



Seminar/Talk

Insights into the crystal chemistry of thermoelectric sulfides, halides and sulfochlorides

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Thermoelectricity offers a promising solution to address energy scarcity by enabling the efficient conversion of waste heat into useful electricity. Continued research and development in this field can lead to the development of more efficient and cost-effective thermoelectric materials, which can play a significant role in addressing the global energy challenge. The scientific challenge is here to synthesize a material in which the electrical and thermal properties are decoupled. In short, how can we develop an electrical conductor that conducts very little heat? In this context, numerous studies have demonstrated the potential of sulfide materials for thermoelectric applications over the temperature range 300 – 700 K. Although most materials have high thermal conductivities, recent works demonstrated that extremely low thermal conductivities could be achieved in sulfides through order/disorder phenomena, rattling dynamics, and lattice anharmonicity. During this presentation, recent advances in synthetic sulfide minerals, halides and sulfochlorides, will be shown. Some peculiar structural features in connection with materials processing, chemical bonds, lattice vibrations and atomic and nanoscale order/disorder phenomena were carefully examined to establish rules and correlations between the crystal structures, nano-microstructures, electronic structures, vibrational and thermoelectric properties.

[1-5] References [1] P. Lemoine, G. Guérou, B. Raveau, E. Guilmeau, *Angew. Chemie Int. Ed.* 61 (2022) e202108686 [2] K. Maji, P. Lemoine, A. Renaud, B. Zhang, X. Zhou, V. Carnevali, C. Candolfi, B. Raveau, R. Al Rahal Al Orabi, M. Fornari, P. Vaquero, M. Pasturel, C. Prestipino, E. Guilmeau, *J. Amer. Chem. Soc.* 144 (2022) 1846 [3] X. Shen, K. Pal, P. Acharyya, B. Raveau, P. Boullay, O. I. Lebedev, C. Prestipino, S. Fujii, C. Yang, I-Y. Tsao, A. Renaud, P. Lemoine, C. Candolfi, E. Guilmeau, *J. Amer. Chem. Soc.* 2024 [4] P. Acharyya, K. Pal, B. Zhang, T. Barbier, C. Prestipino, P. Boullay, B. Raveau, P. Lemoine, B. Malaman, X. Shen, A. Renaud, B. Uberuaga, C. Candolfi, X. Zhou, E. Guilmeau, *J. Amer. Chem. Soc.* 146 (2024) 13477 [5] Z. Zeng, X. Shen, R. Cheng, O. Perez, N. Ouyang, Z. Fan, P. Lemoine, B. Raveau, E. Guilmeau, Y. Chen, *Nature Comm.* 15 (2024) 3007

Friday, February 14, 2025 10:30am - 11:30am

Sunstone Bldg / Ground floor / Big Seminar Room A



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