I. Physikalisches Institut (IA)
Phasenwechselmaterialien
Prof. Dr. rer. nat. Matthias Wuttig

Topic for a Master's Thesis

„Deciphering the Chemical Bonding Mechanism in Layered Bismuth Oxytelluride "

INTRODUCTION…

The Bismuth Oxychalcogenides (Bi_2O_2X, X=S, Se, Te) are potential candidates in various fields such as Thermoelectrics, Ferroelectrics, Piezoelectrics, and photodetectors due to the presence of unique 2D layered structure, i.e., the bismuth oxide layer and chalcogen layer [1]. The relationship between bonding mechanisms and material properties offers a versatile platform for tailoring electronic and phononic properties, potentially leading to other functional characteristics. There are many theoretical and experimental bonding descriptors such as electron transferred and shared values, born effective charge, electrical conductivity, optical dielectric constant, Grüneisen parameter, and Probability of Multiple events (PME). There properties help us to understand the bonding mechanism in Bismuth Oxychalcogenides.

The chemical bonding mechanisms can be separated by the number of electrons transferred and shared between adjacent atoms, as illustrated in Figure 1. Besides the conventional metallic, ionic and covalent bonding, there is another bonding mechanism on the map called metavalent bonding [2]. Many tellurium-related systems like SnTe, GeTe, and PbTe show metavalent bonding. Therefore, it will be interesting to decipher the chemical bonding mechanism with the help of bonding descriptors and find the position of Bi_2O_2Te in the ES and ET map.

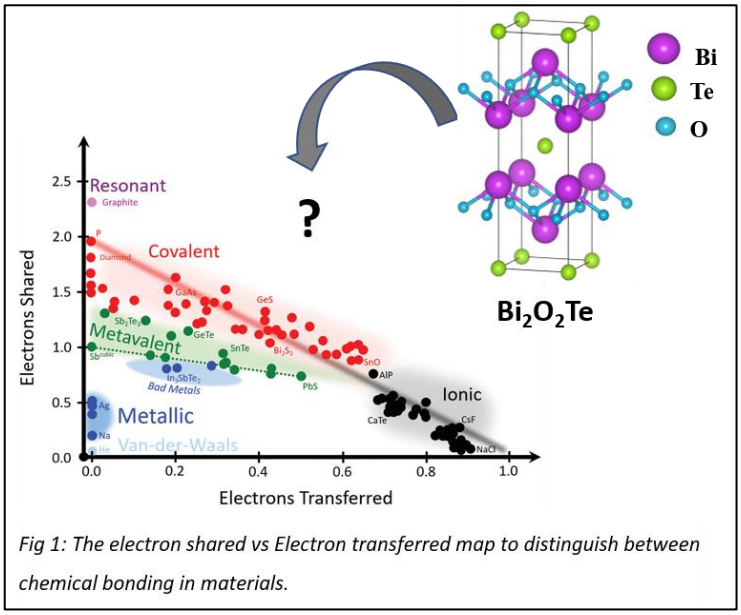

Fig 1: The electron shared vs Electron transferred map to distinguish between chemical bonding in materials.

THESIS DETAILS… In this Master's thesis, we will focus on the chemical bonding mechanism of Bi_2O_2Te. The bonding fingerprints such as the electrical conductivity, optical dielectric constant, the Born effective charge, Grüneisen parameter, Electron shared and transferred values, and PME will be explored. All the theoretical and experimental characterization tools (PPMS, FTIR, and APT) necessary for the successful accomplishment of a Master's thesis are available at I. Institute of Physics, RWTH Aachen University.

References:

[1] Wang et al., InfoMat. 2021; 3:1251–1271.
[2] Kooi et al., Adv. Mater. 2020, 32, 1908302.

M.Sc Sumayya
✉ sumayya@physik.rwth-aachen.de
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