Novel directions for thermoelectric energy materials with record-high power factors

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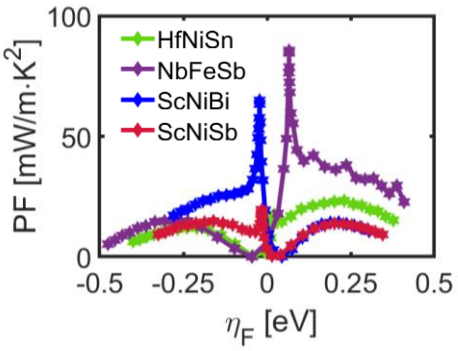

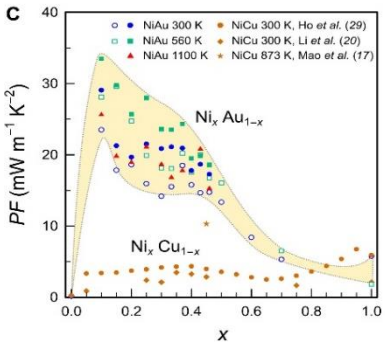

(a) Graziosi et al: Low bandgap material ultra-high power factor peak (2020)
(b) From TU Vienna group: Power factor of an asymmetric metal at ultra-high levels. (2023).

Typical thermoelectric material power factors are at PF = 1-5 mW/mK^2.

Project outline:

The need for energy sustainability and the environmental consequences of fossil fuels make the development of technologies for clean energy imperative. Thermoelectric (TE) materials can harvest enormous amounts of waste heat and convert it into useful electrical power. As 60% of all energy we use is lost into heat during conversion processes, the realization of efficient and scalable TEs can transform the energy-use/savings landscape and play a major role in net-zero sustainability. However, TEs have not found widespread use because of low material efficiencies.

Over the last several years, however, advancements in synthesis and growth have realized many materials with complex electronic structures, with the potential of realizing an advanced energy harvesting technology to contribute towards the net-zero goal. Traditionally, high power factor TE materials have many elongated bands and a sizable bandgap, the latter thus, excludes metals. Very recently, however, the notion that low-bandgap materials, metals, and semimetals are bad TEs, has been strongly challenged. A series of theoretical and experimental works demonstrated that under certain conditions (strong transport energy asymmetry), they can offer record-high TE power factors.

The project uses Density Functional Theory coupled to advanced electronic transport methods, to investigate the TE performance of complex electronic structure materials with low bandgap, metals, and semimetals. It uses machine learning to develop simpler models and descriptors to scan available databases and identify high performance candidates. Through appropriate alloying, the transport energy asymmetry can be further increased, and even higher power factors achieved.

Experimental measurements for optimal materials to be identified, and theory validation, will be available from the literature, and through the work of the co-supervisor (Physics) who can grow materials using molecular beam epitaxy using a wide range of elements.

Links to other research projects:

The project has links to the funded (UKRI undertaken) ERC Grant COMPLEXthermMA

Link to the on-going FET-Open Grant UncorrelaTEd, to the completed Marie Curie project GENESIS and the already completed ERC Grant NANOthermMA:

An EPRSC proposal is under review for low bandgap thermoelectrics, together with experimentalists.

https://warwick.ac.uk/fac/sci/eng/research/grouplist/sensorsanddevices/computational_nanotechnology_lab/projects/#currentprojects

Likely outcomes after 4 years:

1. Development of a theoretical framework and a simulator that utilizes DFT for the electronic structure of low bandgap materials and semimetals and their alloys. It includes the electronic structure of alloys, relevant scattering parameters, and puts them into a form to be used in Boltzmann Transport codes.
2. Develop the generalized design guidelines that will open the pathway for low gap materials and semimetals with asymmetric transport energy features and record-high power factors.
3. Identify a few material designs with exceptional performance which can be tested by experiment. Materials from the Heusler and half-Heusler groups will be targeted.

Possible future collaborations/projects:

Collaborations with experimental partners that will test the design ideas/concepts on different types of alloys materials (St Andrews – J.W. Bos, TU Vienna – E. Bauer, etc.).

Expand modeling studies in a variety of complex bandstructure, low bandgap materials and semimetals to enhance asymmetry and reduce thermal conductivity for high ZT.

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