoelectric ($ZT \sim 0.04$ at room temperature) is revealed to be an exceptional matrix for generating high thermoelectric performances by doping with Cl or an excess of Bi, leading to a thermoelectric figure of merit of 0.30 - 0.43 at 700 K. The low thermal conductivity of these sulphides is also explained by the fact that their structure is essentially built up of heavy $6s^2$ lone pair cations, Bi^{3+} and Pb^{2+} , and shows significant cationic disordering. It is worth pointing out that the present compound which represents the member $x = 1/3$ of a large series of closely related sulphides $(\text{Cu}_{1-x}\square_x)\text{Pb}_{1-x}\text{Bi}_{1+x}\text{S}_3$ with $0 \leq x \leq 1$ opens the way for the investigation of a broad field of thermoelectric materials by varying the chemical composition and by controlling the order-disorder phenomena in this system.

Kindly invited.

Krishnendu Maji,[a] Pierric Lemoine,[b] Adèle Renaud,[b] Bin Zhang,[c,d] Xiaoyuan Zhou,[c,d] Virginia Carnevali,[e] Christophe Candolfi,[f] Bernard Raveau,[a], Rabih Al Rahal Al Orabi,[e] Marco Fornari,[e] Paz Vaqueiro,[g] Mathieu Pasturel,[b] Carmelo Prestipino,[b] Denis Menut,[h], Emmanuel Guilmeau[a]

[a] CRISMAT, CNRS, Normandie Univ, ENSICAEN, UNICAEN, 14000 Caen, France

[b] Univ Rennes, ISCR – UMR 6226, CNRS, F-35000 Rennes, France

[c] College of Physics and Institute of Advanced Interdisciplinary Studies, Chongqing University, Chongqing 401331, China

[d] Analytical and Testing Center of Chongqing University, Chongqing 401331, China

[e] Department of Physics and Science of Advanced Materials Program, Central Michigan University, Mt. Pleasant, MI 48859, USA

[f] Institut Jean Lamour, UMR 7198 CNRS – Université de Lorraine, 2 allée André Guinier-Campus ARTEM, BP 50840, 54011 Nancy Cedex, France

[g] Department of Chemistry, University of Reading, Whiteknights, Reading, RG6 6AD, United Kingdom

[h] Synchrotron SOLEIL, Ligne MARS, L'Orme des Merisiers, Saint Aubin, 91192 Gif-sur-Yvette, France

