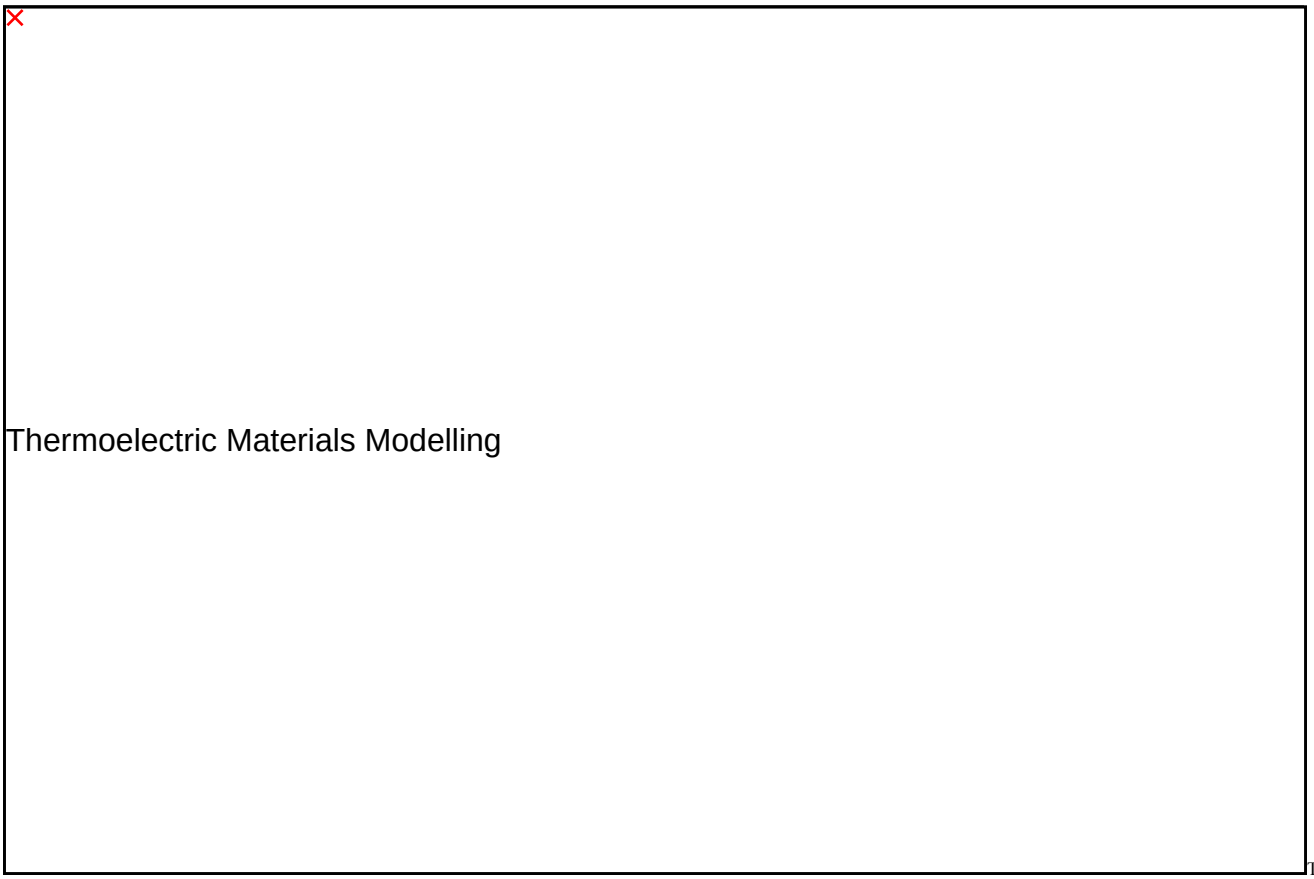
Thermoelectric Materials

First principles modelling of thermoelectric materials

Thermoelectric materials enable conversion between thermal and electrical energy, which makes them attractive for a range of applications, such as waste heat harvesting and powering autonomous wireless sensors.

The key physical properties for good thermoelectric performance are high electrical conductivity, high Seebeck coefficient and low thermal conductivity. In many materials the improvement of one of these characteristics leads to a disimprovement of others, and optimization of the overall thermoelectric performance is highly challenging.



Thermoelectric Materials Modelling

We develop theoretical and computational approaches to understand, interpret and predict thermoelectric transport properties of materials from first principles. Our goal is to develop novel conceptual frameworks to design materials whose thermoelectric efficiency will exceed that of the currently highest-performing materials.

At present we are investigating IV-VI and V2-VI3 materials, which are among few naturally occurring materials that exhibit good thermoelectric efficiency. We aim to identify and manipulate the key physical mechanisms that determine their good thermoelectric properties.

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Related Publications

- Broadband phonon scattering in PbTe-based materials driven near ferroelectric phase transition by strain or alloying
  Physical Review B volume **93** issue **10** (2016)
  Authors: Ronan M. Murphy, Éamonn D. Murray, Stephen Fahy, Ivana Savić

- Dimensionality and heat transport in Si-Ge superlattices
  Applied Physics Letters volume **102** issue **7** page **073113** (2013)
  Authors: Ivana Savić, Davide Donadio, François Gygi, Giulia Galli

- Lattice thermal conductivity of semiconducting bulk materials: atomistic simulations
  Physical Chemistry Chemical Physics volume **14** issue **47** page **16209** (2012)
  Authors: Yuping He, Ivana Savić, Davide Donadio, Giulia Galli

- Precise control of thermal conductivity at the nanoscale through individual phonon-scattering barriers
  Nature Materials volume **9** issue **6** pages **491 to 495** (2010)
  Authors: G. Pernot, M. Stoffel, I. Savic, F. Pezzoli, P. Chen, G. Savelli, A. Jacquot, J. Schumann, U. Denker, I. Mönch, Ch. Deneke, O. G. Schmidt, J. M. Rampnoux, S. Wang, M. Plissonnier, A. Rastelli, S. Dilhaire, N. Mingo