T_CSUH Special Seminar

Texas Center for Superconductivity at the University of Houston

Dr. Yuri Grin

Director, Max-Planck-Institute
for Chemical Physics of Solids (MPI-CP_FS)
Dresden, GERMAN

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Room 102, University of Houston Science Center
11:00 a.m. - 12:00 noon

Chemistry and Physics of Intermetallic Clathrates and Skutterudite-like Compounds

Abstract

Crystal structures of intermetallic clathrates and skutterudite derivatives are formed by the 3D host frameworks with the differently sized filled or non-filled cages. Beside a variety of physical behaviours these compounds attracted the worldwide attention, e.g., as promising thermoelectric materials. Chemical bonding in clathrates and skutterudites is one of the key questions for the creation of the new materials of these classes. While the bonding in intermetallic clathrates may be sufficiently described by the Zintl concept with some modifications, the presence of transition metals in the filled skutterudites does not allow the straight forward description with simple electron counting. A more general description is possible with the new quantum chemical toolbox for bonding analysis in real space - electron localizability indicator [1]. Understanding of the chemical bonding allows to concept new preparation routes for synthesis of new representatives of this materials family. Especially, the (partial) control of the cage filling is achievable on this way [2]. This allows to prepare 'empty' clathrates, e.g., new modification of germanium [3]. Two new groups of filled skutterudites were successfully prepared. The iron-antimonides of the alkali metals $N_aFe_4Sb_{12}$, KFe_4Sb_{12} [4] and $TlFe_4Sb_{12}$ [5] represent the electron-poorest members of this family and reveal a wide spectrum of electronic properties. The novel family of $REPt_4Sb_{12}$ compounds shows i.e., superconductivity at relatively high temperatures [6].

[1] A. Leithe-Jasper et al. Phys. Rev. B. 2004 70 214418.
[2] B. Bo□hme et al. J. Am. CHem. Soc. 2007 129 5348.
[3] A. M. Guloy et al. Nature 2006 443 320-323.
[4] W. Schnelle et al. 2008 submitted.
[5] A. Leithe-Jasper et al. Phys. Rev. B. 2008 in press.
[6] R. Gumeniuk et al. Phys. Rev. Lett. 2008 100 017002.

Bio

Dr. Yuri Grin received his Ph.D. from the Institute of Inorganic Chemistry of the Lviv State University and is currently a member of the Max Planck society and Director at Max-Planck-Institut fur Chemische Physik fester Stoffe in Dresden. He is the author of articles in leading scientific journals. His current research activities are focused on crystal structures of intermetallic clathrates and skutterudite derivatives, which are formed by the 3D host frameworks with the differently sized filled or non-filled cages. Since 2002 he has been a faculty member and honorary professor in chemical metal science at the Technical University of Dresden, Germany.

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