I. Physikalisches Institut (IA)
Physik neuer Materialien
RWTH AACHEN UNIVERSITY

I. Institute of Physics (IA)
Nanocharacterization for advanced functional materials
Dr. rer. nat. Yuan Yu

Topic for a Master's Thesis

„Elemental Te thermoelectrics empowered by metavalent bonding"

INTRODUCTION…

Thermoelectric materials can convert heat into electricity for green energy applications. Elemental Te is a promising thermoelectric material working between room temperature and 600 K with an optimized carrier concentration of 10^{19} cm^{-3}. Pristine pure Te has a low carrier concentration of ca. 10^{17} cm^{-3}, resulting in a low power factor. To increase the carrier concentration, aliovalent doping is typically used in semiconductors. However, extensive research proves that **the carrier concentration of Te can only be effectively optimized by doping As, Sb, and Bi**.

Our previous study shows that **the thermoelectric performance has a close relationship to the chemical bonding mechanism**. Different bonding mechanisms can be distinguished by a unique combination of physical properties. For example, the metavalently bonded compounds show large dielectric constant, large Born effective charge, strong anharmonicity, and a unique bond-breaking behavior with high probability of multiple events characterized by atom probe tomography (APT). Moreover, these bonding mechanisms are well separated on a map coordinated by electrons transferred and shared. As shown in Figure 1, all metavalent compounds are located in the green area as superior thermoelectrics. Interestingly, β-As_2Te_3, Sb_2Te_3, and Bi_2Te_3 all employ metavalent bonding. This implies that **the improved performance of Te by doping As, Sb, and Bi might result from the formation of metavalently bonded compounds**.

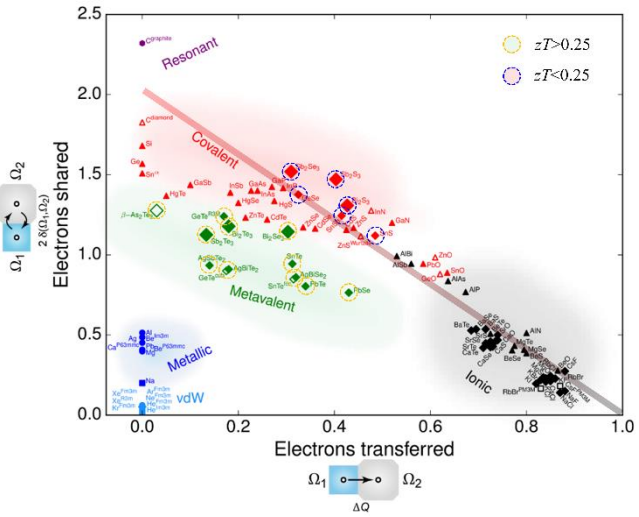

Figure 1: A 2D map of electronic interactions and bonding in materials. Metavalently bonded compounds show zT above 0.25 outperforming other compounds with different bonding mechanisms.

THESIS DETAILS…In this Master thesis, we will **characterize the microstructures by XRD and EDS, measure the optical properties by Ellipsometry and FTIR, and investigate the bond breaking by APT for pure Te and As-, Sb-, and Bi-doped Te**. We then correlate the thermoelectric properties to chemical bonding. Results can help us to design thermoelectrics by selecting promising alloying candidates from the green area of the map. **One $AgSbTe_2$ alloyed Te sample will also be investigated to verify our conclusion**. All the characterization techniques 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 Lin et al., Nat. Commun. **2016**, *7*, 10287.
3 Kooi et al., Adv. Mater. **2020**, *32*, 1908302.

Dr. rer. nat. Yuan Yu
yu@physik.rwth-aachen.de
28A 511 0241 / 80 20335