Inhomogeneity and anisotropy of chemical bonding and thermoelectric properties of intermetallic compounds

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The intermetallic phases attract the attention of materials developer for thermoelectric applications and are currently considered as the main family of thermoelectric materials. Where physical behaviours of intermetallic compounds are widely investigated, their chemistry is still an open research field. These substances are formed by elements located at and left of the Zintl line in the Periodic Table. The valence electron count per atom is usually less than four. The reduced VEC and the presence of transition and/or rare earth metals in this group of inorganic materials allow only restricted application of the traditional chemical concepts based on two-centre interactions, like the Zintl-Klemm model, for interpretation of composition and crystal structure [1]. Therefore, a general picture of interatomic interactions as well as understanding of chemical composition and crystal chemical features is still under debate.

Further progress in this matter require using of the models employing the multi-centre bonding. Use of new quantum chemical tools - bonding indicators in real space - opens the way to qualitative and quantitative interpretation of atomic interactions in thermoelectric materials as combination of covalent polar and non-polar, ionic and multi-centre bonds [2]. Introduction of the terms 'inhomogeneity' and 'anisotropy' for atomic interactions contributes to the understanding of chemical and physical behaviours of thermoelectric materials [3]. In particular, the unusually low thermal conductivity of intermetallic clathrates can be interpreted as a consequence of the inhomogeneously and anisotropically distributed regions with different atomic interactions [4,5]. Furthermore, understanding of chemical bonding allows also a prediction for the new compounds [6].

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