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Physik neuer Materialien
RWTH AACHEN UNIVERSITY

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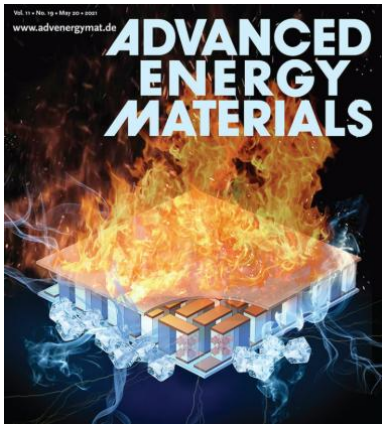
Topic for a Master's Thesis

„Correlating Thermoelectric Performance with Chemical Bonding in 1–2–2 Zintl Phase Materials"

INTRODUCTION…



Thermoelectric materials enable direct solid-state conversion between heat and electricity and play an important role in waste-heat recovery and sustainable energy technologies. Recent advances in high-performance thermoelectric systems such as PbTe, SnTe, and GeTe have revealed that their exceptional transport properties originate from a distinct **metavalent bonding mechanism**. This unconventional bonding regime is characterized by partially delocalized electrons, large optical dielectric constants, anomalously high Born effective charges, soft phonon modes, and strong lattice anharmonicity, which together lead to high carrier mobility and intrinsically low lattice thermal conductivity.

In comparison, **1–2–2 Zintl phase materials**, with the general formula AM_2X_2 (A = alkaline-earth or rare-earth element, M = metal, X = pnictogen), have traditionally been described within the classical Zintl concept as electron-precise compounds stabilized by ionic charge transfer and covalent polyanionic frameworks. Nevertheless, many 1–2–2 Zintl phases exhibit **low lattice thermal conductivity and competitive thermoelectric performance with zT values approaching or exceeding unity**. These favorable properties are commonly attributed to structural complexity and effective phonon scattering.

However, accumulating evidence indicates that the bonding nature of several 1–2–2 Zintl phases deviates from the classical ionic–covalent picture. Enhanced dielectric responses, soft lattice vibrations, and strong sensitivity of electronic transport to chemical substitution closely resemble those of established metavalently bonded materials. These observations suggest that **some 1–2–2 Zintl phases may reside in a borderline bonding regime between classical Zintl behavior and metavalent bonding**, yet this possibility remains largely unexplored. At present, optimization of 1–2–2 Zintl thermoelectrics relies predominantly on empirical doping, alloying, and microstructural engineering, without explicitly considering how such modifications alter the underlying chemical bonding. The lack of a bonding-centered framework limits predictive design and systematic performance optimization in this important material class.

THESIS DETAILS… The objective of this project is to establish a **direct correlation between chemical bonding characteristics and thermoelectric transport in 1–2–2 Zintl phase materials**. The bonding fingerprints, such as the optical dielectric constant, the Born effective charge, and the bond-breaking behavior, will be studied. All the characterization techniques (FTIR and atom probe tomography) necessary to obtain a successful Master's thesis are available at I. Institute of Physics, RWTH Aachen University.

References:

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3 Kauzlarich et al., Dalton Trans. **2007**, 2099-2107.

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