I. Physikalisches Institut (IA)
Phasenwechselmaterialien
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Topic for a Master thesis

Lattice properties of metavalently bonded materials

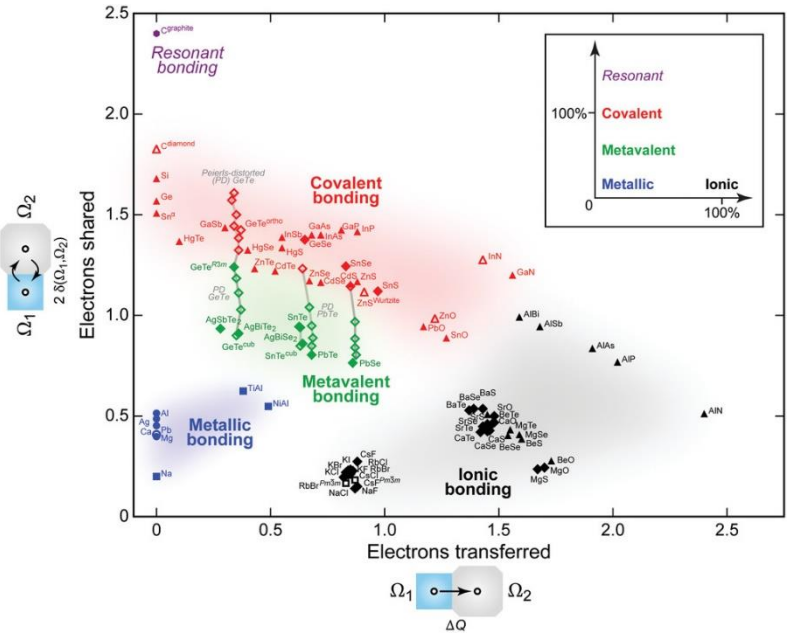

Figure 1: Map with different materials, which are positioned using the two parameters „Electrons transferred“ and „Electrons shared“. The different bonding types are colored accordingly [1].

The metavalent bond (MVB) is a newly proposed type of bond, which is fundamentally different from the ionic or the covalent bond. Materials employing this type of bond are good candidates for phase change materials, thermoelectrics, topological insulators or photovoltaics. An important role in giving MVB materials their respective properties is played by a Peierls distortion of the crystal. A classification of this bonding type has been made using the quantities „Electrons transferred“ and „Electrons shared“, which can be seen in Fig. 1.

Right now the electronic properties of MVB materials have been studied thoroughly (electronic band structure, dielectric function, etc.). Investigating properties of the lattice vibrations could yield further understanding of the role of the Peierls distortion in MVB materials. For that, band structure and the Grüneisen parameter should be calculated using a density functional theory (DFT) code.

The student should be interested in fundamental material research and have an affinity for programming (knowledge of Python recommended).

[1] J. Raty, M. Schumacher, P. Golub, V. L. Deringer, C. Gatti, M. Wuttig: A Quantum-Mechanical Map for Bonding and Properties in Solids, Advanced Materials (2018).

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