# CECAM Workshop Scientific Report

*Workshop:* Nanophononics

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## *I. Summary*

Nanophononics is a quite novel field defined as the control of heat transport in the nanoscale. The technological aspects of nanophononics are very promising. Control of nano-scale heat-flow would improve existing electronic devices, as well as lead to completely new applications in the fields of nano machines, electronics, refrigeration, energy transport and energy generation. It has been suggested that similar devices as those used for electronics can be developed for the control of phonon flows.

The workshop "Nanophononics" was held at the University of Bremen, Germany from September 19$^{th}$ to 23$^{rd}$ 2013. In total, 72 participants from Belgium, Brazil, Finland, Luxemburg, The Netherlands, Spain, Sweden, Switzerland, Finland, Denmark, France, Germany, China, Hongkong, Canada, Israel, Korea, Singapore, Italy, UK and US attended the workshop.

The programme consisted of 29 invited lectures, one poster session presenting 30 posters and many events (reception / conference dinner) to allow for informal exchange. The lectures were scheduled to last 40 min, including 5-10 min discussion time. In addition to this extended time for discussion, the chairpersons were instructed to introduce the subject of the session and to actively participate in the discussion. This "Gordon-conference-style" was essential to guarantee a vivid discussion. The organizers ensured that well-established scientists acted as invited speakers and chairpersons.

Concerning the poster session, we accepted only 30 posters to allow for an intense exchange of ideas at each single poster. Here, we encouraged in particular the young scientists to ask questions. The participation of PhD students was supported by partly covering local accommodation costs.

Due to the compact organization and accommodation in one hotel only all participants had to stay together for the whole time of the conference, which additionally enforced the scientific discussion which was mandatory since scientists from various separated fields, i.e. heat transport, quantum effects, atomistic and nesoscale approaches, scanning probe techniques, optical spectroscopy, phonon transport, electron-phonon interactions, etc. were attending the meeting to merge ideas and formulate a common goal for future directions and collaborations of theory groups with experimental groups.

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## *II. Scientific content, main outcome of key presentations*

Nanophononics is defined as the control of heat transport in the nanoscale. This kind of control would improve existing electronic devices, as well as lead to completely new applications in the fields of nano machines, electronics, refrigeration, energy transport and energy generation. It has been suggested that similar devices as those used for electronics can be developed for the control of phonon flows. The promise of phononics can bring changes as dramatic as the ones brought by electronics.

This field of Nanophononics is reaching a point where, to proceed forward it becomes clear, more exchange between theory, computational methods and experiments is needed. It is also important to have researchers working on different computational methods to exchange ideas in order to bridge methodological gaps. The workshop that brings all these together has contributed to focus the research field, helped to identify challenges and goals.

Scientific steps requiered in the next 3-4 years:

1) We must establish a big international collaboration. This field of Nanophononics is reaching a point where, to proceed forward more efficient exchange between theory, computational methods, and experiments is needed.

2) A new scalable computational method that is efficient and robust on realistic materials including anharmonic effects must be developed. For example, we want something like what TD-DFT did for electron dynamics, but for phonons.

3) Experiments that compare material properties are essential to allow the community to focus on promising materials and build devices.

4) Theoretical understanding of the role of phonon coherence in transport. Many discussions revolved around different aspect of this question, but there is no unified picture.

   Levels of computing from departmental machines to PRACE resources are needed. The system size of nanostructured materials calls for large scale resources e.g. for non-equilibrium molecular dynamics simulations.

## *III. selected discussions*

Finding new ways to control heat, like we control electrons now, will lead to new ways to improve the energy efficiency of devices e.g. via thermoelectric energy harvesting. If Europe wants to grow as a sustainable and innovative economy, EU2020 must incorporate phononics as one of its research initiatives, which will lead to new technologies/industries, which can push the climate/energy goals.

The single most important scientific challenge identified was the need to build a strong collaboration above a critical-mass, that will allow us to connect theory-computation-experiment to characterize materials and enable design of novel devices.

- First, we are now trying to combine efforts from many groups in Europe to establish a coherent collaboration in phononics. After the conference, we have had discussions over the internet to establish such a collaboration under the leading efforts of Clivia Sotomayor, Sebastian Volz, Jouni Ahopelto, Giovanni Cuniberti, and Thomas Frauenheim, among others. The goal is to close the loop of theory-computation-experiment that is necessary to improve the materials and techniques, as needed for phononic devices. We are in the process of identifying possible funding sources. We are also defining possible future conferences.

- Second, and connected to the previous point, we are now trying to combine efforts between Europe and China. Baowen Li is a leader of phononics in China/Singapore, with high visibility for funding agencies there, and is starting a new institute. In this

sense, China has an institutional head start on the field of phononics. However, he is eager to establish a strong collaboration between Chinese and European groups, as Europe has many strengths in experiments and novel computational methods. This seems like a very natural and necessary exchange, as the different groups identified are complimentary to each other. We are currently exploring funding sources to establish a big EU-China Phonon collaboration.

## *IV. Assessment of the results and impact on future direction of the field*

The individual objectives for this workshop which in detail have been achieved are:

- To demonstrate design and build new nanophononic devices. Although there are many systems being considered, an over-arching analysis of the strengths and weaknesses of each one has not been done. By bringing experts from many fields, a broader understanding of the capabilities of different systems has been achieved, such as molecular devices, nanowires, carbon nanotubes, etc. As a community, leading experts build upon this analysis to propose new kind of nanophononic devices.
- To identify the major principles to guide the design of materials. Strategies have been discussed which allow to go from the study of coarse-grained models of heat transport to the identification of nanomaterials with phononic applications. This will lead to a broader approach towards the design of phononic materials, and it will suggest new experiments to be performed.
- To understand the advances and limitations of various theoretical tools and computational methods. Many different theoretical and computational methods were summarized in workshop. The understanding of the realm of validity for many of these methods has been identified and compared. This will also lead to improved computational methods.
- To consolidate a Nanophononics research community. Many of the researchers in this field come from very different research backgrounds. Although it is clear that their research paths are intersecting in the topic of heat transport in nanoscopic systems, a proper community is only forming now. This conference provided the stage to define this field, and create awareness of it. This will have important implications for future publications and grants by the researchers. It will also allow setting new goals and milestones for this emerging field.
- To establish new collaborations between the participants. By achieving the previous goals, the workshop could achieve the goal of building a scientific network between scientists from Europe, United States and Asia that will take this field in future scientific directions.

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The Organizers