

Poster

Polar amalgams: structure-property relations in bad metals**Daniel Kraut, Constantin Hoch***LMU Munich**daniel.kraut@cup.uni-muenchen.de*

The term ‘bad metal’ behavior is used to describe the unusual metallic properties of polar intermetallics. It is the result of a combination of low free electron concentration with a small free electron path length [1,2]. Polar intermetallic phases combine metallic bonding with ionic and covalent bonding contributions [3,4]. Unlike Zintl phases, however, the electron transition from the electropositive to the electronegative constituent remains a partial one, and, therefore, metallic behaviour is retained. Bad metals show an overall relatively high specific resistivity, through the reduction of free charge carrier concentration, and the increase with temperature is linear with a very steep slope only in the low temperature regime. They are, therefore, of particular interest in the development of new thermoelectric materials, microelectronics, data storage, heterogeneous catalysis, and others.

Amalgams of electropositive metals serve as highly interesting and easily accessible model systems to further deepen the understanding of the ‘bad metal’ behavior. Hg is the only noble metal which does not form Zintl-like anions due to its endothermic electron affinity. This together with the high electronegativity differences when combined with electropositive metals (alkali, alkaline or rare earth metals) results in a polar metallic bonding situation. Thus, a plethora of different new metallic materials with extremely rich structural diversity and interesting physical properties are accessible. To identify the parameters of the ‘bad metal’ behavior, binary and ternary amalgams of electropositive metals with varying Hg content were synthesized and subsequently analyzed with respect to crystal structure and physicochemical properties [5].

Three key parameters have been identified to determine mean free path and electron concentration: Coulombic polarity, structural complexity, and disorder phenomena [5,6]. The higher a given parameter the more pronounced the ‘bad metal’ behavior is. Employing amalgams as model systems, each parameter can be studied separately. Coulomb polarity follows the Hg content in polar amalgams. Structural complexity, which can be described with the concept proposed by Krivovichev, seems to have the largest influence on the metallic character, as a decrease in symmetry drastically reduces mean free path [7]. Disorder phenomena, on the other hand, appear to have only a small influence. These can be studied in ternary mixed crystals.

Figure 1. Temperature dependence of the specific resistivity of Hg and the three Li amalgams Li_3Hg , LiHg and LiHg_3

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