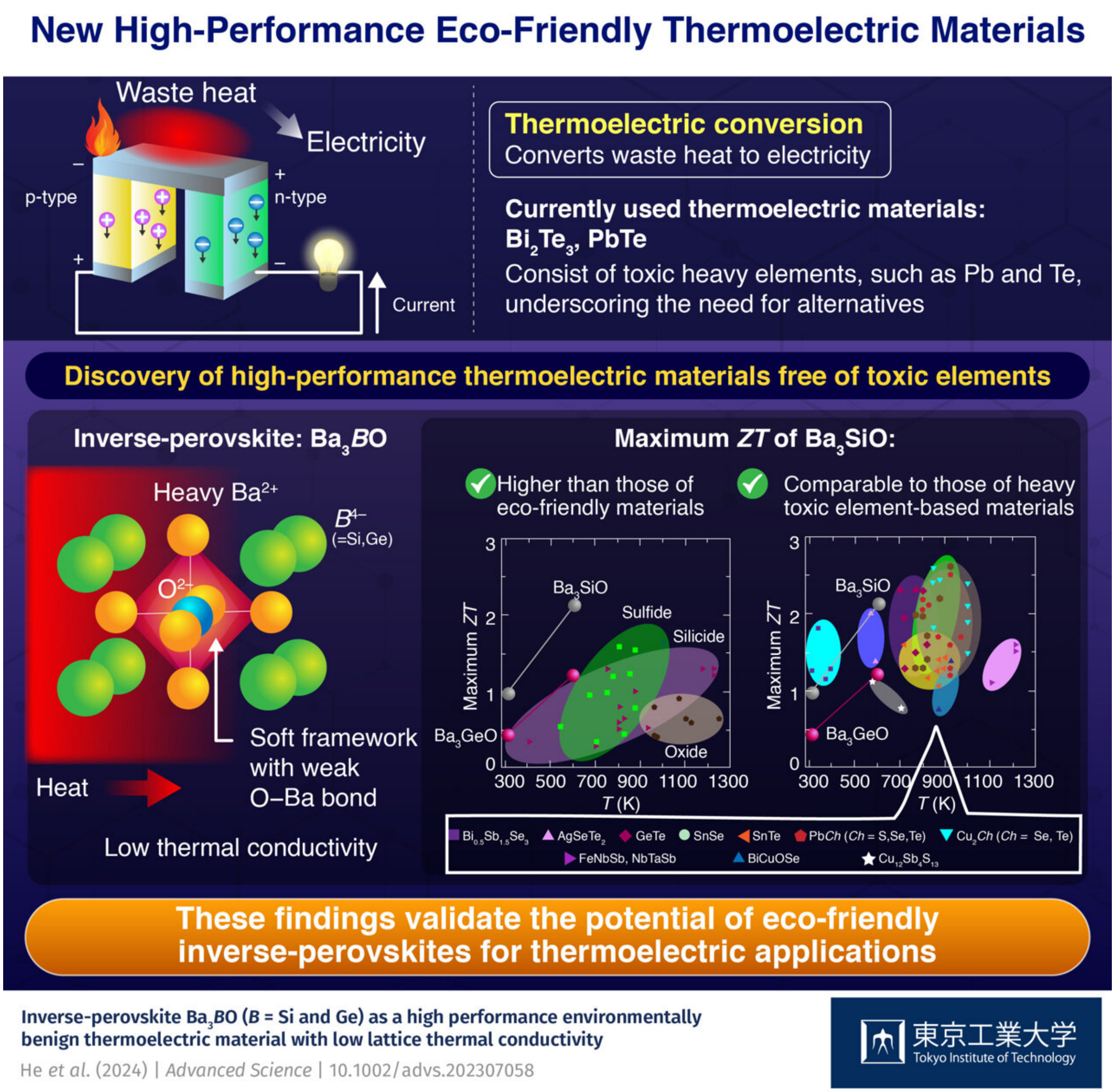
Realizing eco-friendly and high-performance thermoelectric materials

January 11 2024



The new TEMs provide a suitable alternative to TEMs based on toxic elements with better thermoelectric properties than conventional eco-friendly TEMs. Credit: Tokyo Institute of Technology

In a new study, environmentally benign inverse-perovskites with high energy conversion efficiency have been reported by Tokyo Tech scientists with potential for practical application as thermoelectric materials (TEMs). Addressing the limitations typically faced with TEMs, such as insufficient energy conversion efficiency and environmental toxicity due to heavy elements, the new TEMs provide a suitable alternative to TEMs based on toxic elements with better thermoelectric properties than conventional eco-friendly TEMs.

Thermoelectric materials (TEMs) capable of converting thermal energy to electrical energy and vice versa have become an essential part of our world, which needs better waste-energy harvesting systems and cooling systems for electronic gadgets.

The energy conversion efficiency of TEMs depends on a dimensionless figure of merit (ZT), which is a product of two different factors: the inverse of thermal conductivity (k) and the power factor (PF).

A high-performance TEM exhibits a high ZT if it possesses low k and high PF. Over the years, scientists developed several high-performance heavy metal chalcogenide-based TEMs, such as Bi_2Te_3 and PbTe, that fulfill these criteria. While these materials were ideal for energy conversion, they were toxic to the environment and the health of living organisms—they contained toxic heavy elements, such as lead (Pb) and tellurium (Te), which limited their practical applications.

On the other hand, although oxide-based TEMs, such as $SrTiO_3$, have several advantages of non-toxicity and abundant natural resources, their ZT has been limited due to their high k.

To address this, a research team led by Associate Professor Takayoshi Katase from Tokyo Institute of Technology explored efficient yet environmentally benign toxic-element-free TEMs. In their study published in *Advanced Science*, the researchers present "inverse"-perovskite-based high ZT TEMs with the chemical formula Ba_3BO, where B refers to silicon (Si) and germanium (Ge).

"Unlike normal perovskites, such as $SrTiO_3$, the positions of cation and anion sites are inverted in inverse-perovskites Ba_3BO. So, they contain a large amount of the heavy element, Ba, and their crystal structure is formed by a soft flamework made up of weak O-Ba bonds. These characteristics realize the low k in inverse-perovskites," says Dr. Katase, elaborating on the standout properties of the materials.

The research team clarified the synthesized bulk polycrystals of Ba_3BO possess extremely low k of 1.0–0.4 W/mK at a T of 300–600 K, which is lower than those of Bi_2Te_3 and PbTe bulks. As a result, the Ba_3BO bulks exhibit rather high ZT of 0.16-0.84 at T = 300–623 K.

Additionally, the team carried out theoretical calculations which predicted a potential maximum ZT of 2.14 for Ba_3SiO and 1.21 for Ba_3GeO at T = 600 K by optimizing hole concentration. The maximum ZT of these non-toxic TEMs is much higher than that of other eco-friendly TEMs and comparable to the toxic heavy element ones in the same temperature range.

In addition, the team clarified that the high ZT of Ba_3BO is due not only to its low k but also its high PF: B ion, which usually behaves as a positively charged cation but as a negatively charged anion in Ba_3BO. The B anions are responsible for the carrier transport, which achieves high PF.

In summary, this study validates the potential of the newly designed Ba_3BO as a high-performing and eco-friendly alternative to conventional toxic, heavy element-based TEMs.

The results establish inverse-perovskites as a promising option for developing advanced environmentally benign TEMs. In this regard, Dr. Katase concludes, "We believe that our unique insight into designing high ZT materials without using toxic elements would have a strong impact on the materials science and chemistry communities as well as among innovators looking to expand the horizon of thermoelectric material applications beyond laboratories into our everyday life."

More information: Xinyi He et al, Inverse-Perovskite Ba_3BO (B = Si and Ge) as a High Performance Environmentally Benign Thermoelectric Material with Low Lattice Thermal Conductivity, *Advanced Science* (2023). DOI: 10.1002/advs.202307058

Provided by Tokyo Institute of Technology