2018 Helmholtz – OCPC – Program

for the involvement of postdocs in bilateral collaboration projects

KIT-02

PART A

Title of the project:
Anharmonic lattice dynamics in materials for energy applications

Helmholtz Centre and institute:
Karlsruhe Institute of Technology (KIT), Institute for Solid State Physics (IFP)

Project leader:
PD Dr. Frank Weber

Web-address:
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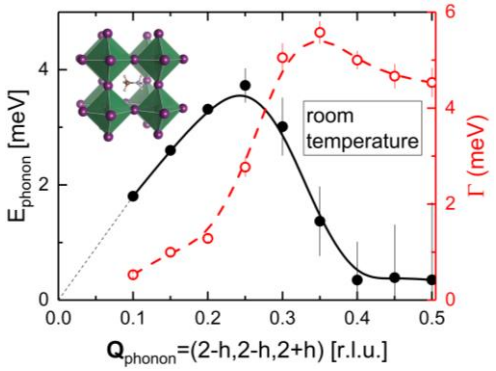
Description of the project (max. 1 page)**:**

The aim of this project is to study anharmonic lattice dynamics in two important classes of materials for energy applications. We want to elucidate the impact of phonon properties on the ultra-low thermal conductivity in thermoelectric PbTe and on the exciting optical properties in organic-inorganic lead halide perovskites employed for high-performance solar cell applications.

Thermoelectric materials are interesting for energy applications as they can transform heat into useful electricity. The energy transformation efficiency of a thermoelectric material is determined by the figure of merit, $ZT = \sigma S^2 T/(\kappa_L + \kappa_E)$ [κ_L (κ_E): lattice (electronic) component of thermal conductivity, σ: electrical conductivity, S: Seebeck coefficient, T: absolute temperature]. This formula expresses the fact that the electrical energy produced is in the form of a current driven by the thermoelectric voltage, which is given by $-S\Delta T$, whereas heat conduction and electrical resistance are parasitic. Thus, efficient thermoelectric materials must have a low thermal conductivity, to preserve the temperature gradient exploited to generate a voltage. Therefore, reducing κ_L is central to obtaining high-performance thermoelectrics. Recent inelastic neutron scattering experiments in one of the most studied thermoelectric materials **PbTe** [1] revealed strongly anharmonic behaviors in phonon scattering which were proposed to play an important role in producing the extremely low lattice thermal conductivity of $\kappa_L = 2\ \mathrm{Wm^{-1}K^{-1}}$ [2]. ***Within this project*****,** we seek at exploring the relation between these anomalous phonons and κ_L by tuning the crystal structure of PbTe with pressure. The successful applicant will study the evolution of lattice dynamics as function of pressure ($p \leq 6\ \mathrm{GPa}$) and temperature employing high energy resolution inelastic x-ray (IXS) and neutron scattering (INS) experiments on single crystals of PbTe. Our measurements and accompanying *ab-initio* modelling will provide a detailed understanding of the intriguing lattice dynamical properties of PbTe, and pave the path for the designs of new high-performance thermoelectric materials.

The past five years have seen an unprecedented increase of the efficiency of solar cells based on **organic-inorganic halide perovskites** (OIHPs). In fact, the power-conversion efficiencies of the best research-cells are coming close to those of Silicon-based devices while promising cheaper production and a larger variety of cell structures adoptable to different environments. Various reports suggest strong phonon-phonon as well as electron-phonon interaction of photo-excited electrons. In 2017, it was suggested [3] that phonons are responsible for the slow carrier recombination and, hence, for long carrier life times. ***Within this project*****,** the successful applicant will study the lattice dynamics of OIHPs using IXS and INS. While IXS mostly reveals the dynamics of the heavy ions, e.g., lead, INS on deuterated samples grown at IFP enables the investigation of vibrations of the lighter ions and also rotational movements of the organic molecule. Preliminary IXS data for an OIHP (see figure) reveal a pronounced anomaly at $h > 0.25$ of a transverse acoustic (TA) phonon. The evolution of this ultra-soft phonons in the operating temperature range of OIHP solar-cells will be relevant for the low thermal conductivity of OIHPs and might be related to the phonon-assisted carrier recombination.



Dispersion E_{phonon} and linewidth Γ of the TA soft phonon mode in an OIHP.

[1] Delaire *et al.*, Nat. Mat. **10**, 614 (2011); [2] Chen et al., Phys. Rev. Lett. **113**, 105501 (2014); [3] Hutter et al., Nat. Mat. **16**, 115 (2017).

Description of existing or sought Chinese collaboration partner institute (max. half page)**:**

The University of Hong Kong Shenzhen Institute of Research and Innovation (HKU-SIRI) established in 2011 with the support of the Shenzhen Municipal Government, is an integral part and an extension into mainland China of the research conducted by the University of Hong Kong (HKU). HKU-SIRI is a member institution of Shenzhen Virtual University Park, which has developed a postdoctoral research station registered with the Office of the China Postdoctoral Council (OCPC) to integrate postdoctoral stations of member institutions. HKU-SIRI plays an important role in transferring science and technology from HKU to mainland China.

The group of Dr. Yue Chen at HKU-SIRI specializes in the studies of materials physics for thermal and electrical transports, such as lattice dynamics and electronic structures. In particular, he has been focusing on the phonon coupling problems in thermoelectric materials using density functional theory-based first-principles methods. He is experienced in studying the intrinsic ultralow thermal conductivities of crystalline solids with strong lattice anharmonicity and the related phonon scattering mechanisms.

In 2017, a collaboration between the group of Dr. Yue Chen and the neutron scattering group at the Institute for Solid State Physics, KIT, was established in order combine our efforts in lattice dynamical investigations of materials of current interest. This collaboration takes advantage of the combination of the experimental and theoretical expertise of the KIT and HKU-SIRI groups, respectively, and will allow us to microscopically understand the lattice dynamics in the above proposed materials PbTe and OIHPs.

Required qualification of the post-doc:

- PhD in physics or a related subject
- Experience with solid state physics
- Additional skills in neutron scattering and/or ab-initio calculations are beneficial

PART B

Documents to be provided by the post-doc, necessary for an application to OCPC via a postdoc-station in China, which is affiliated to a research institution like a university:

- Detailed description of the interest in joining the project (motivation letter)
- Curriculum vitae, copies of degrees
- List of publications
- 2 letters of recommendation
- Proof of command of English language

PART C

Additional requirements to be fulfilled by the post-doc:

- Max. age of 35 years
- PhD degree not older than 5 years
- Very good command of the English language
- Strong ability to work independently and in a team