New material holds promise to create more flexible, efficient technologies

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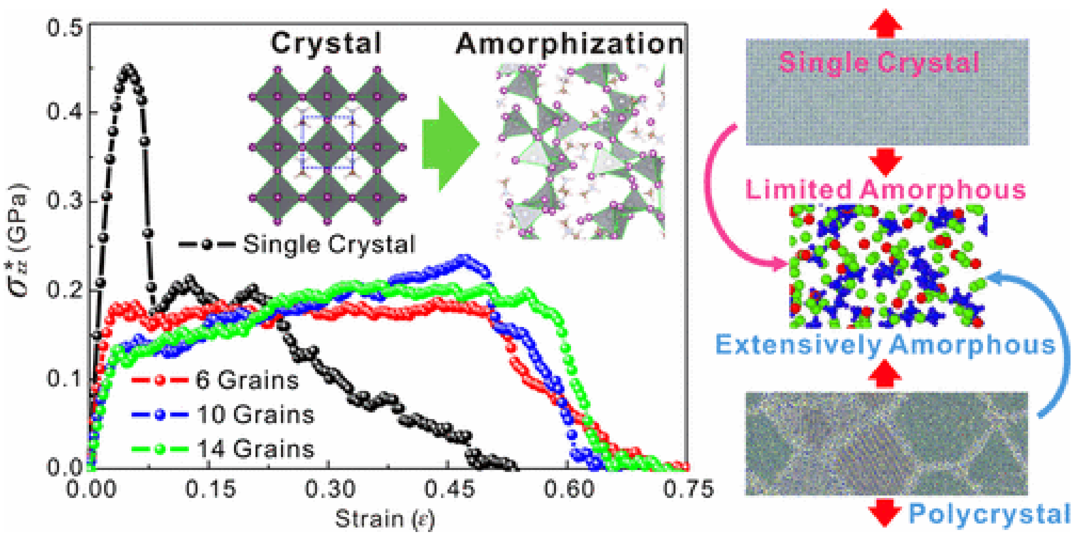

Credit: ACS

An organic-inorganic hybrid material may be the future for more efficient technologies that can generate electricity from either light or heat or devices that emit light from electricity.

FAMU-FSU College of Engineering Assistant Professor Shangchao Lin has published a new paper in the journal *ACS Nano* that predicts how an organic-inorganic hybrid material called organometal halide perovskites could be more mechanically flexible than existing silicon and other inorganic materials used for solar cells, thermoelectric devices and light-emitting diodes.

In a separate study, Lin found that they might be more energy efficient as well.

"We're addressing this from a theoretical perspective," Lin said. "Nobody has really looked at the mechanical and thermal properties of this new material and how it could be used."

Through mathematical simulations, Lin found that organic-inorganic hybrid perovskites should be extremely malleable and flexible. Although plenty of researchers have looked at perovskites for energy technologies, they did not think they were viable for certain devices because of their crystal structure. Scientists thought they would shatter if used for something like a solar panel.

However, Lin found that hybrid perovskites are predicted to fracture slowly through a crystalline-to-amorphous transition, which would make them very damage-tolerant.

Before mechanical failure, they might absorb twice as much elastic energy from external loading than currently used materials in electronic devices, such as silicon and gallium arsenide.

In a previous paper published in the journal *Advanced Functional Materials*, Lin and his team predicted that hybrid perovskites possess very low thermal conductivity due to the organic component. This could make them ideal materials for high efficiency thermoelectric energy conversion.

Specifically, his work suggested that hybrid perovskites are twice as efficient as the current state-of-art thermoelectric material, bismuth telluride, which is very expensive and composed of rare-earth elements.

"The amazing energy conversion efficiency found in hybrid perovskites has put it at the frontier of material discovery," Lin said. "Even more exciting, hybrid perovskites-based solar cells are four times as efficient, in terms of quantum yield, than polymer-based ones. They are also as efficient as the current, mainstream silicon-based solar cells but are much more flexible and cheaper to make from a solution phase through a procedure very similar to inkjet printing."

Lin hopes to follow these two studies by teaming with experimental chemists, material scientists and device engineers who could put his theoretical framework to the test.

"Computational materials-by-design will be a powerful predicting tool for researchers at FSU and at other universities and industry to use as they move forward in this field," he said.

More information: Mingchao Wang et al. Anisotropic and Ultralow Phonon Thermal Transport in Organic-Inorganic Hybrid Perovskites: Atomistic Insights into Solar Cell Thermal Management and Thermoelectric Energy Conversion Efficiency, *Advanced Functional Materials* (2016). DOI: 10.1002/adfm.201600284

Jingui Yu et al. Probing the Soft and Nanoductile Mechanical Nature of Single and Polycrystalline Organic–Inorganic Hybrid Perovskites for Flexible Functional Devices, *ACS Nano* (2016). DOI: 10.1021/acsnano.6b05913

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