From crystals to glasses: a new unified theory for heat transport

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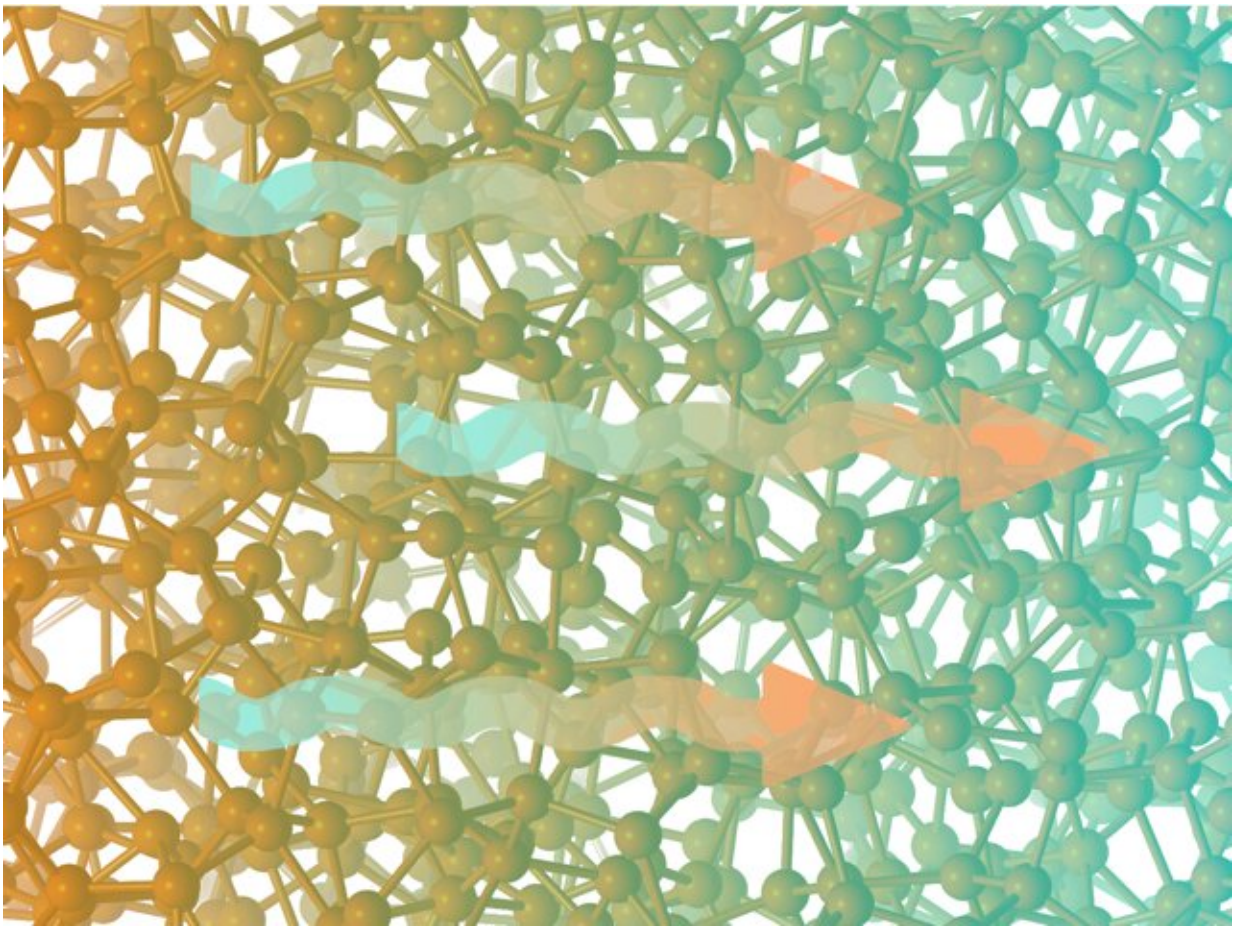

Heat flows from warmer to cooler regions of amorphous silicon. Credit: Leyla Isaeva

Theoretical physicists from SISSA and the University of California at Davis have developed a new approach to heat transport in materials, which finally allows crystals, polycrystalline solids, alloys and glasses to be treated on the same solid footing. It opens the way to the numerical simulation of the thermal properties of a vast class of materials in important fields such as energy saving, conversion, scavenging, storage, heat dissipation, shielding and the planetary sciences, which have thus far dodged a proper computational treatment. The research has been published in *Nature Communications*.

Heat dissipates over time. In a sense, heat flow is the defining feature of the arrow of time. In spite of the foundational importance of heat transport, the father of its modern theory, Sir Rudolph Peierls, wrote in 1961, "It seems there is no problem in modern physics for which there are on record as many false starts, and as many theories which overlook some essential feature, as in the problem of the thermal conductivity of nonconducting crystals."

A half-century has passed since, and heat transport is still one of the most elusive chapters of theoretical materials science. As a matter of fact, no unified approach has been able to treat crystals and (partially) disordered solids on equal footing, thus hindering the efforts of generations of materials scientists to simulate certain materials, or different states of the same material occurring in the same physical system or device with the same accuracy.

This major gap has been finally closed by a group of researchers from SISSA and UC Davis, led by Stefano Baroni and Davide Donadio in the framework of the MAX EU Centre for Supercomputing Applications. The researchers have developed a new methodology based on the Green-Kubo theory of linear response and concepts from lattice dynamics that nicely bridges different approaches applying to crystals and glasses. The new methodology naturally accounts for quantum mechanical effects,

thus finally enabling the predictive modeling of heat transport in complex disordered materials in the low-temperature quantum regime to which no existing technique applied.

This feat will thus empower scientists and engineers to understand and design heat transport for a broad variety of applications. Achieving extremely low thermal conductivity is essential for thermoelectric energy harvesting and solid-state cooling, thermal insulation and thermal barrier coating, while high thermal conductivity is key for heat management in high-power electronics, batteries and photovoltaics. Finally, nanostructured, polycrystalline, highly defective or even glassy materials can be studied with high accuracy within a unified and practicable framework.

More information: Leyla Isaeva et al. Modeling heat transport in crystals and glasses from a unified lattice-dynamical approach, *Nature Communications* (2019). DOI: 10.1038/s41467-019-11572-4

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