Interdisciplinary Approaches to Functional Electronic and Biological Materials

Science Meeting: Workshop

Reference number: 2921

Title of Science Meeting:
New materials for thermoelectric applications: theory and experiment.

Location : Hvar, Croatia.

Date of Science Meeting : 02/10/2010 - 07/10/2010

Scientific report

Abstract

The workshop reviewed new materials and examined mechanisms relevant for new thermoelectric devices with an enhanced figure-of-merit. The main topic was the heat, charge and spin transport in strongly correlated systems. The objective was to acquire the basic knowledge about the relevant quantum degrees of freedom, which is required to achieve the control and engineer new thermoelectric and magneto-caloric materials with specific quantum mechanical properties. The organization and form of the workshop encouraged the informal exchange of ideas, and promoted discussion.

General report

Thermoelectric devices are heat engines that either convert heat into electricity or use the electricity to pump the heat from a cold to hot reservoir. The possibilities arising from the fact that electricity can be generated directly from heat, the Seebeck effect known since 1821, are beginning to be more widely appreciated. This is due to current environmental concerns to reduce waste heat loss and to find new, sustainable energy sources. The thermoelectric devices can reduce the petrol consumption in motor vehicles by 5 to 10%, reducing significantly the oil needs. They are also used for power generation in remote regions, where the thermoelectricity ensures a continuous power supply of electronic equipment. This is an important, but only one type of application of a thermoelectric effect. The other thermoelectric effects, the Peltier effect and Thompson effect, can be used for cooling without moving parts, providing microcooling for the electronics industry and refrigeration without the use of environmentally damaging CFCs and FCs. All of these can play an important role in development and efficient use of sustainable energy resources. The scientific and technological advances in this field could have important implication for modern society.

The main problem in nearly all of these applications is the rather low efficiency of the processes of energy conversion. The important factor which determines the efficiency is the dimensionless ratio, ZT, known as the figure of merit. This needs to be optimized to give a value of ZT of the order of 1 or higher for the more widespread use of thermoelectric devices. A value of ZT of the order 1 requires use of a material with a large thermopower and electrical conductivity and a low thermal conductivity. These tend to be incompatible requirements; for example, a good metal has a high electrical conductivity but also a high thermal conductivity. Materials which have a high thermopower tend also to have a low electrical conductivity. The aim of this research field, therefore, is to find or fabricate materials with the properties that enhance ZT. It is a multidisciplinary field, requiring the expertise of material physicists, chemists, metallurgists and the support of theory. There have been important recent developments in innovative synthesis techniques, the discovery of new materials, and a deeper understanding of the parameters that affect the performance of materials in thermoelectric devices. These have brought the goal of producing materials with the required characteristics for commercial application a significant step closer. There have been important developments in the fabrication and design of these materials, and they have considerable potential, due to the possibility of combining materials with quite different attributes to influence the various factors which contribute to the overall figure of merit.

Detailed activity report

The workshop brought together the experts in the different fields, to exchange the latest results and ideas, and to discuss the directions for future work. The focus was on a particular issue each day, as can be seen from the program. Here we mentioned just a few talks that we find particularly illuminated.

E. Bauer, R. Baumbach, A. Goncalves, P. Rogl and B. Sales discussed the systematic approaches to find new materials and how to improve the thermoelectric response of already known promising materials.

J. Snyder, and Y. Grin discussed new ways of identifying good candidates for thermoelectric effects.

U. Stockert discussed the thermoelectric response as a way of identifying the nature of the low lying excitations in strongly correlated compounds, and distinguishing between competing energy scales.

J. Fauque talked about using the Nernst effect as a probe in Bi and graphite.

V. Oganessyan complemented the experimental work of using the thermoelectric response as a probe, on the Nernst effect as a probe in the high Tc superconduc-

tors and graphene.

D. Jaccard explained how to a probe with the Hall effect for unusual superconductors under pressure.

J. Malone discussed how the thermopower in a high magnetic field throws some light on the hidden order and unusual behavior of URu2Si2

Nanostructured, layered materials and composites were covered by J. Freericks. Continuing the nanoscale theme, T. Costi explained the potential of the Kondo effect in quantum dots for thermoelectric devices— with the conclusion that way to obtain an enhanced density of states just above the Fermi level for a strong thermopower would be via a charge Kondo effect rather than spin Kondo effect.

S. Maekawa covered some particularly interesting and novel ideas about involving directly the spin degrees of freedom, using a ferromagnet in a temperature gradient to generate a spin current and induce a spin Seebeck effect.

E. Tosatti and M. Fabrizio discussed various topics related to Kondo screening in nanocontacts.

P. Prelovsek discussed thermal transport in Fe pnictides.

One of the problems confronting the theorist is that of taking into account both the strongly correlated electrons and the phonons, and we had a number of talks from theorists taking on aspects of this challenge. Pruschke and Ueda both considered the interplay of the electrons and phonons in different heavy fermion systems, and there was a poster by Bonca on a similar topic.

There were many poster contributions. The one-hour poster session was held each afternoon, before the afternoon lecture session. The posters were continuously on the display and the organizers printed-out all the presentations and put them on poster-boards as well. The lecturers wwere available at their posters for answering additional questions.

The lectures and discussions were recorded and put on the web, together with the PowerPoint presentations. The material will edited and presented as virtual proceedings which will be available to the public over the Internet. This material should provide an up-to-date summary of the thermoelectricity of correlated systems. The DVD with the virtual proceedings will be made available free of charge to all the participants and at the cost of the postage to everyone else. Depending on the willingness of the contributors to provide the manuscripts, we might also edit a book with selected lectures from the workshop., as we did on two previous occasions.

List of speakers and participants and titles of the presentations:

Aviani I. Dr., Institute of Physics, Zagreb, Croatia Phase diagram of 4f heavy fermion compounds

Bagaric I., Institute of Physics, Zagreb, Croatia

Bauer E. Prof. , Technical University, Vienna, Austria How high performance skutterudites may loose efficiency in thermoelectric devices

Baumbach R. E. Dr. , University of California, San Diego, USA Correlated Electron Materials for Thermoelectric Applications

Bonca J. Dr. ,J. Stefan institute and Faculty of Mathematics and Physics, University of Ljubljana, Slovenia Gain of the kinetic energy of bipolarons in the t-J-Holstein model based on electron-phonon coupling

Costi T. Dr. , Institute of Solid State Research, Research Centre J?lich, Germany Thermoelectric properties of strongly correlated quantum dots

Fabrizio M. Dr. , Scuola Normale Superiore and Democritos CNR-IOM, Trieste, Italy Lack of Kondo screening at nanocontacts of nearly magnetic metals?

Falmbigl M. , Insitute of Physical Chemistry, University of Vienna, Austria Thermal Expansion and Mechanical Properites of clathrates

Fauque B. Dr., LPEM/ESPCI (CNRS), Paris, France Nernst effect as a probe of the quantum limit of bismuth and graphite

Freericks J. Prof., Georgetown University, Washington DC, USA Transport and static properties of strongly correlated multilayers

Goncalves A. P. Dr., Instituto Tecnologico e Nuclear, Sacavem, Portugal Recent advances on thermoelectric glasses

Grin J. Prof., Max Planck Institute, Dresden, Germany Chemistry and Physics of New Cage Compounds

Hartmann S. Dr., Max Planck Institute for Chemical Physics of Solids, Dresden, Germany Thermopower Evidence for an Abrupt Fermi Surface Change at a Quantum Critical Point

Hewson A. Dr., Imperial College, London, UK

Jaccard D. Prof., Ecole de Physique, Geneva, Switzerland Thermoelectricity in extreme conditions

Koshibae W. Dr., CMRG, RIKEN, Saitama, Japan

Madunć M.., Institute of Physics, Zagreb, Croatia

Maekawa S. Prof., ASRC, Japan Atomic Energy Agency, Tokai, Ibaraki, Japan Seebeck Effect, Spin Seebeck Effect and Spin-Electronics

Malone L. Dr., CNRS, Grenoble, France Thermoelectricity of URu2Si2

Maple B. Prof., University of California, San Diego, USA Matsuo M., ASRC, Japan Atomic Energy Agency, Tokai, Ibaraki, Japan Magnetic field dependence of thermopower in strongly correlated electron systems

Mori M. Dr., ASRC, Japan Atomic Energy Agency, Tokai, Ibaraki, Japan Quantum transport in nano-structure of superconductor and ferromagnet

Ocko M. Dr., Institute of Physics, Zagreb, Croatia Report on the recent investigations of the systems which assume some of the good thermoelectric properties

Oganessyan V. Prof., City University of New York, USA Theory of dissipationless Nernst effects

Ohe J. Dr., Advanced Science Research Center JAEA,Tokai, Ibaraki, Japan Numerical study on the thermal spin transport in ferromagnetic insulators

Oles A. M. Prof., Max-Planck-Institut FKF, Stuttgart, Germany Compass-Heisenberg Model on the Square Lattice: Spin Order and Elementary Excitations

Paschen S. Prof., Technical University, Vienna, Austria Towards phonon and electron engineered thermoelectrics

Prelovsek P. Prof., Faculty of Mathematics and Physics, University of Ljubljana, and Institute Jozef Stefan, Ljubljana, Slovenia Anomalous Transport Properties of Iron Pnictides: A Phenomenological Theory

Pruschke T. Prof., Goettingen University, Germany Monte-Carlo approach to stationary transport through correlated nano-structures beyond the linear response limit

Pudalov V. Prof., Lebedev Physics Institute, Moscow, Russia Strongly correlated electrons in 2D and 2D metal-insulator transition

Rogl G. Mag.,Institute of Physical Chemistry, University of Vienna, Austria Mechanical Properties of Skutterudites

Rogl P. Prof., Institute of Physical Chemistry, University of Vienna, Austria Multicomponent Clathrates for Thermoelectric Applications

Sales B. Prof., Oak Ridge National Lab, USA Exploring FeSi and Related alloys for Thermoelectric Refrigiraion: Evidence for Strong Electron-Phonon Scattering

Snyder J. Prof., California Institute of Technology, USA Use of Semi-Emperical Models of High Temperature Thermoelectric Transport to Improve zT

Stockert U. Dr., Max Planck Institute for Chemical Physics of Solids, Dresden, Germany Energy scales in 4f systems studied by thermopower

Tosatti E. Prof., Scuola Normale Superiore and Democritos CNR-IOM, Trieste, Italy Electrical Conductance Through Magnetic Impurities in Gold Nanocontacts and in Nanotubes

Ueda K. Prof., Institute of Solid State Physics, Tokio, Japan Kondo Effect of a Vibrating Magnetic Ion

Zeiringer I. Mag.,Institute of Physical Chemistry, University of Vienna, Austria
Thermoelectric Clathrates: Ba8Ag,AuxSi,Ge46?x?yΔy

Zlatic V. Dr., Institute of Physics, Zagreb, Croatia