Structural complexity, chemical and physical behaviours and chemical bonding in intermetallic compounds

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While - from the physical point of view – the behavior of intermetallic compounds is considered as well studied and understood, the chemical aspects of physical properties and especially the relationships between chemical and physical aspects are still under consideration. This slows down the search and the development of new materials with interesting prospective. Analysis of chemical bonding in intermetallic and related materials with the quantum chemical techniques in positional space shows that atomic interactions play a key role in their chemical and structural organization. It is a substantial reason for their crystallographic complexity and physical behaviors. Atomic interactions (bonding) form a basis for the total electron balance in the material regulating e.g. the charge carrier concentration and transport. Moreover, they influence also the heat transport in the material. Spatial distribution of the regions with different types of chemical bonding - inhomogeneity and anisotropy – seems to be connected with the thermal and electronic transport more than other – solely crystallographic - features.

[1] Yu. Grin, J. Solid State Chem. **274** (2019) 329.
[2] F. R. Wagner, R. Cardoso-Gil, B. Boucher, M. Wagner-Reetz, J. Sichelschmidt, P. Gille, M. Baenitz, Yu. Grin, Inorg. Chem. **57** (2018)12908.

Fig.1: The image of X.

Fig.2: The figure of Y.