



Holger Kleinke

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Research Interests:

Inorganic Materials, Solid State Chemistry, Thermoelectric Energy Conversion, Crystal Structure Predictions

Academic Background:

Vordiplom, 1988, Chemistry,
WWU Münster (Germany)

Diplom, 1991, Chemistry,
WWU Münster (Germany)

Ph.D., 1994, Science, J.-G.
Universität Mainz (Germany)

Habilitation, 2001, Inorg.
Chem., Philipps-Universität
Marburg (Germany)

Selected Awards:

Liebig Fellow, 1997-99
(Philipps-Universität
Marburg)

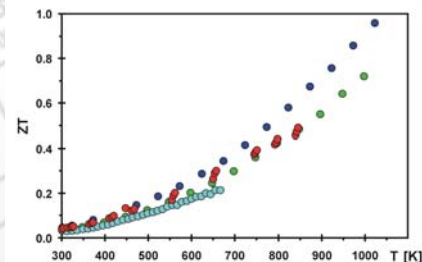
Premier's Research
Excellence Award, 2000

Canada Research Chair in
Solid State Chemistry (tier II,
NSERC), 2001

Ontario Distinguished
Researcher Award (OIT),
2002.

Our main focus lies on finding and optimizing new thermoelectric materials. Thermoelectrics are capable of converting heat into electrical energy and vice versa. This environmentally friendly energy conversion currently has several applications; but this is inhibited by the low efficiency. We are attempting to increase the efficiency so that thermoelectrics may be used to recover electricity from the nowadays abundant waste heat, e.g. in the exhaust of automobiles.

One of the synthetic goals is the discovery of new materials with rattling metal atoms in Sb/Te cages. A challenging task is the synthesis of small-gap semiconductors within this class, a necessity for enhanced thermoelectric energy conversion. Since the thermoelectric properties depend on the thermopower as well as on the electrical and thermal conductivity, various property measurements are routinely carried out in our group. The syntheses are guided by calculations performed by students who are fascinated by the theoretical aspects of chemical research. Other high profile research projects that also combine theory and experiment are available in the areas of hypervalent bonding including square net distortions, and structure predictions.



Selected Publications:

C. R. Sankar, S. Bangarigadu-Sanasy, A. Assoud, H. Kleinke, *Crystal structure and physical properties of Tl_4MQ_4 ($M = Zr, Hf, Q = S, Se$)*, Inorg. Chem. **50**, 245 (2011).
• H. Kleinke, *New bulk Materials for Thermoelectric Power Generation: Clathrates and Complex Antimonides*, Chem. Mater. **22**, 604 (2010). • Y. Cui, J. He, G. Amow, H. Kleinke, *Thermoelectric properties of n-type double substituted $SrTiO_3$ bulk materials*, Dalton Trans. **39**, 1031 (2010). • H. Xu, K. M. Kleinke, T. Holgate, H. Zhang, Z. Su, T. M. Tritt, H. Kleinke, *Thermoelectric performance of $Ni_yMo_3Sb_{7-x}Te_x$ ($y \leq 0.1, 1.5 \leq x \leq 1.7$)*, J. Appl. Phys. **105**, 053703 (2009). • C. Graf, A. Assoud, O. Mayasree, H. Kleinke, *Solid State Polyselenides and Polytellurides: a Large Variety of Se-Se and Te-Te Interactions*, Molecules **14**, 3115 (2009). • J. Xu, H. Kleinke, *Unusual Sb-Sb bonding in High Temperature Thermoelectric Materials*, J. Comput. Chem. **29**, 2134 (2008). • N. Soheilnia, H. Xu, H. Zhang, T. M. Tritt, I. Swainson, H. Kleinke, *Thermoelectric Properties of $Re_3Ge_{0.6}As_{6.4}$ and Re_3GeAs_6 in comparison to $Mo_3Sb_{5.4}Te_{1.6}$* , Chem. Mater. **19**, 4063 (2007).