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I. Institute of Physics (IA)
Nanocharacterization for advanced functional materials
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Topic for a Master's Thesis

„Thermoelectric ZnSb empowered by metavalent bonding"

INTRODUCTION…

Thermoelectric materials provide a promising solution to convert waste heat into electricity and facilitate the goal of carbon-neutrality in the next decades. As early as 1959, Ioffe et al. built a kerosene lamp generator using ZnSb as the p-type leg and PbS as the n-type leg to generate 80-90 volts to operate a portable radio, see the Figure. The first semiconductor thermoelectric cooler was also made of ZnSb and PbTe. With the renaissance of thermoelectric research in recent decades, the thermoelectric figure-of-merit, zT, of PbS and PbTe has been enhanced from about 1 to 2 due to the deep understanding of the intrinsic properties of materials such as the energy band structure, anharmonicity, and chemical bonding mechanism. In contrast, the development of ZnSb is much slower maybe due to the less knowledge of the fundamental properties of this compound.

The outstanding thermoelectric transport properties of PbS and PbTe, such as the high electrical conductivity, optimal bandgap, and low thermal conductivity, can be attributed to the metavalent bonding mechanism [1]. Thus, it would be very interesting to study the chemical bonding mechanism of ZnSb. Atom probe tomography results show a high value of "probability of multiple events" (PME) for ZnSb, as shown in the figure, which is an indicator of metavalent bonding [1]. More chemical-bonding fingerprints, such as the optical dielectric constant, the Born effective charge, and the number of electrons transferred and shared [2] between Zn and Sb, should be characterized to corroborate the unconventional chemical bonding mechanism. In turn, the thermoelectric properties of ZnSb could be further improved by rationally choosing dopants to modify the chemical bonding mechanism.

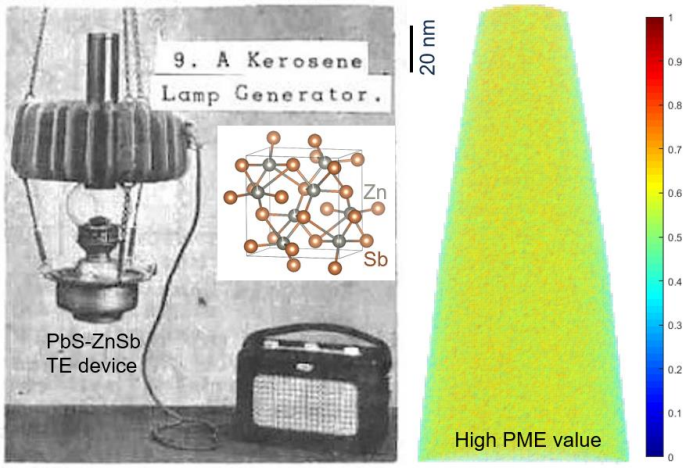

Figure. The first semiconductor thermoelectric generator made of PbS and ZnSb by Ioffe in 1959. Inset is the atomic arrangement of ZnSb. The high PME value measured by APT indicates the abnormal bond-breaking and chemical bonding mechanism.

THESIS DETAILS…In this Master thesis, we will focus on **the chemical bonding mechanism of ZnSb. The bonding fingerprints such as the optical dielectric constant, the Born effective charge, and the bond-breaking behavior will be studied. Finally, the thermoelectric transport properties will be measured by TTO option with PPMS and to correlate the bonding mechanism.** All the characterization techniques (FTIR, atom probe tomography, and PPMS with TTO) necessary to obtain a successful Master thesis are available at I. Institut of Physics, RWTH Aachen University.

References:

1 Yu et al., Adv. Funct. Mater. **2020**, *30*, 1904862.
2 Kooi et al., Adv. Mater. **2020**, *32*, 1908302.

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