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TU Vienna team developing new class of thermoelectric material: intermetallic clathrates

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Researchers at the the Vienna University of Technology (TU Vienna) are developing a new and more efficient class of thermoelectric materials—intermetallic clathrates (crystals in which host atoms are enclosed in cage-like spaces) containing cerium. A paper on their work is published in the journal *Nature Materials*.

> *These clathrates show remarkable thermal properties. We came up with the idea to trap cerium atoms, because their magnetic properties promised particularly interesting kinds of interaction.*
>
> —Professor Silke Bühler-Paschen

Earlier attempts to incorporate magnetic atoms such as the rare-earth metal cerium into the clathrate structures failed. With the help of a crystal growth technique in a mirror oven, Professor Andrey Prokofiev (TU Vienna) has now succeeded in creating clathrates made of barium, silicon and gold, encapsulating single cerium atoms.

> *The thermal motion of the electrons in the material depends on the temperature. On the hot side, there is more thermal motion than on the cold side, so the electrons diffuse towards the colder region. Therefore, a voltage is created between the two sides of the thermoelectric material*
>
> —Professor Bühler-Paschen

Experiments show that the cerium atoms increase the material’s thermopower by 50%, so a much higher voltage can be obtained. Furthermore, the thermal conductivity of clathrates is very low. This is also important, because otherwise the temperatures on either side would equilibrate, and no voltage would remain.

Bühler-Paschen attributes the “remarkably good material properties” to a special kind of electron-electron correlation—the Kondo effect. The Kondo effect is an unusual scattering mechanism of conduction electrons in a metal due to magnetic impurities, resulting in a change in electrical resistivity with temperature. The Kondo effect is known from low-temperature physics, close to absolute zero temperature.

In the clathrate, the electrons of the cerium atom are quantum mechanically linked to the atoms of the crystal. These quantum mechanical correlations also play an important role in the novel clathrate materials, even at a temperature of hundreds of degrees Celsius.

> *The rattling of the trapped cerium atoms becomes stronger as the temperature increases. This rattling stabilizes the Kondo effect at high temperatures. We are observing the world’s hottest Kondo effect.*
>
> —Professor Bühler-Paschen

The research team at TU Vienna will now try to achieve this effect also with different kinds of clathrates. In order to make the material commercially more attractive, the expensive gold could possibly be substituted by other metals, such as copper. Instead of cerium, a cheaper mixture of several rare-earth elements could be used.

Resources

- A. Prokofiev, A. Sidorenko, K. Hradil, M. Ikeda, R. Svagera, M. Waas, H. Winkler, K. Neumaier & S. Paschen (2013) Thermopower enhancement by encapsulating cerium in clathrate cages. *Nature Materials* doi: 10.1038/nmat3756
