
TCSUH Special Seminar

Skutterudites: high performance thermoelectric materials – from band-structure calculations towards industrial production



Prof. E. Bauer

Institute of Solid State Physics and
Christian Doppler Laboratory for Thermoelectricity
Vienna University of Technology

Wednesday, February 10, 2016

HSC 102 • 12:00 N – 1:00 p.m.

ABSTRACT

Filled skutterudites $E_p T_4 X_{12}$ (T is a group VIII transition element; X is a pnictide and the electropositive element E_p fills the icosahedral voids in Wyckoff position 2a of space group Im-3) are among the most promising thermoelectric materials fulfilling the PGEC concept as worked out by G. Slack. While the rigid host structure of skutterudites maintains electronic transport, the guest atoms in the icosahedral voids of the skutterudite structure exhibit localized vibrational (“rattling”) modes. This perturbs the propagation of phonons, and thereby significantly reduces the phonon contribution to the thermal conductivity. Besides a large variety of interesting ground state properties like superconductivity, or heavy fermion behavior – some of them will be reviewed here. The possibility of substituting and doping at the various lattice sites of the crystalline unit cell allows fine-tuning the charge carrier density of this material class in order to reach those optimal levels required for superior thermoelectricity. Further improvements of the thermoelectric performance, which is measured by the dimensionless figure of merit, are possible considering nanostructuring of bulk materials as previously proposed by M. Dresselhaus.

In the present work, we will show how promising thermoelectric materials can be derived within the family of filled skutterudites and how auspicious routes for further improvements of this material class can be read-off from *ab-initio* electronic structure calculations carried out for some members of the family of filled skutterudites. Furthermore, we will show how this knowledge, initially derived on a laboratory scale, can be used to set-up an industrial production process of filled skutterudites.

BIO

Ernst Bauer obtained his Ph.D. in 1984 from the Vienna University of Technology. He got his postdoctoral lecture qualification in 1991 and became associate professor at the Vienna University of Technology in 1997. In 2009 he was awarded University Professor at the Vienna University of Technology. His research is focused on strongly correlated electron systems at extreme conditions, on superconductivity and thermoelectric materials built up by cage-forming compounds. In 2004, he detected superconductivity in heavy fermion materials without inversion symmetry. He was the head of European Union COST program P16 “ECOM”, was chairman of the International Conference on Strongly Correlated Electron Systems, SCES’05, of the Austrian Chemical-Physical Society and of the Austrian Neutron and Synchrotron User Community (NESY). In 2013, he received a “Christian Doppler Laboratory for Thermoelectricity”. He has published more than 450 papers in international journals.

Persons with disabilities who require special accommodations in attending this lecture should call (713) 743-8213.
