A simple crystal with ultralow thermal conductivity has applications in thermal insulation and thermoelectrics

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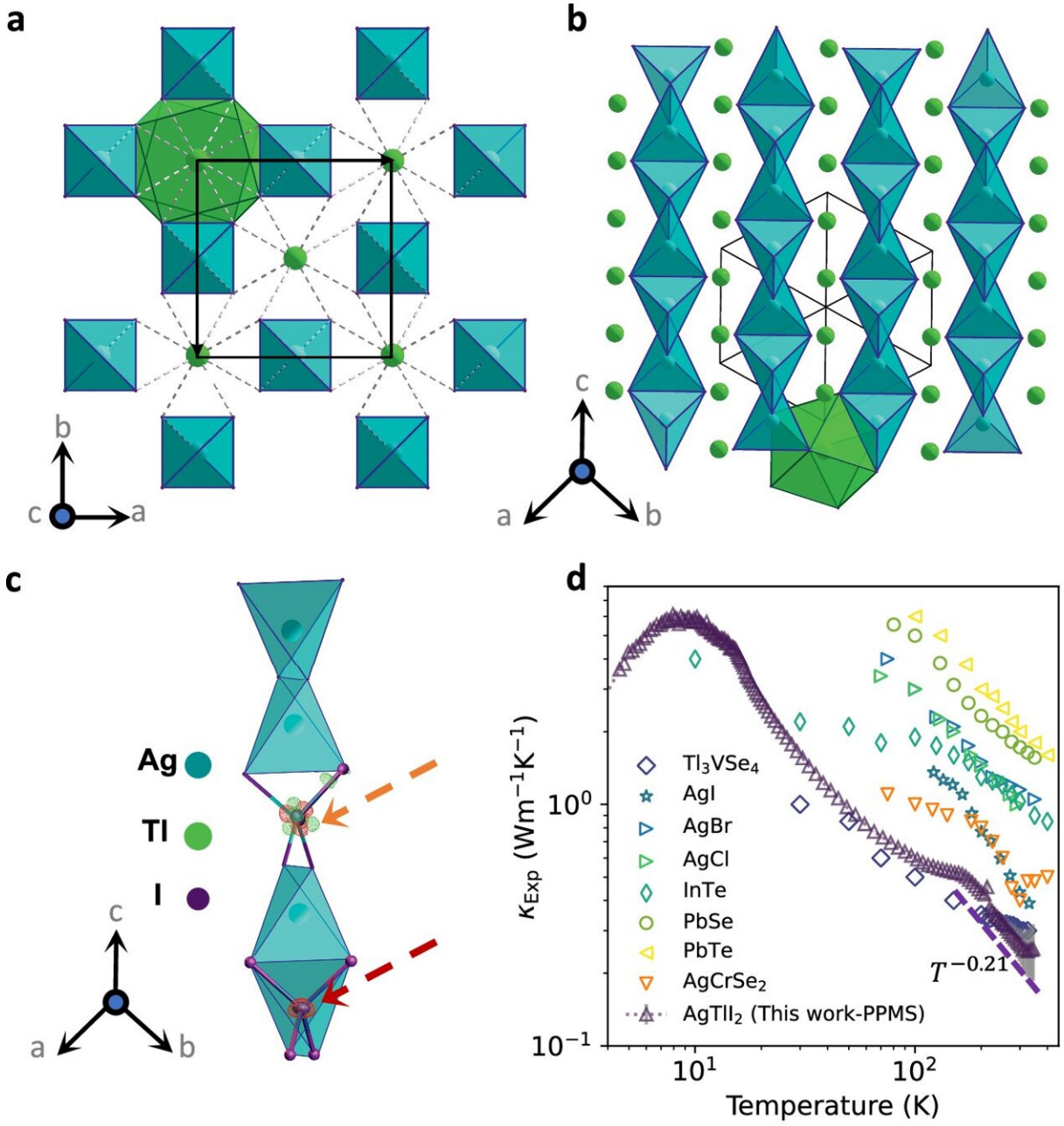

Structure analysis and experimental thermal conductivity of $AgTlI_2$. Structural projection a along c-axis, b along [111] and focus on a $[AgI_2]_\infty$ chain. Ag, Tl, and I atoms are drawn using blue, green, and purple circles, respectively. **c** Orange arrow: Residual electron density (red: positive and green: negative) in the area of the Ag site for a harmonic description of Ag. Red arrow: Anharmonic three-dimensional probability density function (pdf) isosurfaces of Ag (red cloud); displacements are pointing toward the faces of the tetrahedron. **d** Experimental

thermal conductivity of $AgTlI_2$ from 4 to 325 K measured by Physical Property Measurement System (PPMS). Credit: *Nature Communications* (2024). DOI: 10.1038/s41467-024-46799-3

An engineering research team led by Professor Yue Chen from the Department of Mechanical Engineering at the University of Hong Kong (HKU) has achieved a remarkable milestone in the realm of thermal transport in crystals.

The research highlights the potential of simple crystal structures to achieve low thermal conductivity. This discovery not only underscores the importance of exploring new materials for applications in thermal insulation and thermoelectrics but also calls for further experimental investigations to expand the repertoire of materials with ultralow thermal conductivity.

The work is published in the journal *Nature Communications*.

Traditionally, efforts to lower the lattice thermal conductivity of materials have focused on complex material systems, where lower thermal conductivity is typically observed. However, the pursuit of simple crystals with ultralow thermal conductivity has proven to be a challenging task.

In their research, the team identified an exceptional candidate, $AgTlI_2$, which defies conventional expectations by exhibiting an extraordinarily low thermal conductivity of 0.25 W/mK at room temperature—a rarity among simple crystals.

Through a combination of state-of-the-art experimental techniques, including X-ray diffraction experiments and ab initio molecular

dynamics simulations, coupled with advanced anharmonic lattice dynamics, the team gained comprehensive insights into the complex thermal transport mechanisms of $AgTlI_2$ at room temperature.

Their findings revealed the coexistence of ultralow particle-like and wavelike phonon thermal transports in $AgTlI_2$, elucidating the underlying nature of its ultralow thermal conductivity.

Moreover, leveraging their understanding of thermal transport in $AgTlI_2$, the team proposed an effective alternative approach for identifying other simple materials with ultralow thermal conductivity, promising to expand the repertoire of materials with strongly suppressed thermal transport.

This interdisciplinary study was conducted in collaboration with Professor Emmanuel Guilmeau's team from CRISMAT at Normandie University in France, Professor Zheyong Fan's team from Bohai University, China, and Professor Pierric Lemoine from Institute Jean Lamour, France.

The collaborative effort allowed for the integration of expertise from multiple research groups, including sample preparation, synchrotron X-ray scattering, low-temperature thermal conductivity measurement, and ab initio simulations.

"The discovery of the ultralow thermal conductivity of $AgTlI_2$ is a result of a combined effort of both theorists and experimentalists," stated the first author of the paper, Dr. Zezhu Zeng.

He is currently a Post-doctoral Fellow in Professor Geoff Thornton's group at University College London and Professor Bingqing Cheng's group at University of California, Berkeley and Institute of Science and Technology, Austria. Dr. Xingchen Shen from CRISMAT at the French

National Center for Scientific Research (CNRS) also contributed as a co-first author.

"This work implies the important role of simple crystals on thermal insulation, paving the way for new research directions," said Professor Chen.

More information: Zezhu Zeng et al, Pushing thermal conductivity to its lower limit in crystals with simple structures, *Nature Communications* (2024). DOI: 10.1038/s41467-024-46799-3

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