Scientists discover mechanisms behind thermoelectric material

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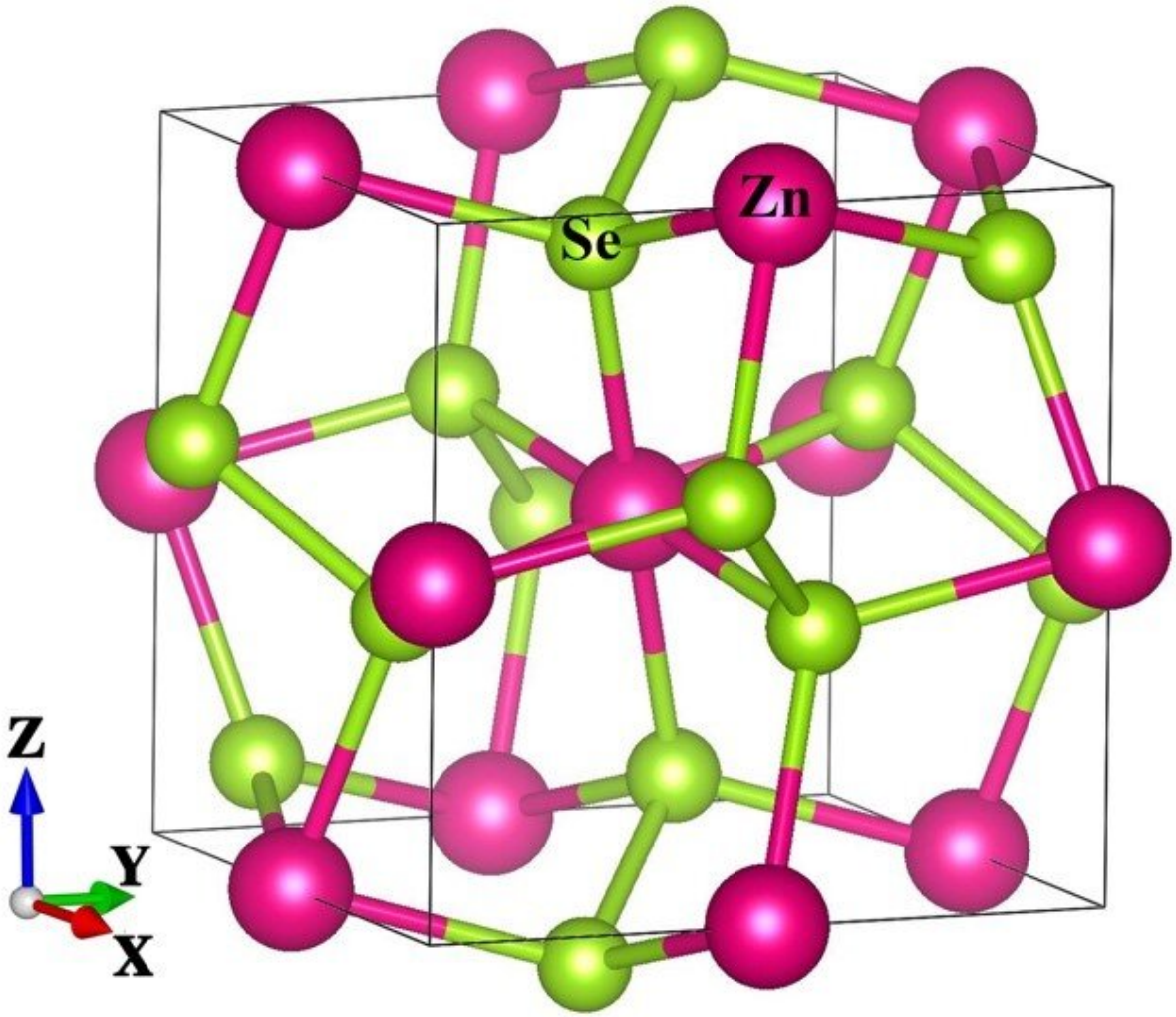

The pyrite-type crystal structures of $ZnSe_2$. Credit: JIA Tiantian

Recently, a research group led by Prof. Zhang Yongsheng from the Institute of Solid State Physics, Hefei Institutes of Physical Science successfully explained the novel physical mechanisms behind pyrite-type $ZnSe_2$.

Pyrite-type $ZnSe_2$ compound was predicted as a strong anharmonicity and promising thermoelectric by the same team early this year, while the underlying physical mechanism behind the compound remained ambiguous.

The researchers analyzed the vibrational spectrums and electrical properties of $ZnSe_2$, and verified its thermoelectric properties.

Their findings showed that the vibrational spectrums of $ZnSe_2$ were characterized by both the isolated high-frequency optical phonon modes due to the stretching of Se-Se dimers, and the low-frequency optical phonon modes with a strong anharmonicity due to the rattling modes of Zn atoms, especially the rotations of Zn atoms around these dimers.

Therefore, they proposed that the existence of localized Se-Se dimers leads to the strong anharmonicity of low-frequency optical phonon modes and the low thermal conductivity.

Furthermore, their analysis of electronic properties showed that $ZnSe_2$ possessed the complex energy isosurfaces of both valence and conduction bands near the Fermi-level, which could contribute to the promising electrical transport properties of p-type and n-type $ZnSe_2$. The low thermal conductivities and promising electrical transport properties led to a large thermoelectric figure of merit of $ZnSe_2$ for both p-type (ZT=2.21) and n-type (ZT=1.87) doping.

Their studies revealed the effect of the physical mechanism behind this thermoelectric phenomena which could be used to guide researchers to

seek promising thermoelectric materials containing strong nonmetallic dimers.

More information: Tiantian Jia et al. Localized dimers drive strong anharmonicity and low lattice thermal conductivity in ZnSe2, *Physical Review B* (2020). DOI: 10.1103/PhysRevB.102.125204

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