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Research Highlights

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MANA Scientists Employ Active Machine Learning to Enhance Thermoelectric Performance of Materials

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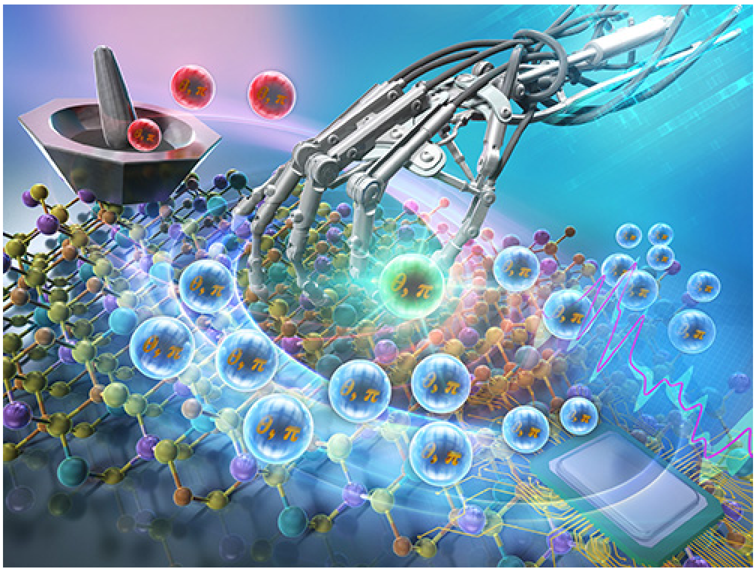
Scientists from the Research Center for Materials Nanoarchitectonics (MANA) have integrated machine learning with traditional materials science to expedite the discovery of kesterite-type thermoelectric materials, paving the way for efficient energy conversion technologies.



Kesterite-type materials, like Cu_2ZnSnS_4, are promising thermoelectric (TE) materials that convert waste heat into electricity. These non-toxic materials are composed of abundant, easily accessible elements and exhibit a figure of merit (zT), a quantity that measures thermoelectric efficiency, of greater than 1 at temperatures between 300 and 800K (26 to 526°C). Around 500K, kesterites undergo a transition from an ordered to a disordered one cationic structure, which affects their TE properties significantly. However, identifying optimal manufacturing conditions is time-consuming and requires multiple experiments.

Researchers from MANA used machine learning to accelerate this process. In just four experimental cycles, they optimized the sintering process, improving the thermoelectric performance of $Cu_{2.125}Zn_{0.875}SnS_4$ by 60%. The study was led by Dr. Cédric Bourgès from the International Center for Young Scientists, along with Guillaume Lambard from Center for Basic Research on Materials as well as Naoki Sato, Makoto Tachibana, Satoshi Ishii, and Takao Mori from MANA, NIMS, Japan.

The researchers employed Active Learning with Bayesian Optimization (ALMLBO), which analyzes sintering parameters—such as heating rate, sintering temperature, holding time, cooling rate, and applied pressure—alongside thermoelectric properties obtained from experiments. This approach recommended new experimental conditions, and the process was repeated until the thermoelectric properties improved, indicated by a stabilized zT.

The team began with data from 11 samples prepared using spark plasma sintering, combining copper, zinc, tin, and sulfur powders under partial vacuum. The ALMLBO model predicted sintering conditions that achieved a record maximum zT of 0.44 at 725K. "This method showcases how integrating machine learning with traditional materials science accelerates discovery and optimization in complex material systems," say the authors. This approach has the potential to be extended to other materials, enabling rapid innovations in photovoltaics, batteries, and electronics.

Reference

Journal	Acta Materialia
Title	Process optimization on kesterite-based ceramics for enhancing their thermoelectric performances assisted by active machine learning approach: A tool for metal-sulfide ceramics development
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