Chemistry of strongly correlated systems

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Design of the new materials with strongly correlated electronic systems may be realized on the experimental way. Here the development of the new preparation routes for obtaining intermetallic compounds, e.g. utilizing the redox reactions, allows synthesis of the phases, which were previously inaccessible for thermodynamic or kinetic reasons. Another possibility for the design of new materials with strongly correlated electronic systems may be opened by investigations of chemical bonding in intermetallic compounds which seems to play an important role for observation of distinct physical behaviors. Especially for preparation of new intermetallic compounds the understanding of the atomic interactions may open also new opportunities. In particular the covalent interactions between the metal atoms seem to have an effect on physical behavior. Detection and visualization of covalent interactions in intermetallic compounds is an emerging object of research.

For this kind of investigations, new quantum chemical tools based on the electron localizability approach [1,2] were developed. In this approach, the correlations in the electron's motion in the real space are analyzed. Study of the chemical bonding using the electron localizability indicator (ELI-D representation) was shown to by especially suitable for metallic systems. Decomposition of ELI-D into contributions of the states belonging to certain energy ranges in the electronic density of states [2] allows visualizing and investigation of the role of electrons of the inner shells in the atomic interactions in $EuRh_2Ga_8$ [3] and $La_7Os_4C_9$ [4]. In particular for $EuRh_2Ga_8$, two types of atomic interactions were found between the europium cations and the $[Rh_2Ga_8]$ anion: ionic (non-directed) interaction via transfer of the electrons of the sixth shell to the polyanion and (directed) covalent interaction using the electrons of the penultimate (fifth) shell.

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[2] F. R. Wagner et al. Chem. Eur. J. **13** (2007) 5724.
[3] O. Sichevich et al, Inorg. Chem. **48** (2009) 6261.
[4] E. Dashjav et al. J. Solid State Chem. **181** (2008) 3121.