WORKSHOP ANNOUNCEMENT

Thermoelectric Transport: progress in first principles and other approaches and interplay with experiment

July 22, 2009 – July 24, 2009
Lausanne, Switzerland

Organizers
Natalio Mingo (CEA-Grenoble, France)
Nathalie Vast (Ecole Polytechnique, France)
David Brodid (Boston College, USA)
Derek Stewart (Cornell Nanoscale Facility, USA)

Invited Speakers
E. Bertranandy (Ecole Polytechnique), G. Cuniberti (TU-Dresden), Keivan Esfarjani (UC Santa Cruz), Giulia Galli (UC Davis), Gang Chen (MIT), Joseph Heremans (Ohio State University), Peter Kratzer (University of Duisburg-Essen), A. Lyakhov (SUNY, Stony Brook), Gerald Mahan (Pennsylvania State University), Takao Mori (National Institute for Materials Science, Namiki, Japan), A. Rastelli, (Leibnitz Institute, Dresden), M. Roger (CEA-Saclay, France), Ivana Savic (CEA Grenoble), J Sjakste (CNRS/Ecole Polytechnique), Ali Shakouri (UC Santa Cruz), Sebastian Volz (Ecole Centrale Paris), Paul Von Allmen (Jet propulsion Laboratory, Cal Tech), Shidong Wang (CEA Grenoble), Mona Zebarjadi (UC Santa Cruz).

Registration:
The workshop is open to all researchers interested in thermoelectric transport. Students and postdocs are especially encouraged to participate. Poster presentation slots are available. There is no registration fee.

To register please sign up on the Cecam website (http://www.cecam.org/signup.html), and then email the organizers (natalio.mingo@cea.fr) the following information, preferably by June 15:

First and last name: 
Job title:
Institution: 
Country:
E-mail: 
Telephone number:
Webpage (if any):
Presenting a poster? (Yes/No)
Description of Program

The program will cover a broad array of topics at the forefront of thermoelectrics research. Predicitve theoretical methods (such as first principles, molecular dynamics and monte carlo approaches) will be highlighted and their utility in addressing materials design issues for thermoelectrics will be elucidated.

Each day will consist of morning and afternoon sessions with oral presentations. Ample time for discussion will be provided in each session. In addition, there will be a late afternoon poster session on the Day 1 and a late afternoon panel discussion on Day 2. The focus of this panel discussion will be: a) to highlight the major current thermoelectrics challenges, b) to elucidate promising future directions and c) to identify and promote possible collaborative efforts between the international group of workshop participants. A summary of the tentative session workshop organization is provided below:

Day 1: Novel Materials for Thermoelectrics (2 Sessions)

Wednesday morning: Powder and nanoparticle composites

Gang Chen: (title unavailable)
A. Shakouri: Metal/semiconductor nanocomposites for thermoelectric energy conversion
M. Zebarjadi: thermoelectric materials with embedded nanoparticles
N. Mingo: nanoparticle composites: from simple modeling to ab-initio calculations.

Wednesday afternoon: New bulk materials

T. Mori: "Critical role of disorder in the thermoelectric properties of boron-rich compounds"
Nathalie Vast, E. Bertranhandy: "Boron and boron carbides from first principles"
Joseph Heremans: "Designing chemical bonds to enhance the thermoelectric figure of merit"
M. Roger: "Nanoscale patterning of sodium ions in thermoelectric Cobaltates. Consequences on transport properties"

Poster session

Day 2: Thermal transport (2 sessions)

Thursday morning: Nano-materials

S. Volz: (title unavailable)
A. Rastelli: Growth and thermal conductivity characterization of self-assembled SiGe/Si(001) nanocrystal multilayers.

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I. Savic: Green’s function approach to thermal transport in SiGe/Si(001) nanocrystal multilayers.

David Broido: First principles approach to thermal transport in bulk and nanostructured materials.


Thursday afternoon: Complex interfaces

Gerald Mahan: Kapitza thermal resistance between a metal and an insulator.
Keivan Esfarjani: Lattice thermal transport in point contacts and nanojunctions
Derek Stewart: A first principles approach to thermal resistance at interfaces

Panel Discussion: “Beating the ZT Barrier: Issues and Future Directions”

Day 3: Materials by Design (2 sessions)

Friday morning: Large scale ab-initio computations

G. Cuniberti: (title unavailable)
A. Lyakhov: "Evolutionary crystal structure prediction as a tool in materials design"
Giulia Galli: (title unavailable)
P. Von Allmen: (title unavailable)

Friday afternoon: Advances in electron transport theory

P. Kratzer, V. Fomin: Theory of Miniband Transport in Quantum Dots
Shidong Wang: Green’s function approaches to electron filtering in thermoelectric nanocomposites.
J. Sjakste: "Electron-phonon coupling in Si and semiconducting nanostructures: ab initio description of transport properties"