Ab-initio investigation of thermoelectric properties of low-dimensional and topological systems

Keywords: low-dimensional systems, thermoelectricity, energy applications, topology, numerical simulations

Scientific description:

In the last years it has become evident that fossil fuels, like coal and gas, need to be replaced by more sustainable (in terms of pollution and availability) sources such as solar or thermal energy. However, in order to do so, it is important to find suitable materials allowing for optimal energy conversion.

The present (M2) master project focuses on the theoretical ab-initio study of low-dimensional materials for thermoelectric applications (e.g. Bismuth-based systems [1,2] or Janus 2D materials [3,4]).

The *thermoelectric effect* refers to phenomena by which either a temperature difference creates an electric potential or an electric current creates a temperature difference. Thermoelectric materials are used in thermoelectric systems for cooling or heating in niche applications, and are being studied as a way to regenerate electricity from waste heat. Their performance is evaluated by the figure of merit ZT (where T is the temperature):

$$ZT = \frac{S^2 \sigma T}{\kappa}$$

where S is the Seebeck coefficient, σ is the electrical conductivity and κ is the thermal conductivity. An optimal thermoelectric material has a high value of ZT: while the simultaneous optimization of electronic and thermal parameters is not easily feasible, low-dimensionality and topological states seem to be promising for the actual decoupling of these two aspects [5,6].

The aim of the students will be to use state-of-the art ab-initio techniques to investigate the effect of low-dimensionality and/or topological phase transition on the electronic structure as well as transport (electronic and thermal) properties.

[1] J. Mater. Chem. C, 3, 11999 (2015)
[2] Phys.L Rev. Mat. 6, 074204 (2022)
[3] J. Phys. Chem. C 125, 20 (2021)
[4] ACS Appl. Mater. Interfaces 12, 41 (2020)
[5] npj Quantum Materials 2, 51 (2017)
[6] Phys. Rev. Mat. 5, 025404 (2021)

Methods in use:

Density Functional Theory (DFT), GW corrections, anharmonicity (SSCHA), tight-binding methods

Applicant skills:

A strong background in solid state physics as well as knowledge of electronic structure theory and computataional languages (Fortran, C++, Python, Julia).
Previous experience of DFT codes (e.g. Quantum ESPRESSO) would be advantageous.

Possibility for a PhD:

Yes, subject to funding availability

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