

## Workshop IV: Energy Conservation and Waste Heat Recovery

### Monday November 18, 2013

- 8:00–9:00 *Check-In/Light Breakfast (Hosted by IPAM)*
- 9:00–9:15 *Welcome and Opening Remarks*
- 9:15–9:40 **Claudia Draxl** (Humboldt-Universität)  
*Overview Workshop 1*
- 9:50–10:05 *Break*
- 10:05–10:30 **Matthias Scheffler** (Fritz-Haber-Institut der Max-Planck-Gesellschaft)  
*Overview Workshop 2*
- 10:40–11:05 **Graeme Henkelman** (University of Texas at Austin)  
*Overview Workshop 3*
- 11:15–11:30 *Break*
- 11:30–12:10 **Jennifer Lukes** (University of Pennsylvania)  
*Hybrid Atomistic-Continuum Simulations of Thermal-Fluid Transport at Interfaces*
- 12:30–2:30 *Lunch (on your own)*
- 2:30–3:10 **Giulia Galli** (University of California, Davis (UC Davis))
- 3:30–4:00 *Break*
- 4:00–4:40 **Carlos Levi** (University of California, Santa Barbara (UC Santa Barbara))  
*High temperature coatings technology for gas turbine systems: materials issues and fundamental research needs*
- 5:00–6:30 *Reception and Poster Session (Hosted by IPAM)*

### Tuesday November 19, 2013

- 8:00–9:00 *Continental Breakfast*
- 9:00–9:40 **Ivana Savic** (Tyndall National Institute, University College Cork)  
*Thermal Conductivity of SiGe Nanostructured Materials from Large Scale Atomistic Simulations*
- 10:00–10:15 *Break*
- 10:15–10:55 **Christian Carbogno** (Fritz-Haber-Institut der Max-Planck-Gesellschaft)  
*Thermal Transport from First Principles*
- 11:15–11:30 *Break*

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11:30–12:10 **Anton van der Ven** (University of California, Santa Barbara (UC Santa Barbara))

12:30–2:00 *Lunch (on your own)*

2:00–2:40 **Jayathi Murthy** (University of Texas at Austin)  
*Fast Computational Techniques for Sub-continuum Transport*

3:00–3:15 *Break*

3:15–3:55 **Irena Knezevic** (University of Wisconsin-Madison)  
*Semiclassical Phonon Transport in the Presence of Rough Boundaries*

4:15–4:30 *Break*

4:30–5:10 **Irene Gamba** (University of Texas at Austin)  
*Transport thermalization by electron-phonon interactions in nano scale devices*

### **Wednesday November 20, 2013**

8:00–9:00 *Continental Breakfast*

9:00–9:40 **Jorge Sofo** (Pennsylvania State University)  
*Thermoelectrics: A theoretical approach to the search for better materials*

10:00–10:15 *Break*

10:15–10:55 **Boris Kozinsky** (Bosch)  
*Path to predictive computations of thermoelectric effects for automotive waste heat recovery*

11:15–11:30 *Break*

11:30–12:10 **Derek Stewart** (Cornell University)  
*Using First Principles Thermal Transport to Aid in Energy Recovery and Conservation*

12:30–2:30 *Lunch (on your own)*

2:30–3:10 **Matthieu Verstraete** (Université de Liège)  
*Advanced ab initio methods in thermoelectrics: working more to relax more accurately*

3:30–4:00 *Break*

4:00–4:40 **Xiulin Ruan** (Purdue University)  
*First Principles-Enabled Simulations of Thermal Conductive and Radiative Properties of Solids*

## Thursday November 21, 2013

- 8:00–9:00 *Continental Breakfast*
- 9:00–9:40 **Yann Chalopin** (Centre National de la Recherche Scientifique (CNRS))  
*Thermal properties of phonon systems from fluctuations*
- 10:00–10:15 *Break*
- 10:15–10:55 **Yintao Song** (University of Minnesota, Twin Cities)  
*Energy Conversion by Multiferroic Phase Transformation*
- 11:15–11:30 *Break*
- 11:30–12:10 **Pinar Mengüç** (Özyeğin Üniversitesi)  
*Near Field Radiation Transfer for Energy Harvesting and Characterization'*
- 12:30–2:30 *Lunch (on your own)*
- 2:30–3:10 **Liping Liu** (Rutgers University)  
*A continuum theory of thermoelectric bodies and proposed large-scale application in energy conversion*
- 3:30–4:00 *Break*

## Friday November 22, 2013

- 8:00–9:00 *Continental Breakfast*
- 9:00–9:40 **Gang Chen** (Massachusetts Institute of Technology)  
*Simulating and Probing Phonon and Electron Transport for Thermoelectric Applications*
- 10:00–10:15 *Break*
- 10:15–10:55 **Emmanouil Kioupakis** (University of Michigan)  
*Electronic structure calculations of materials for efficient light emitters*
- 11:30–12:10 **Claudia Draxl** (Humboldt-Universität)  
*Organic molecular materials for light-emitting applications: a first-principles view*
- 12:30 *Conclusion*

