Elemental 'cookbook' guides efficient thermoelectric combinations

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A repository developed by Duke University engineers that they call a "materials genome" will allow scientists to stop using trail-and-error methods for combining electricity-producing materials called "thermoelectrics."

Thermoelectric materials produce electricity by taking advantage of temperature differences on opposite sides of a material. They are currently being used in deep space satellites and camp coolers. But until now, scientists have not had a rational basis for combining different elements to produce these energy-producing materials.

The project developed by the Duke engineers covers thousands of compounds, and provides detailed "recipes" for creating most efficient combinations for a particular purpose, much like hardware stores mix different colors to achieve a particular tint of paint. The database is free and open to all (aflowlib.org).

"We have calculated the thermoelectric properties of more than 2,500 compounds and have calculated all their energy potentials in order to come up with the best candidates for combining them in the most efficient ways," said Stefano Curtarolo, associate professor of mechanical engineering and materials sciences and physics at Duke's Pratt School of Engineering. "Scientists will now have a more rational basis when they decide which elements to combine for their thermoelectric devices."

The results of the Duke team's work were published online in the journal *Physics Review X*.

A thermoelectric device takes advantage of temperature differences on opposite sides of a material – the greater the temperature difference, the greater energy potential.

Thermoelectric devices are currently used, for example, to provide power for deep-space satellites. The side of the device facing the sun absorbs heat, while the underside of the device remains extremely cold. The satellite uses this temperature difference to produce electricity to power the craft.

Different material combinations may be a more efficient method of turning these temperature differences into power, according to Shidong Wang, a post-doctoral fellow in Curtarolo's lab and first author of the paper.

Thermoelectric materials can be created by combining powdered forms of different elements under high temperatures – a process known as sintering. Not only does the new program provide the recipes, but it does so for the extremely small versions of the particular elements, known as nanoparticles. Because of their miniscule size and higher surface areas, nanoparticles have properties unlike their bulk counterparts.

"Having this repository could change the way we produce thermoelectric materials," Wang said. "With the current trial-and-error method, we may not be obtaining the most efficient combinations of materials. Now we have a theoretical background, or set of rules, for many of the combinations we now have. The approach can be used to tackle many other clean energy related problems."

The Duke researchers believe that the use of thermoelectric devices –

which the new database should help fuel – could prove especially effective in cooling microdevices, such as laptop computers.

Provided by Duke University