



Contents lists available at ScienceDirect

Journal of Materiomics

journal homepage: www.journals.elsevier.com/journal-of-materiomics/

Disruptive new concepts in thermoelectricity

Over the last few years, alongside a remarkable effort to improve the efficiency and reliability of various classes of thermoelectric materials, several novel ideas have surfaced to overcome factors limiting heat conversion and refrigeration, both on the materials side and at the device level. On the first count, new strategies have emerged taking advantage of the growing capabilities of modeling charge carrier and phonon transport in defective materials, engineering defects to evade the materials efficiency limits set by the contrasting need of decreasing materials thermal and electrical conductivity. On the other count, attention has been focused on novel device layouts and on the possibility of reusing mature thermoelectric materials in high-demanding contexts such as heat harvesting from non-planar surfaces. Overall, thermoelectric research appears to be on the cusp of a new breakthrough, potentially comparable to the nanotechnology revolution it underwent in the 1990s [1].

Considering such recent advancements, this special issue of the *Journal of Materiomics* aims at presenting such disruptive new concepts, disseminating them toward the growing community of scholars working on thermoelectrics – and to current and prospective end-users of the thermoelectric technologies.

On the device side, geometry-engineered thermoelectric devices are discussed by Haiyang Li *et al.* [2], showing how the geometric design of thermoelectric legs has emerged as a transformative strategy to regulate thermal and electrical transport and ultimately improve efficiency. To this aim, computational modelling methods are advanced for designing geometry-optimized devices, including gradient-based and non-gradient-based techniques as well as machine learning approaches.

On the materials side, Hang Yin *et al.* [3] shows how the photothermoelectric performance of SnSe strongly depends on the crystallographic quality of single-crystal films. Undoped and Na, Cu-doped SnSe films were deposited *via* pulsed laser deposition on SrTiO₃ substrates. Authors found that the growth mode of SnSe films transitions from island-by-layer to 3D island growth as the film thickness increases. Notably, Na, Cu-doped SnSe films reported enhanced performances, enabling its potential for integrated photoelectric-thermoelectric applications.

The role played by suitably engineered grain boundaries also in high-temperature thermoelectric materials is discussed by Duncan Zavanelli *et al.* [4]. Although electrical resistance from grain boundaries decays exponentially with increasing temperature, authors demonstrate that grain boundary resistance remains pivotal even in high temperature thermoelectrics. Paradoxically enough, thermoelectric performance of La₃Te₄ is found to be more

dependent on grain size at high rather than low temperatures, suggesting an unprecedented form of boundary resistance, linearly increasing with temperature as expected in metals – remarking how grain boundary engineering remains needed even for high temperature applications.

A novel strategy to reduce thermal conductivity in half-Heusler compounds is proposed by Rahidul Hasan *et al.* [5], reporting about a new n-type Ti₂CoNiSb₂ compound with 18.5 valence electrons, thus intentionally breaking the conventional valence balance. When Cu, Bi cooping is carried out, both phonon scattering and weighted mobility simultaneously increase, particularly at high temperatures. As a result, a peak figure of merit is achieved at 973 K, where it reaches a value four times higher than in the pristine compound, therefore highlighting the effectiveness of co-doping strategies to concurrently optimize thermal and electronic transport properties.

Device layout and materials co-optimization are finally discussed in the making of flexible thermoelectric generators, which have emerged as promising candidates to power wearable electronics. Kun Hu *et al.* [6] report about strategies to qualify inorganic thermoelectric material to make efficient, flexible thermoelectric generators. More factors are shown to govern output power density, namely, the power factor of thermoelectric materials, device geometry, packaging, and the effective temperature gradient that is applied across the device. Concerning materials properties, carrier scattering and density modulation along with energy band engineering are shown as the most promising methods to enhance the power factor, while integration of hydrogels and phase change materials into flexible heat sinks are reported as effective ways to establish and maintain sufficiently large temperature differences.

In summary, this Special Issue will provide readers with a collection of highly inspiring perspective papers that, beyond summarizing the state of the art in the thermoelectric field, is expected to disseminate new, promising ways to enhance the efficiency of thermoelectrics, leveraging their use for both microgeneration, supplying energy to distributed, low-power sensors and actuators, and waste heat recovery at a larger scale.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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This article is part of a special issue entitled: New Concepts in Thermoelectricity published in Journal of Materiomics.

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Available online 31 December 2025