MONASH University

Monash Centre for Electron Microscopy

Monash Centre for Electron Microscopy Seminar

Structural Thermoelectrics

MONDAY 27 MARCH, 2017

11.00AM

SCIENCE THEATRE S9
16 RAINFOREST WALK
MONASH UNIVERSITY
CLAYTON CAMPUS

Presenter

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Abstract

The figure of merit, $zT = TS^2\sigma/\kappa$, has a central standing in thermoelectrics, and the individual components (thermopower S, electrical conductivity σ, thermal conductivity κ) relate to the transport properties of the thermoelectric material. Thus, the major part of thermoelectric science has focus on measuring and interpreting transport properties. However, all understanding of physical or chemical properties of molecular scale systems relies of precise knowledge of the atomic structure. Without knowledge of the composition and three dimensional disposition of the atoms in space, rigorous interpretation of properties is impossible. Structural techniques therefore must have a central standing in thermoelectrics

In this talk I will discuss structural thermoelectrics exemplified through recent studies of various high performance materials. The PbX and SnX (X = S, Se, Te) systems have received immense interest due to record breaking figures of merit.[1] The crystal structures have been analyzed with the nuclear enhanced maximum entropy method (NXMEM),[2] and the unexpected low thermal conductivity appears to have contributions from atomic disorder, vacancies and strong anharmonic motion.[3] In search for new materials, computational screening methods have been advanced, but they are no better than the structural information used to calculate the properties. Furthermore, they often lack simple measures to relate the properties to the crystal structures. A new method coined “orbital engineering” provides a simple predictive measure related to the crystal structure of layered compounds,[4] and this has been used to discover the new breakthrough n-type material $Mg_3Sb_{1.5}Bi_{0.5}$.[5]

1. (a) Biswas et al., Nature 2012, 489, 414, (b) Zhao et al. Nature 2014, 508, 373–377.
2. Christensen et al, Acta Crystallogr. Sect. A 2015, 71, 9–19
3. (a) Kastbjerg et al., Adv. Func. Mat. 2013, 23, 5477-5483, (b) Christensen et al., PCCP 2016, 8, 15874-15883, (c) Sist et al., IUCr-J 2016, 3, 377-388, (d) Sist et al., Acta Crystallogr. Sect. B. 2016, 72, 310–316.
4. Zhang et al., Nature Comm. 2016, 7, 10892
5. Zhang et al., Nature Comm. 2017, 8, 13901

About the Presenter:

Bo Brummerstedt Iversen received his PhD in Chemistry from Aarhus University in 1995. Following a postdoc appointment at UCSB, he returned to Denmark to take a position as Assistant Professor at the Department of Chemistry, Aarhus University. In 2000 he was promoted to Associate Professor and in 2004 he became Chair of Inorganic Chemistry there. Bo has during the last decade every year spent extended periods as guest professor at University of Western Australia in Perth. He is Director of the Center for Materials Crystallography, which is a Center of Excellence funded by the Danish National Research Foundation. Bo is one of the few Danish Scientists holding both a Doctor of Science degree (2002) and a Doctor of Technology degree (2010). He is a Fellow of the Royal Danish Academy of Science and Letters and he has won many awards including the Elite Researcher Award from the Danish Ministry of Science. His research interests revolve around topics in materials chemistry and materials crystallography including synthesis, characterization and application of energy materials (thermoelectrics, Li ion batteries, solar energy, catalysis), chemical bonding, electron density analysis, application of synchrotron and neutron radiation in chemistry, nanoparticles, supercritical fluids, and hydrothermal liquefaction (bio-oil). He has published ~280 papers in peer-reviewed journals

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