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Topic for a Bachelor Thesis

Density Functional Theory Investigation of Chemical Bonding in Solids using the Bulk Modulus and Grüneisen Parameter

Differentiating materials by their types of chemical bonding has a long tradition. Recently, it has been shown that characteristic bonding descriptors can be used to separate solids into distinct bonding classes: covalent, metallic, ionic, and metavalent bonding. Metavalent compounds exhibit a unique combination of properties[1] that offers strong potential for thermoelectric and phase-change applications.

Many state-of-the-art thermoelectric compounds (notably among chalcogenides) are located close to the covalent–metallic boundary and frequently exhibit unusual combinations of properties that lead to low lattice thermal conductivity, a key ingredient for high thermoelectric efficiency. In this context, the bulk modulus, which is directly tied to the speed of sound provides a direct and experimentally/computationally accessible bridge between bonding, lattice dynamics, mechanical properties, and thermal transport.

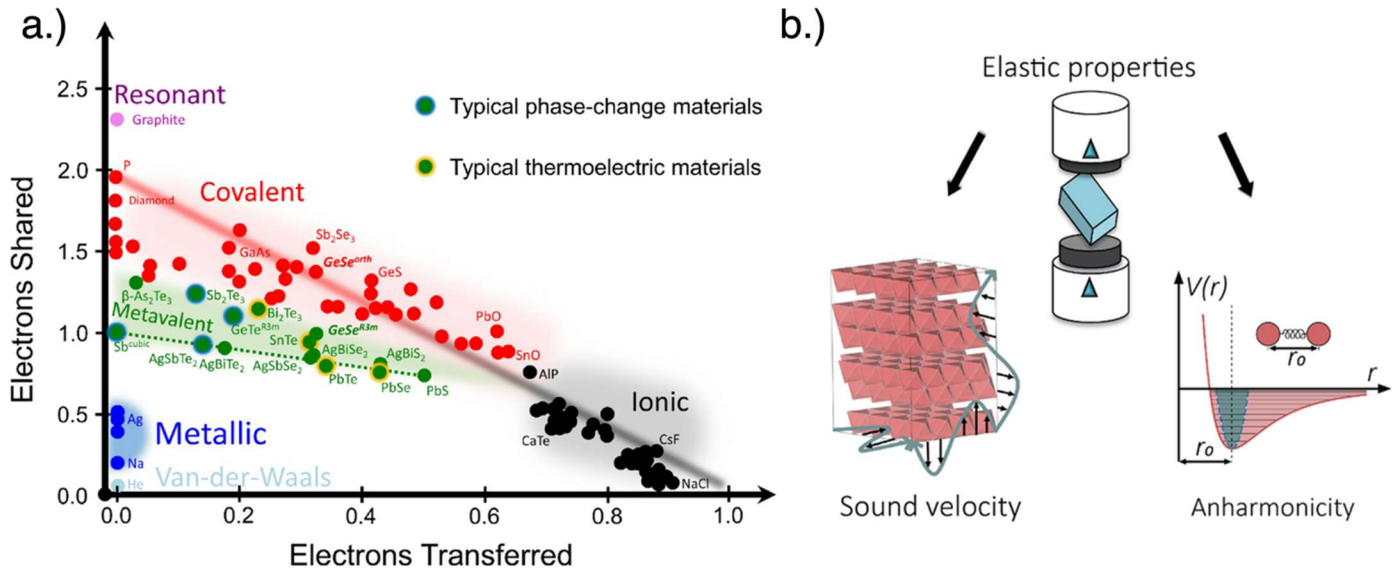

Figure 1: a.) Chemical bonding map spanned by the number of electrons transferred (ET) and electrons shared (ES) between adjacent atoms, derived from the quantum theory of atoms in molecules. Taken from [3]. b.) Schematic representation of the information gained by compressing solid-state structures. Taken from [2].

This bachelor project will use two descriptors, the bulk modulus B and the Grüneisen parameter γ (bond anharmonicity), to differentiate materials by their bonding type and to support the interpretation of thermoelectrically relevant phonon and thermal-transport trends. B will be obtained from energy–volume equations-of-state, and γ from volume-dependent vibrational properties (e.g., phonons at multiple volumes), enabling a direct comparison of elasticity (B) and anharmonicity (γ) and their connection to chemical bonding.

The thesis offers an excellent opportunity to learn the fundamentals of density functional theory calculations, which is a state-of-the-art ab-initio method. It is particularly well suited for students interested in theoretical and computational work and provides training in a methodology of quantum-mechanical calculations based on the electron density.

[1] Schön, Carl-Friedrich, et al. „Classification of properties and their relation to chemical bonding: Essential steps toward the inverse design of functional materials" Science Advances 8.47 (2022)

[2] Isotta, Eleonora, et al. "Elastic moduli: a tool for understanding chemical bonding and thermal transport in thermoelectric materials." *Angewandte Chemie* 135.12 (2023).

[3] Yu, Yuan, and Matthias Wuttig. "From phase-change materials to thermoelectrics: The role of metavalent bonding." *Journal of Materials Research* (2025): 1-10.).

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