The 2nd Forum of Integrated Research and Education Center for Energy Production, Storage, Saving, and Transfer Technologies: Energy Conversion and Storage I

Organized by: Research and Education Center for Advanced Energy Materials, Devices, and Systems, Kyushu University

Co-organized by: Research and Education Center of Carbon Resources, Kyushu University
Green Asia Education Center, Kyushu University

Cutting-edge Materials and Devices for Thermoelectric Energy Conversion and Electrochemical Energy Storage

We are delighted to announce that the Second Forum of the Integrated Research and Education Center for Energy Production, Storage, Saving, and Transfer Technologies will be held on power generation and storage technologies. This Forum aims at holding an open discussing opportunity for academicians, scientists, and faculty members in Kyushu University, with world-famous scientists in thermoelectrics, energy storage, and related technologies. Participation of graduate students and external researchers are also highly welcome. Materials and devices to optimize efficiency and cost/performance aspects will be enlightened with emphasis on tailoring electrical, thermal, and electrochemical properties to the demand of applications.

Date and Time: 13:00, August 27th (Wed.), 2014
Place: #112 Lecture Room, IGSES Building A, Chikushi-campus, Kyushu University, Kasuga, Fukuoka, Japan

Time Table

13:00 - 13:10 Opening Remarks

13:10 - 14:00 "Thermoelectrics: From Space to Terrestrial Applications – Successes, Challenges and Prospects"
Dr. Thierry Caillat (Jet Propulsion Laboratory, NASA/Caltech, USA)

14:00 - 14:50 "Thermoelectric Materials – From Basic Science to Energy Applications"
Dr. Qiang Li (Brookhaven National Laboratory, USA)

14:50 - 15:00 Break

15:00 - 15:50 "Novel Sulphate Compounds as High-voltage Fe-based Cathodes"
Dr. Prabeer Barpanda (Indian Institute of Science, India)

15:50 - 16:30 Q&A, General Discussion

16:30 Closing Remarks

Point of Contact:

Prof. Michitaka Ohtaki
Research and Education Center for Advanced Energy Materials, Devices, and Systems
Department of Applied Science for Electronics and Materials, Interdisciplinary Graduate School of Engineering Sciences, Kyushu University, Japan
Phone&Fax +81-(0)92-583-7947
E-mail: ohtaki@kyudai.jp

Thermoelectrics: From Space to Terrestrial Applications - Successes, Challenges and Prospects

Thierry Caillat

Jet Propulsion Laboratory/California Institute of Technology

4800 Oak Grove Drive, Pasadena, CA 91109, USA

Despite their relatively low efficiency, thermoelectric coolers have been used for many years for a variety of applications, typically in which their high reliability outweigh their relatively low performance compared to compressor based systems. Radioisotope Thermoelectric Generators (RTGs) generate electrical power by converting the heat released from the nuclear decay of radioactive isotopes (typically plutonium-238) into electricity using a thermoelectric converter. RTGs have been successfully used to power a number of space missions including the Apollo lunar surface science packages, the Viking Mars landers, Pioneer 10 and 11, and the Voyager, Ulysses, Galileo, Cassini and New Horizons to Pluto outer planet spacecrafts. Following the spectacular lading of the Mars Science Laboratory rover in the summer of 2012, the rover, powered by the Multi-Mission RTG, began its science mission. These generators have demonstrated their reliability over extended periods of time (tens of years) and are compact, rugged, radiation resistant, and produce no noise, vibration or torque during operation. These properties have made RTGs suitable for autonomous missions in the extreme environment of outer space and on the surface of Mars. Additionally, approximately a third of the energy consumed by the U.S. manufacturing industry is released in the form of waste heat, offering opportunities to convert the industrial waste energy into electrical energy using various technologies, including thermoelectrics. A review of the various prospective applications including automobile and industrial waste heat recovery is provided and the technical and economical challenges are highlighted. One of the key-enabling technologies for these applications is high-temperature, high-efficiency thermoelectric materials and converters. A review of state-of practice and state-of-the art high-temperature thermoelectric materials and converters is presented including recent development at the NASA Jet Propulsion Laboratory (JPL). Key challenges are summarized and future prospects for large-scale application of thermoelectrics are discussed.

1. J. Yang and T. Caillat, MRS Bulletin, Vol. 31, March 2006 (You can find all the special issue articles as a single pdf file by searching this literature information “J. Yang…..2006” on the web).
2. T. Caillat, Section 4, Chapter 2 in "Handbook of Thermoelectric Conversion Technology" Takenobu Kajikawa, Ryoji Funahashi, et al. editors (2008, in Japanese).

Thermoelectric Materials – From Basic Science to Energy Applications

Qiang Li
Brookhaven National Laboratory, Upton, NY 11973-5000, USA

In this lecture, I will discuss some recent works on thermoelectric materials aimed at fundamental understanding of their electronic and phonon structures, as well as exploring their energy applications. In the first part, I will describe the Angular Resolved Photoemission Spectroscopy (ARPES) used for probing the electronic structure of correlated materials, for example: thermoelectric cobaltates,[1] which is influenced not only by charge, but also by the spin, lattice and orbital degrees of freedom, leading to giant responses to small perturbations. In the second part, I will describe the measurements of the phonon density of states by inelastic neutron time-of-flight scattering and specific-heat measurements along with first-principles calculations. In the case of filled skutterudites, the combined results not only provide compelling evidence for the existence of an Einstein oscillator (rattler) at low energy (5 meV) in the filled skutterudite $Yb_{0.2}Co_4Sb_{12}$, but also revealed multiple dispersionless modes in the measured density of states of $Yb_{0.2}Co_4Sb_{12}$ at intermediate transfer energies which suggests these modes are owed to a complementary mechanism for the scattering of heat-carrying phonons in addition to the low energy mode, and hence offers a plausible explanation for the significantly higher dimensionless figures of merit of filled skutterudites.[2] In the third and the last part, I will present a brief review of recent progress on bulk thermoelectric materials synthesized via non-equilibrium routes at Brookhaven National Laboratory. A family of high performance thermoelectric materials has been developed by converting rapid solidified precursor into crystalline bulks. This family includes tellurides, silicites, half-Heuslers, and filled skutterudites. In the case of filled skutterudites, percentage of cage-filling elements can be substantially increased during non-equilibrium processing, extending the range of chemical tuning, or position of the Fermi-level. Reduction of lattice thermal conductivity and increase of power factor can be achieved simultaneously. The selection of filled skutterudites for vehicle waste heat recovery using thermoelectric power generators will be discussed and emphasized. Other promising materials such as $CuSe_2$ may also be discussed briefly.[3]

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References:

1) T. Valla, Q. Li, *et al.*, “Coherence-incoherence and Dimensional Crossover in Layered Strongly Correlated Metals”, *Nature*, **417**, 627 (2002).
2) I. K. Dimitrov, Q. Li, *et al.*, “Einstein Modes in the Phonon Density of States of the Single-filled Skutterudite $Yb_{0.2}Co_4Sb_{12}$”, *Phys. Rev. B*, **81**, 17431 (2010).
3) H. L. Liu, Q. Li, *et al.*, “Copper Ion Liquid-like Thermoelectrics”, *Nature Materials*, **11**, 422-425 (2012).

Novel Sulphate Compounds as High-voltage Fe-based Cathodes

Prabeer Barpanda

Faraday Materials Laboratory,
Materials Research Centre,
Indian Institute of Science, Bangalore, 560012, India

prabeer@mrc.iisc.ernet.in

Abstract. Rechargeable batteries based on Li-ion and Na-ion have been growing leaps and bound since their inception in the seventies. The steady demand for building better batteries calls for discovery, optimization and implementation of novel positive insertion (cathode) materials. In this quest, chemists have tried to unravel many future cathode materials taking into consideration their eco-friendly synthesis, material/ process economy, high energy-density, safety, easy handling and sustainability. Interestingly, sulphate-based cathodes offer good combination of sustainable syntheses and high energy-density owing to their high-voltage operation stemming from electronegative SO_4^{2-} units. The current paper will showcase some recent discovery of sulphate-containing cathode materials highlighting (i) the highest Fe redox potential cathode (triplite, 3.9 V) for Li-ion batteries, (ii) the highest Fe redox potential cathode (alluaudite, 3.8 V) for Na-ion batteries and (iii) new hydrated cathodes e.g. bihydrated fluorosulphates [$AMSO_4F.2H_2O$] and hydrated bisulphates [$A_2M(SO_4)_2.nH_2O$].[1-3] These materials offer the highest ever Fe(III)/Fe(II) redox potentials for both Li-ion and Na-ion batteries made from low-cost earth-abundant Li-Na-Fe-S-O-H system. Comparative study of some key sulphate-based cathodes will be presented to offer an outlook on the future development of high-voltage polyanionic cathode materials for next generation batteries.

Keywords: batteries, cathodes, fluorosulphates, polysulphates, tavorite, alluaudite.

1. P. Barpanda et al, *Nature Communications*, **5**, 4358 (2014).
2. P. Barpanda et al, *Nature Materials*, **10**, 772 (2011).
3. P. Barpanda et al, *Chem. Mater.*, **26**, 1297 (2014).

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