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Gegründet im Jahre 1869 von H. Hasiwetz,  
J. Loschmidt, J. Petzval und J. Stefan

## EINLADUNG

zum Vortrag von

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über

## Understanding of intermetallic compounds: layers vs cages

am Dienstag, 25. November 2008, um 17.30 Uhr

Ort: Großer Hörsaal der Experimentalphysik, Universität Wien,  
1090 Wien, Strudlhofgasse 4 / Boltzmanngasse 5, 1. Stock

#### Abstract:

Cage compounds attract recently the worldwide attention because of their variety of emerging physical behaviours, especially thermoelectric and superconducting properties were in focus of the investigations. Crystal structures of intermetallic clathrates and skutterudite derivatives are formed by the 3D host frameworks with the differently sized, filled or non-filled cavities. The complexity of the crystal structures increases rapidly by partial ordering of the constituents and/or defects [1]. Relatively few representatives of the rare-earth metals (RE) containing clathrates are known, e.g., two modifications of the  $\text{Eu}_8\text{Ga}_{16-x}\text{Ge}_{30+x}$  [2-4] or their variations with the two different cations, i.e.,  $\text{Sr}_4\text{Eu}_4\text{Ga}_{16}\text{Ge}_{30}$  [5] or  $\text{K}_6\text{Eu}_2\text{Cd}_5\text{Ge}_{41}$  [6].

The RE compounds of boron with at least one relatively short (.4 Å) lattice parameter were traditionally interpreted as 2D (layer) compounds. Analysis of the chemical bonding of  $\text{TmAlB}_4$  with the electron localizability tools reveal covalent bonding between the boron and aluminium atoms which interconnect the boron layers to a 3D framework with the Tm atoms located in the cavities. This interpretation allows understanding of the nature of complex magnetic ordering [7]. In the isotopic compounds  $\text{RERhB}_4$  rhodium is also a part of the 3D polyanion embedding rare earth metals, which interacts mainly as ions with the polyanion [8]. Analysis of the chemical bonding in this class of intermetallic compounds allows their novel interpretation as framework structures.

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[2] V. Pacheco et al. Phys. Rev. Lett. 87 (2001) 099601.

[3] B. C. Sales et al. Phys. Rev. B 63 (2001) 245113.

[4] V. Pacheco et al. Phys. Rev. B 71 (2005) 165205.

[5] J. L. Cohn et al. Phys. Rev. Lett 82 (1999)7915.

[6] S. Paschen et al. Physica B 383 (2006) 89.

[7] T. Mori et al. Phys. Rev. B 76 (2007) 064404.

[8] I. Veremchuk et al. J. Solid State Chem. 181 (2008) 1983.

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Vorsitzender 2007/08: Ao.Univ.Prof. Dr. Ernst Bauer, Institut für Festkörperphysik, Technische Universität Wien