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Graz University of Technology Team Decodes Heat Conduction of Complex Materials

Using machine learning workflows developed in-house, the researchers were able to establish that heat conduction is much more intricate than previously thought. Findings offer potential for developing specific materials.

Complex materials such as organic semiconductors or the microporous metal-organic frameworks known as MOFs are already being used for numerous applications such as OLED displays, solar cells, gas storage and water extraction. Nevertheless, they still harbour a few secrets. One of these has so far been a detailed understanding of how they transport thermal energy. Egbert Zojer's research team at the Institute of Solid State Physics at Graz University of Technology (TU Graz), in collaboration with colleagues from TU Vienna and the University of Cambridge, has now cracked this secret using the example of organic semiconductors, opening up new perspectives for the development of innovative materials with customised thermal properties. The team has published its findings in the reputable journal npj Computational Materials (https://doi.org/10.1038/s41524-025-01514-8).

Little attention given to heat transport up to now

"Scientists have been conducting research on charge transport in organic semiconductors for around 40 years, but no one has ever really looked at the detailed mechanisms relevant to heat transport," explains Egbert Zojer. "However, the fundamental properties of materials are very interesting for us and the insights we have gained into heat transport in organic semiconductors are also directly relevant for many other complex materials. This applies both to materials in which low thermal conductivity is intended to achieve a large thermoelectric effect and to materials that are intended to efficiently supply or dissipate thermal energy through a high thermal conductivity. The fact that we can now determine and understand heat transport so precisely is unparalleled."

The research team achieved this breakthrough by utilising machine learning in a context typically not in the focus when discussing applications of artificial intelligence. Instead of looking for correlations in empirical observations, the researchers searched for causalities based on the strategies they had developed in the past for the use of particularly efficient machine-learned potentials. They wanted to work out how and why heat is distributed in a certain way within a material. Previous explanations for heat transport assumed solely a particle-like transport of phonons also for complex crystalline materials like organic semiconductors. Phonons in this context are energy packets assigned to lattice vibrations, whose transport is typically described similarly to the transport of gas particles. However, the new findings show that an additional mechanism plays a decisive role: the tunnelling transport of phonons.

Molecular length is a decisive factor

Tunnelling transport is based on the wave-like character of atomic vibrations in solids and is particularly important in complex materials with low thermal conductivity. It has been shown that this transport mechanism becomes more

important with the size of the molecules that form an organic semiconductor crystal.

“You can imagine that heat transport is not only determined by the collisions of the vibrational quanta, but also by a ‘tunnelling effect’ that couples two separate vibrational states with each other,” says Lukas Legenstein, author of the publication. “This finding not only explains why certain organic semiconductors exhibit an unusually low temperature dependence of their thermal conductivity, but also enables a more targeted design of materials with specific thermal properties. We can now influence heat conduction by specifically designing the molecular structure.” As a consequence, the researchers would like to apply this new knowledge to the versatile MOFs, as heat transport plays a crucial role in practically all potential applications for this class of materials – even more so than for organic semiconductors.

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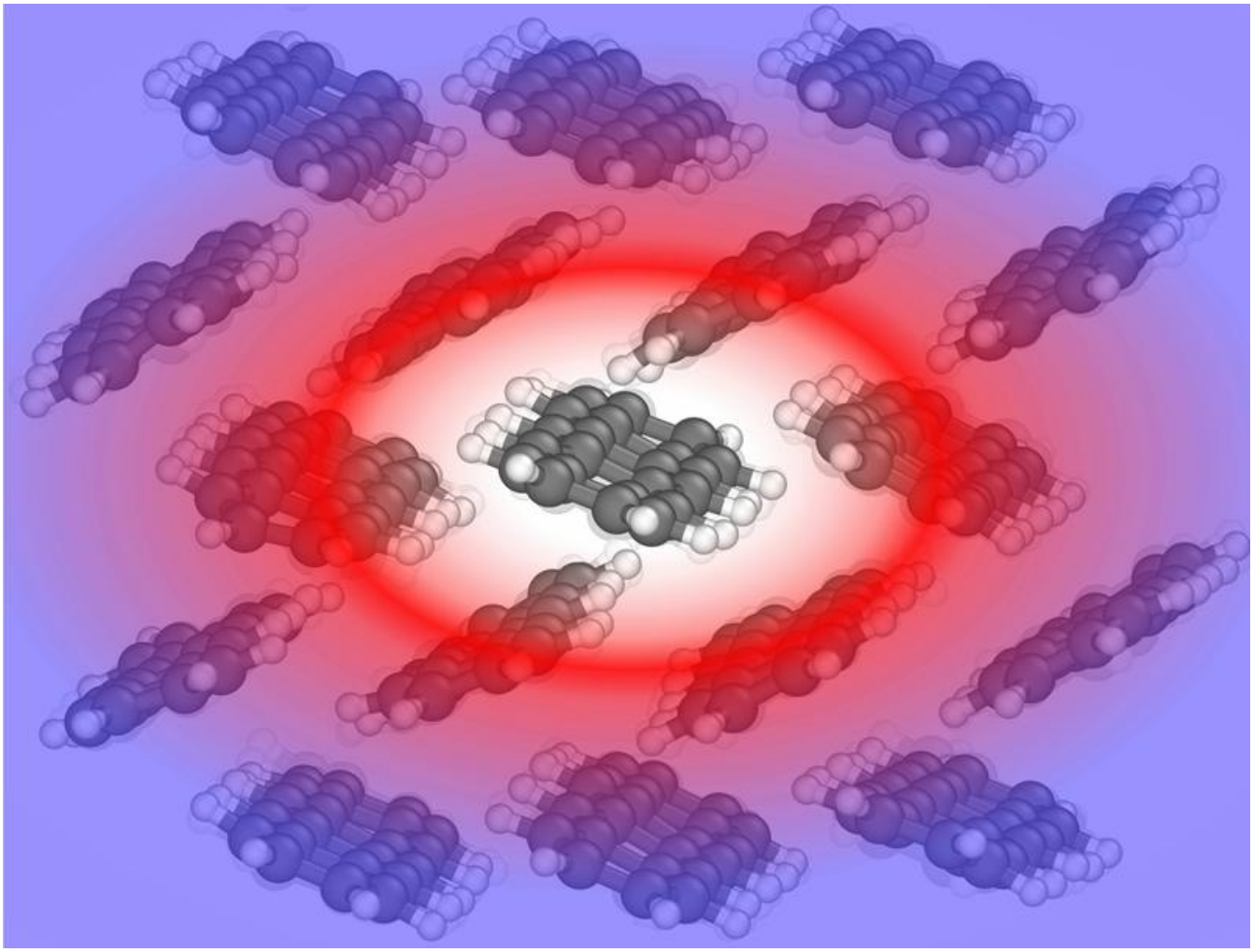
Organic solar cells.
Helmut Lunghammer
Lunghammer - TU Graz



The efficiency of heat transport varies depending on the orientation and length of the pentacene molecules.
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