


# Towards more efficient and eco-friendly thermoelectric oxides with hydrogen substitution

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## Towards More Efficient and Eco-Friendly Thermoelectric Oxides with Hydrogen Substitution



Thermoelectric material can convert waste heat into electricity

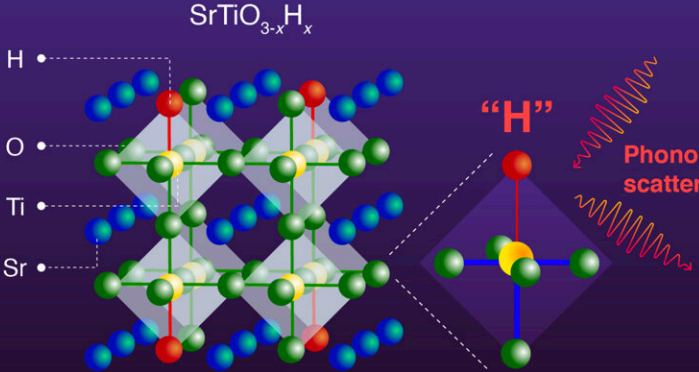
Requirements:

- Low thermal conductivity  $\kappa$
- High electrical conductivity

	$\text{Bi}_2\text{Te}_3$	$\text{SrTiO}_3$
Resource	×	⊙
Toxicity	×	⊙
Efficiency	High	Low
$\kappa$	⊙ Low	×

**Hydrogen anion ( $\text{H}^-$ ) substitution in polycrystalline  $\text{SrTiO}_3$  reduces:**

**Thermal conductivity**



$\text{SrTiO}_{3-x}\text{H}_x$

H

O

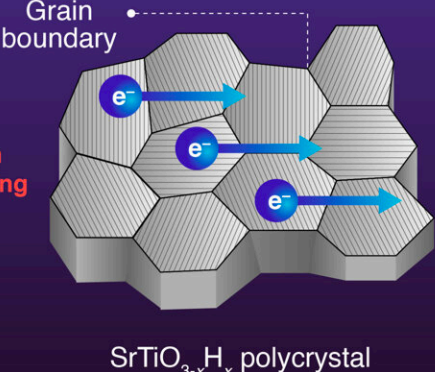
Ti

Sr

“H”

Phonon scattering

**Grain boundary barrier**



Grain boundary

$\text{SrTiO}_{3-x}\text{H}_x$  polycrystal

**The  $\text{H}^-$  substitution approach can realize excellent environmentally benign thermoelectric materials without the use of heavy elements**

Hydride anion substitution boosts thermoelectric performance of polycrystalline  $\text{SrTiO}_3$ , via simultaneous realization of reduced thermal conductivity and high electronic conductivity

He et al. (2023) | *Advanced Functional Materials* | DOI: 10.1002/adfm.202213144

Credit: Tokyo Tech

Today, over half of the total energy produced from fossil fuels is discarded as waste heat, which accelerates global warming. If we could convert the waste heat into a more useful form of energy like electricity, we could minimize fuel consumption and reduce our carbon footprint. In this regard, thermoelectric energy conversion has gained momentum as a technology for generating electricity from waste heat.

For efficient conversion, a [thermoelectric material](#) must have a high conversion efficiency (ZT). So far, realizing a high ZT has been possible only with the use of heavy elements like lead, bismuth, and tellurium. However, the use of rare, expensive, and environmentally toxic elements such as these has limited the large-scale application of thermoelectric energy conversion.

To tackle these issues, [transition metal oxides](#) based on platforms such as  $\text{SrTiO}_3$  have emerged as a more inexpensive and benign alternative. However, their ZT is typically limited by a [high thermal conductivity](#) ( $\kappa$ ), since for a high  $\kappa$ , the temperature across the material becomes uniform more quickly, and the lowered temperature difference—the [driving force](#) behind the thermoelectric conversion—causes electric power generation to decrease as well.

Against this backdrop, a research team including Associate Professor Takayoshi Katase from Tokyo Institute of Technology (Tokyo Tech), Japan recently discovered a new approach to reducing  $\kappa$  and boosting the performance of  $\text{SrTiO}_3$  by hydrogen substitution.

Conventionally, the use of light elements is expected to increase the  $\kappa$  originating from lattice vibration ( $\kappa_{\text{lat}}$ ), leading to the adoption of heavy elements to reduce the  $\kappa_{\text{lat}}$ . In contrast, in their study published in *Advanced Functional Materials*, the team discovered that the  $\kappa_{\text{lat}}$  of  $\text{SrTiO}_3$  could be reduced to less than half its original value by substituting a light element, namely hydrogen.

They clarified the mechanism underlying their observation using first-principles calculations, which showed that substituting a portion of the oxygen anions ( $\text{O}^-$ ) with hydrogen anions ( $\text{H}^-$ ), yielding compounds of the form  $\text{SrTiO}_{3-x}\text{H}_x$ , results in a mixture comprising a strong Ti-O bond and a weak Ti-H bond. These randomly distributed Ti-(O,H) bonds, in turn, largely decrease  $\kappa_{\text{lat}}$ .

The team also found that  $\text{SrTiO}_{3-x}\text{H}_x$  polycrystals exhibit high electron mobility comparable to that of single-crystal materials without any deterioration in electron conduction across grain boundaries. Based on these two effects, a [low thermal conductivity](#) along with a high electrical output power are realized at the same time, resulting in an improved thermoelectric conversion efficiency in the  $\text{SrTiO}_{3-x}\text{H}_x$  polycrystal.

Overall, these findings can open doors to innovative strategies for developing next-generation thermoelectric materials. "In future, the hydrogen substitution approach would realize excellent environmentally benign thermoelectric materials that do not require the use of heavy elements," concludes Dr. Katase.

**More information:** Xinyi He et al, Hydride Anion Substitution Boosts Thermoelectric Performance of Polycrystalline  $\text{SrTiO}_3$  via Simultaneous Realization of Reduced Thermal Conductivity and High Electronic Conductivity, *Advanced Functional Materials* (2023). [DOI: 10.1002/adfm.202213144](https://doi.org/10.1002/adfm.202213144)

Provided by Tokyo Institute of Technology

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