# Researchers report record performance for bismuth-based Zintl material

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An international team led by researchers from the University of Houston has reported record thermoelectric performance from rarely studied bismuth-based Zintl phases, work that could lead to a new class of thermoelectric material.

The new material is non-toxic and can be used at temperatures between 500 degrees and 600 degrees Celsius, or around 1,000 degrees Farenheit. The research is described in a paper published this week in the *Proceedings of the National Academy of Sciences*.

Thermoelectric materials produce electricity by exploiting the flow of thermal current from a warmer area to a cooler area and are currently used in both subsea and aerospace applications. Widespread adoption of this form of clean energy has been hampered, however, by the relatively low efficiency of available materials; that is, they convert heat to electricity at a relatively low rate, which is determined by the figure of merit, or ZT.

Zintl compounds - a class of materials named after the German chemist Eduard Zintl, who developed the idea of a metal/nonmetal compound - are considered potential candidates for thermoelectric materials.

But bismuth-based Zintl compounds haven't been widely studied, said Zhifeng Ren, MD Anderson Chair Professor of physics at the University of Houston and lead author on the paper. Zintl materials in general are often overlooked as potential thermoelectric materials because they

usually don't efficiently convert heat to electricity, Ren said.

The researchers reported that the new material - described by the formula $(Eu_{0.5}Yb_{0.5)1-x}Ca_xMg_2Bi_2$ - had a figure of merit of 1.3 at 873 Kelvin (600 degrees Celsius), higher than that recorded for antimony-based Zintl compounds.

That translates to an efficiency of about 10 percent, said Ren, who also is a principal investigator at the Texas Center for Superconductivity at UH. Top efficiency for current single thermoelectric materials is about 12 percent.

"This new Bi-based Zintl phase with high thermoelectric properties could be a good thermoelectric material candidate in the future," the researchers wrote.

In the paper, they describe the use of band engineering and multi strain field fluctuation to enhance the figure of merit for the material. "This ZT value is the highest ever reported in a CaAl2Si2-based structure, especially compared to the most popular Sb-based Zintl compounds," they wrote. "We confirm chemical disorder has no effect on valence band, but does affect the conduction band, resulting in good p-type TE properties."

In addition to Ren, authors on the paper include Ching-Wu "Paul" Chu, chief scientist at the Texas Center for Superconductivity at UH; Jiming Bao, associate professor of electrical and computer engineering at UH; Zhuan Zhu and Jing Shuai, graduate students at UH; Zihang Liu, Huiyuan Geng and Jiehe Sui of the Harbin Institute of Technology in China; Chao Wang of the University of Electric Science and Technology in China, and Yucheng Lan of Morgan State University.

**More information:** Higher thermoelectric performance of Zintl

phases (Eu0.5Yb0.5)1−xCaxMg2Bi2 by band engineering and strain fluctuation, *PNAS*, www.pnas.org/cgi/doi/10.1073/pnas.1608794113

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