Thermoelectric energy conversion via inorganic metal halide perovskites under tailored mechanical deformation

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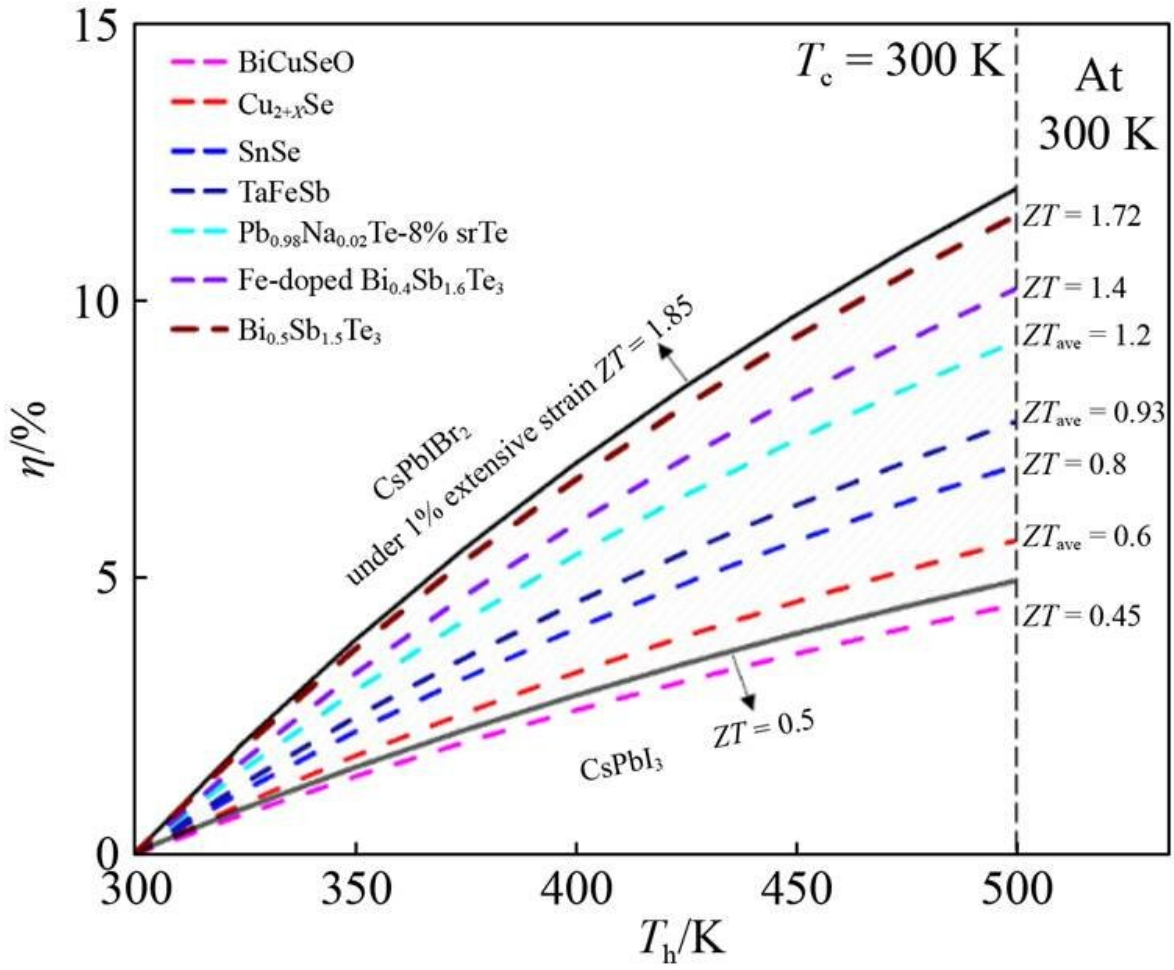

Thermoelectric energy conversion efficiency of inorganic halide perovskites compared with other thermoelectric materials. Credit: HIGHER EDUCATION PRESS LIMITED COMPANY

Solid-state thermoelectric energy conversion devices attract broad research interests because they show great promise in waste heat recycling, space power generation, deep water power generation, and temperature control, but the search for the essential thermoelectric materials with high performance remains challenging.

A research group of Lingling Zhao from Southeast University and Shangchao Lin from Shanghai Jiao Tong University just investigated inorganic metal halide perovskites $CsPb(I_{1-x}Br_x)_3$ under mechanical deformation systematically using the first-principle calculations and the Boltzmann transport theory. They demonstrate that intrinsic strains can be introduced into thermoelectric devices under mechanical deformation, which opens up a new technical approach for improving the stability and thermoelectric performance of perovskite materials.

Halogen mixing and mechanical deformation are efficient methods to tailor the electronic structures and charge transport properties in $CsPb(I_{1-x}Br_x)_3$ synergistically. The strain effect is related to the energy level shift of the electronic band structure CBM of perovskite. The power generation efficiency of the thermoelectric device can reach as high as approximately 12% using mixed halide perovskites under tailored mechanical deformation when the heat-source is at 500 K and the cold side is maintained at 300 K, surpassing the performance of many existing bulk thermoelectric materials.

Published in *Frontiers in Energy*, this study can provide theoretical guidance for the transport performance regulation of perovskite and the performance improvement of thermoelectric devices.

More information: Lifu Yan et al, High performance solid-state thermoelectric energy conversion via inorganic metal halide perovskites

under tailored mechanical deformation, *Frontiers in Energy* (2022). DOI: 10.1007/s11708-022-0831-y