Porous materials measure temperature at molecular level

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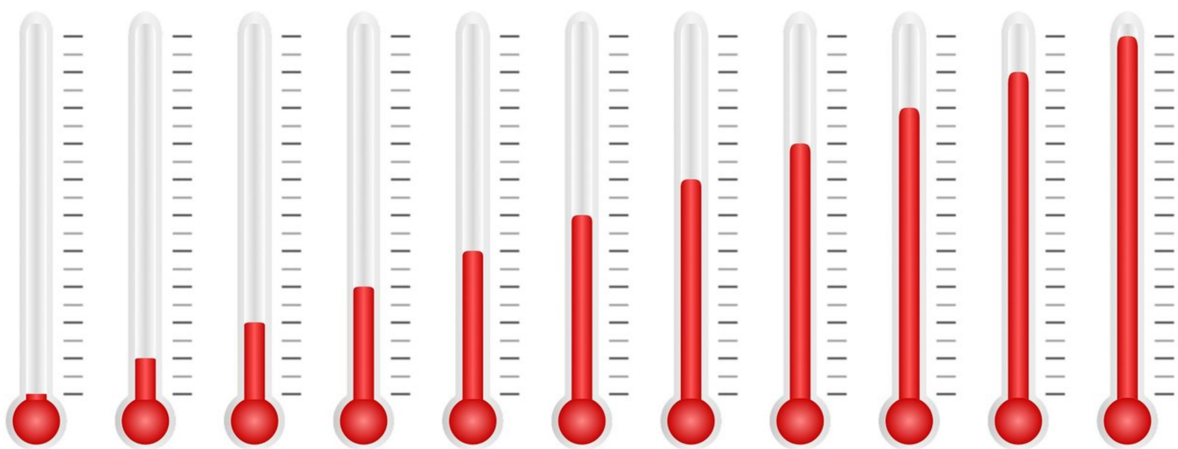

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Researchers of Ghent University investigated how so-called metal-organic frameworks breathe as it gets hotter or colder. Using advanced computer simulations, they found that the temperature at which these materials suddenly expand or shrink is tuneable. Their results allow the design of thermostats that work at the molecular level.

The research was conducted at the Center for Molecular Modeling at Ghent University supervised by Prof. V. Van Speybroeck and in collaboration with the University of Vienna. It appears in *Nature Communications* this week.

Ingenious pores

Metal-organic frameworks are riddled with minuscule pores, no more than a billionth of a meter in diameter. Despite this limited size, the pores offer opportunities for a wide array of cutting-edge applications. Metal-organic frameworks thus far attracted attention for the detection of chemical weapons, the transport of drugs in blood or the capture of greenhouse gases.

Materials design through computer simulations

The researchers of the Center for Molecular Modeling focused on the breathing versions of metal-organic frameworks. The pores of these materials open or close as they heat up or cool down. This breathing behaviour gives rise to a sudden increase or decrease of the volume. The UGent scientists now showed that the temperature at which this phenomenon occurs is dependent on the composition of the metal-organic frameworks. Their molecular building blocks can therefore be selected as a function of the temperature at which a reaction is required. In particular, the switching temperature results from a subtle balance between the attraction between the pore walls and the mobility of the atoms.

Molecular thermostat

The findings of the study open new perspectives for the design of thermostats limited to a handful of atoms. Such materials are necessary to be able to deal with the progressive miniaturization of various applications, ranging from electronics to biology. The conversion of heat into volume change moreover offers possibilities for the exploitation of energy at the smallest length scales.

More information: J. Wieme et al. Tuning the balance between dispersion and entropy to design temperature-responsive flexible metal-organic frameworks, *Nature Communications* (2018). [DOI: 10.1038/s41467-018-07298-4](https://doi.org/10.1038/s41467-018-07298-4)

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