Interdisciplinary Approaches to Functional Electronic and Biological Materials

Science Meeting: Workshop

Reference number: 3596

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

Location : Hvar, Croatia.

Date of Science Meeting : 19/09/2011 - 25/09/2011

Directrors: V. Zlatić and A. Hewson.

Scientific report

Summary

This workshop was the continuation of the workshop held on the same location in 2010. 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 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. The organization and form of the workshop encouraged the informal exchange of ideas, and promoted discussion.

The program of the workshop was spread over five and a half days. An abstract booklet of all the talks was prepared and given to all participants on arrival. The key presentations were for 50 minutes with 10 minutes for discussion. Most of the participants were given an opportunity to talk and present the results of their work as we had a number of shorter 1/2 hour talks each day. A poster session was also arranged for most days which provided an additional forum for discussion and for participants to present their work. On the final day a round table discussion was organized to reflect on the work presented at the workshop and to discuss plans for further research work and cooperation.

Description of the scientific content of and discussion at the event

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.

The search for new materials for thermo-electric devices is a multidisciplinary one,and the workshop reflected the full range of research activities in the field. The efficiency of thermoelectric devices depends on the figure of merit, ZT, of the materials used, and suitable materials should have a figure of merit of 1 or higher. Suitable materials should have a high thermopower (Seebeck coefficient), high electrical conductivity and a low thermal conductivity. As these tend to be incompatible requirements, simple metals for instance have a high electrical conductivity but also a high thermal conductivity whereas the opposite is the case

for insulators. As a result the search for suitable materials has mainly focussed on semiconductors, semi metals and composites. A more recent development has been the investigation of compounds with strongly correlated electrons, because these compounds tend to have enhanced many-body excitations in the neighborhood of the Fermi level which lead to a large Seebeck coefficients. One strategy, therefore, to enhance ZT is to find or fabricate materials of this kind, and to characterize and understand their properties. The better we understand these materials the greater the chance of being able to manipulate them to improve on their prospect for thermoelectric applications. Some way also has to be found for lowering their thermal conductivity.

A few talks that we find particularly illuminated are mentioned below. The webcasts of all the lectures and the prower-point presentations used for the lectures can be found at the website http://hvar2011.ifs.hr

- The lattice contribution to the thermal conductivity can be reduced in materials which have rigid cages holding loosely bound ions that act as rattlers. The most promising materials of this type are skutterudites and clathrates, and these classes of compounds were fully reviewed in the workshop by Bauer and Rogl.

- It is clear that simple band models of these complex compounds cannot take into account strong correlation effects in many of these compounds. An important theoretical activity, therefore, has been in devising and applying new techniques that can handle these strong correlation effects to make useful predictions to guide the experimental work. These methods have improved significantly in recent years such that predictions of the thermoelectric properties of specific compounds can be predicted with some confidence. These methods depend on a combination of density functional band calculations with the techniques of dynamical mean field theory and an overview of this activity was presented in the talks of Kotliar, Held, Delaire and Mori.

- Other theoretical approaches depend on working with simplified models which capture the essence of strong correlation effects to predict their effects on thermoelectric response functions. There were two talks by Shastry based on the t-J model, in which he described a completely new way of calculating the electronic behavior of this model.

- Thermal transport in one dimensional systems was discussed in the talks of Prelovsek and Zotos. The non-linear aspects of charge and heat transport were discussed by Pruschke, Bonca, Mierzejewski and Fabrizio.

- The Nernst effect, which is also of interest for thermoelectric applications, was discussed by Hess, Behnia and Oganessyan. A special tutorial lecture on Nernst effect was given by Oganessyan.

- At the other end of the spectrum were talks on different ways of processing materials, some of which are already in use, to improve their figure of merit. These ranged from grain size reduction, glassy materials, nanopowdering, spark plasma sintering, severe plastic deformation and high pressure torsion, and were covered in the talks of Gonclaves, Gelbstein and G. Rogl.

- On the theoretical side Freericks gave a talk on the calculations (performed jointly with Zlatic) of enhanced thermal transport in multilayers of strongly correlated materials and Costi considered a possible mechanism of enhancing the thermopower via the charge Kondo effect in a molecular quantum dot (proposed jointly with Zlatic).

There were also several 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.

Assessment of the results and impact of the event on the future direction of the field

There were 36 talks in total ranging from investigations on specific compounds to those with the more general aim of understanding the relation between thermoelectric properties and other electronic response functions in strongly correlated materials. We were very pleased with the high quality of the talks and for the many questions and discussion sessions they stimulated.

Nearly all the lectures were recorded and have been put on the website together with the power-point presentations and are available for the general public at the website: http://hvar2011.ifs.hr

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.

There was an optimistic but confident conclusion from the workshop for future work that real progress is being made, not only in finding new materials, understanding them at a more fundamental level, but also in improving on compounds already in use. The progress may only be incremental—it is unlikely that we will suddenly have an ideal material, cheap and easy to manufacture with a high figure of merit— but nevertheless significant and important and will lead to more, and more widespread, applications both in power generation and cooling.

One specific outcome of the workshop was several participants combining forces to put in a joint proposal to the European Science Foundation for a project on 'Thermoelectric Applications and Materials'. There was also the declared intention to continue the cooperation and organize another workshop in three years time.

List of participants supported by the ESF grant:

Name	Surname	Gender	Country	
Ana	Akrap	F	Geneva	Switzerland
Ivica	Aviani	M	Zagreb	Croatia
Katica	Biljaković	F	Zagreb	Croatia
Matthias	Falmbigl	M	Vienna	Austria
Benot	Fauqu	M	Paris	France
Jonathan	Hänel	M	Vienna	Austria
Matthias	Ikeda	M	Vienna	Austria
Oleg	Matveev	M	Lviv	Ukraine
Michiyasu	Mori	M	Tokai	Japan
Jernej	Mravlje	M	Palaiseau	France
Andriy	Shvayka	M	Lviv	Ukraine
Hugo	Vieyra	M	Dresden	Germany
Isolde	Zeiringer	F	Vienna	Austria
Sanja	Žonja	F	Zagreb	Croatia

The grant enabled us to cover the hotel accommodation (bed and breakfast) of fourteen participants listed in the above table. The full addreses and emails of these participants have been entered on the ESF web site.

Final programme of the meeting

Tuesday, September 20.

8:50 - 9:00 Zlatić V. and Hewson A. *Opening of the workshop.*

9:00 - 10:00 Bauer E., Technical University, Vienna, Austria. *From superconductivity towards thermoelectricity: Germanium based skutterudites.*

10:00 - 11:00 Kotliar G., Rutgers University, Piscataway, NJ, USA. *First principles calculations of thermoelectric properties of materials: Quo Vadis?*

11:00 - 11:30 Break

11:30 - 12:30 Behnia K., Ecole Normale Superier, Paris, France. *Nernst effect in Bismuth and graphite beyond the quantum limit.*

12:30 - 15:30 Lunch & afternoon break

15:30 - 16:30 Posters and discussion session

16:30 - 17:30 Snyder J., California Institute of Technology, CA, USA. *Carrier Pocket Engineering to Improve Thermoelectric Transport in Semiconducting PbTe.*

17:30 - 18:30 Delaire O., Oak Ridge National Laboratory, Oak Ridge, USA. *Phonons in thermoelectrics probed with neutron scattering experiments and DFT calculations: electron-phonon and phonon-phonon couplings in FeSi and PbTe.*

18:30 - 20:30 Dinner break

20:30 - 21:30 After dinner talk Shastry S., University of California Santa Cruz, CA, USA. *Extreme Correlations: or How I learned Not to Worry and Love the Infinite U limit.*

Wednesday, September 21.

9:00 - 10:00 Gelbstein Y., Ben-Gurion University of the Negev, Beer-Sheva, Israel. *General Trends in Thermoelectrics.*

10:00 - 11:00 Maple B., University of California, San Diego, USA. *Experiments on new correlated electron systems.*

11:00 - 11:30 Break

11:30 - 12:30 Rogl P. F., University Vienna, Austria. *Clathrate Type I Thermoelectrics:* $Ba, Sr_8 M_x Ge, Si_{46-x-y}[]_y$

12:30 - 13:00 Mravlje J., Ecole Polytechnique, Palaiseau, France. *Thermopower in strongly correlated Sr2RuO4 from first principles.*

13:30 - 15:30 Lunch & afternoon break

15:30 - 16:30 Posters and discussion session

16:30 - 17:30 Mori M., Advanced Science Research Center, JAEA, Tokai, Japan. *Thermopower in correlated electron systems revisited: non-monotonic temperature dependence.*

17:30 - 18:00 Pruschke T., Goettingen University, Germany. *Monte-Carlo Approach to Stationary Non-equilibrium of Mesoscopic Systems.*

18:00 - 18:30 Hewson A., Imperial College, London, UK. *Fusion of energy scales on the approach to a local quantum critical point.*

Thursday, September 22.

9:00 - 10:00 Buehler-Paschen S., Vienna University of Technology, Vienna, Austria. *Anisotropic Kondo insulators.*

10:00 - 11:00 Fauque C., Ecole Normale Superier, Paris, France. *Entropy transport in (topological insulator) Bi2Se3.*

11:00 - 11:30 Break

11:30 - 12:30 Tomczak J., Rutgers University, Piscataway, NJ, USA. *Signatures of correlation effects and thermopower in FeSi.*

12:30 - 13:00 Shastry S., University of California Santa Cruz, CA, USA. *Universal features of Thermopower in High Tc systems and Quantum Criticality.*

14:30 - 19:30 Workshop trip

Friday, September 23.

9:00 - 10:00 Held K., Technical University, Vienna, Austria. *Enhancement of the Na0.7CoO2 thermopower due to electronic correlations.*

10:00 - 10:30 Arsenault L-F., Universite de Sherbrooke, Canada. *Optimal doping and entropic origin of giant thermopower in doped Mott insulators.*

10:30 - 11:00 Hess C., Leibniz Institute, Dresden, Germany. *Nernst effect of iron pnictide and stripe ordering cuprate superconductors.*

11:00 - 11:30 Break

11:30 - 12:00 Goncalves A. P., Instituto Tecnologico e Nuclear, Sacavem, Portugal. *Alternative strategies for thermoelectric materials development.*

12:00 - 12:30 Pernau H-F., Fraunhofer Institut, Freiburg, Germany. *Contributions to physical clarification of high ZT-Bi2Te3/Sb2Te3 nanoscale superlattices.*

12:30 - 13:00 Prelovšek P., University of Ljubljana, Slovenia. *Transport in disordered systems of interacting fermions.*

13:00 - 15:30 Lunch & afternoon break

15:30 - 16:30 Posters and discussion session

16:30 - 17:30 Costi T., Forschungsyentrum Juelich, Germany. *Charge Kondo effect in molecular quantum dots and Pb1?xTeTlx and a mechanism for large thermopower.*

17:30 - 18:30 Freericks J., Georgetown University, Washington DC, USA. *Enhanced thermal transport in strongly correlated multilayers.*

18:30 - 19:00 Kirchner S., Max Planck Institute for Complex Systems, Dresden, Germany. *A superperturbation theory approach to thermoelectric transport in strongly correlated quantum dots.*

20:00 Workshop Dinner

Saturday, September 24.

9:00 - 9:30 Fabrizzio M., Scuola Normale Superiore, Trieste, Italy. *Out-of-equilibrium dynamics in correlated systems: a variational approach.*

9:30 - 10:00 Mierzejewski M., Institute of Physics, University of Silesia, Poland. *Nonlinear Current Response of an Isolated System of Interacting Fermions.*

10:00- 10:30 Oles, A., Max-Planck-Institut fur Festkorperforschung *Spin-Orbital Entangled States in Transition Metal Oxides.*

10:30 - 11:00 Svaika A., Institute of the Academy of Sciences, Lviv, Ukraine. *Many-body dynamics and inelastic scattering in strongly correlated electron systems.*

11:00 - 11:30 Break

11:30 - 12:00 Bonča J., J. Stefan institute and University of Ljubljana, Slovenija. *Nonequlibrium dynamics of many-body systems driven by a constant electric field.*

12:00 - 12:30 Zotos X., University of Crete, Heraklion, Greece. *Open issues on the*

transport phenomena of 1D quantum magnets.

12:30 - 15:30 Lunch & afternoon break

15:30 - 16:30 Posters and discussion session

16:30 - 17:30 *Oganesyan V., City University of New York, USA. Tutorial lecture: Magnetothermoelectric effects - experiments and theories.*

17:30 - 18:00 Rogl, G., University Vienna, Austria. *Severe Plastic Deformation (SPD) using High Pressure Torsion (HPT) a new route to high ZTs?*

18:00 - 18:30 Pfau H., MPI for Chemical Physics of Solids, Dresden, Germany. *Thermoelectric transport across the metamagnetic transition in CeRu2Si2.*

18:30 - 19:30 Očko M., Institute of Physics, Zagreb, Croatia. *Silicon goes thermoelectric.*

19:30 - 19:45 Zlatić V. and Hewson A. *Closing of the workshop.*

Sunday, September 24.

10:00 - 12:00 Round-table discussion on the future of the thermoelectric research.