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New aspects of an old class of compounds: Tetrelphosphides and their thermoelectric performance

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The tetrelphosphides $Ag_6Ge_{10}P_{12}$ is the prototype of a class of compounds which is known since the mid of the 1970s. In the subsequent years, various experimental results were published. However, due to a lack of accurate quantum chemical investigations, the interpretation of the data was not unambiguous at this time. After three decades of silence, these compounds attracted attention again, due to the promising thermoelectric performance. The figure of merit (zT) of pristine $Ag_6Ge_{10}P_{12}$ is already 0.6 at 700 K, leaving room for improvements in this class of compounds. Reason for this relatively large zT value is the small thermal conductivity, $k<1\ W{\cdot}m^{-1}{\cdot}K^{-1}$, which is related to the exceptional bonding characteristics. According to recent density functional calculation and a thorough bonding analysis, the crystal structure consists of a zinc blende like arrangement of germanium and phosphorus atoms with large voids. This covalent framework encloses subvalent silver octahedra. Four of the faces of the Ag_6^{4+} clusters are capped by another germanium atom, respectively. The atoms within the voids are weakly bound. Concerning the bonding types, there exists a hierarchy with a wide range of bond strength, giving rise to local, low-frequency phonon modes which lead to the reduced lattice contribution to the thermal conductivity. The electronic as well as the dynamic properties of the compound can be modified by substituting elements at the various tetrel sites in the crystal. The covalent framework becomes more rigid when replacing germanium by silicon. Tin as capping atoms of the silver octahedral resulted in a blue shift of the low-lying frequencies and a smaller band gap. By these controlled modifications, new insight can be gained into the complex interplay of electrical and thermal transport properties in thermoelectric materials.

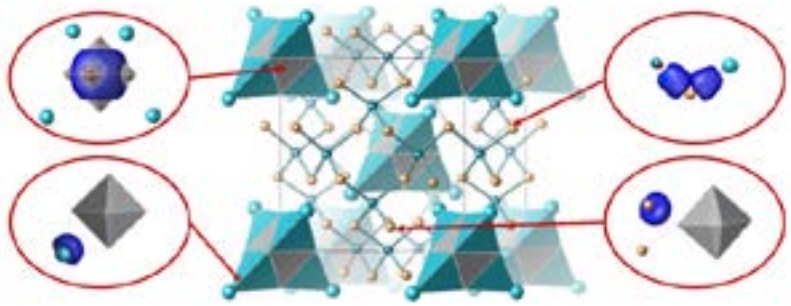

Figure 1: Structure of $Ag_6Ge_{10}P_{12}$ and selected maximally localized Wannier functions.

Biography

Ulrich Wedig research interests include Solid State Chemistry and Physics. Having a sound background in quantum chemistry, he collaborates with experimenters in order to elaborate a deeper understanding of the behaviour and properties of molecular and solid state systems. Special emphasis is put on the relation between quantum chemical data and chemical concepts, bridging the gap between more or less rigorous *ab initio* calculations and a local description of bonds in chemistry.

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