MS18-P08 | Structure and Thermoelectric Characterization of Lithium-substituted Bismuth Palladium Oxide

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Over the last decades, thermoelectric (TE) oxides have gained increasing interest as potential materials for the direct conversion of waste heat into electricity for applications in the mid- to high temperature range up to 1200°C. To overcome a major drawback of oxides - a typically low electrical conductivity σ - the use of square planar structural motifs has recently been theoretically proposed based on an inverse band structure design approach [1] and, in combination with stereo-chemically active lone-electron pairs on heavy constituent atoms, the system Bi_2PdO_4 has been proposed as a promising TE oxide [2]. The material is predicted to display an intrinsically low thermal conductivity and good electrical properties, specifically a high power factor $PF=\sigma S^2$ attainable upon hole doping. In this talk, I will present experimental work on the synthesis of polycrystalline and bulk samples of Bi_2PdO_4 and Li-substituted $Bi_2Pd_{1-x}Li_xO_4$ and report on their structural characterization by means of powder X-ray and high-resolution neutron diffraction measurements. I will further discuss the results of our macroscopic characterization of the TE properties which show that the experimental validation of theoretical predictions is a crucial step towards a better understanding and proper design of novel TE materials.

[1] E.B. Isaacs and C. Wolverton, Chem. Mater. 2018, 30, 1540-1546
[2] J. He et al., Chem. Mater. 2017, 29, 2529-2534