

**UNIVERSITY OF SOUTH FLORIDA
DEPARTMENT OF PHYSICS**

COLLOQUIUM

Friday, Mar 7th 2008

4:00 pm

PHY 130

**CHEMISTRY AND PHYSICS OF INTERMETALLIC
CHLATHRATES AND SKUTTERUDITE-LIKE COMPOUNDS**

Yuri Grin

**Max-Planck Institute for Chemical Physics of Solids
Dresden, Germany**

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 $\text{NaFe}_4\text{Sb}_{12}$, $\text{KFe}_4\text{Sb}_{12}$ [4] and $\text{TlFe}_4\text{Sb}_{12}$ [5] represent the electron-poorest members of this family and reveal a wide spectrum of electronic properties. The novel family of $\text{REPt}_4\text{Sb}_{12}$ compounds shows i.e., superconductivity at relatively high temperatures [6].

[1] A. Leithe-Jasper et al. Phys. Rev. B. **2004** 70 214418. [2] B. Böhme 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.