Charting the Lattice Thermal Conductivities of I–III–VI2 Chalcopyrite Semiconductors

Chalcopyrite-structured semiconductors have promising potential as low-cost thermoelectric materials, but their thermoelectric figures of merit must be increased for practical applications. Understanding their thermal properties is important for engineering their thermal conductivities and achieving better thermoelectric behavior. We present here a theoretical investigation of the lattice thermal conductivities of 20 chalcopyrite semiconductors with an ABX_2 composition (I–III–VI_2) (A = Cu or Ag; B = Al, Ga, In, or Tl; X = S, Se, or Te). To afford accurate predictions across this large family of compounds, we solve the Boltzmann transport equation with force constants derived from density functional theory calculations and machine learning-based regression algorithms, reducing by between 1 and 2 orders of magnitude the computational cost with respect to conventional approaches of the same accuracy. The results are in good agreement with available experimental data and allow us to rationalize the role of chemical composition, temperature, and nanostructuring in the thermal conductivities across this important family of semiconductors.

Fuente de la publicación:

- Jose J. Plata, Victor Posligua, Antonio M. Márquez, Javier Fernandez Sanz, and Ricardo Grau-Crespo. Charting the Lattice Thermal Conductivities of I–III–VI2 Chalcopyrite Semiconductors. *Chemistry of Materials* 2022 34 (6), 2833-2841.
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Noticias relacionadas:

- La prestigiosa revista "Chemistry of materials" publica en portada los resultados de un trabajo científico que ha requerido la infraestructura de supercómputo de CénitS [CénitS [2]].

Links
[1] https://doi.org/10.1021/acs.chemmater.2c00336 [2] http://www.cenits.es/noticias/31032022-prestigiosa-revista-chemistry-materials-publica-portada-resultados-trabajo