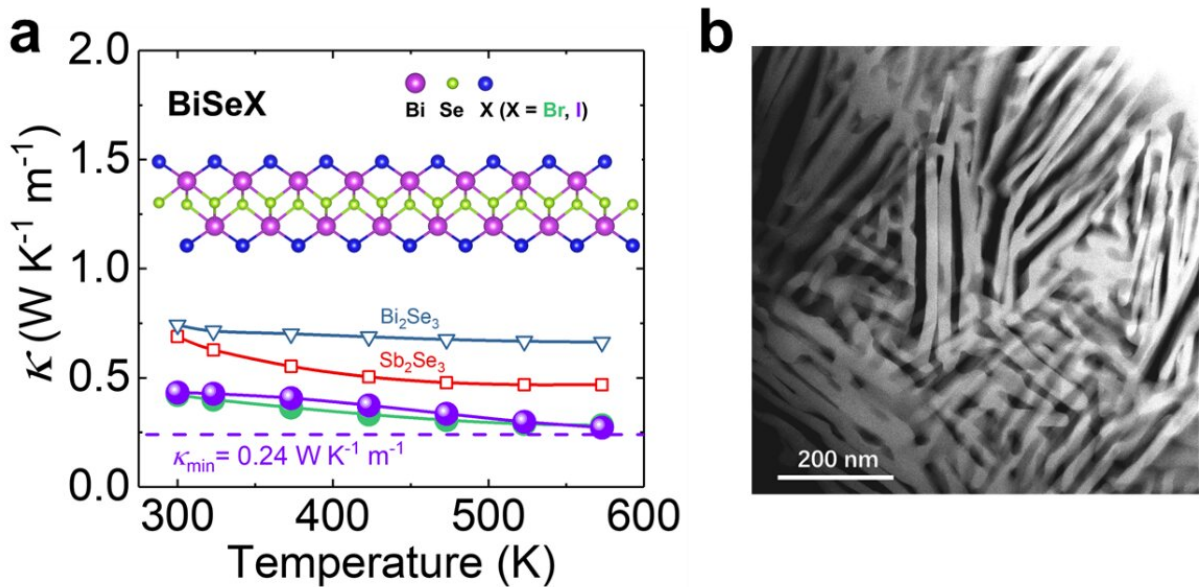


Extremely low thermal conductivity in 1-D soft chain structure

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(a) The thermal conductivity as function of temperature. Insert is the chain structure of BiSeI. (b) The morphology of wire shape chains in 1D BiSeI. Credit: ©Science China Press

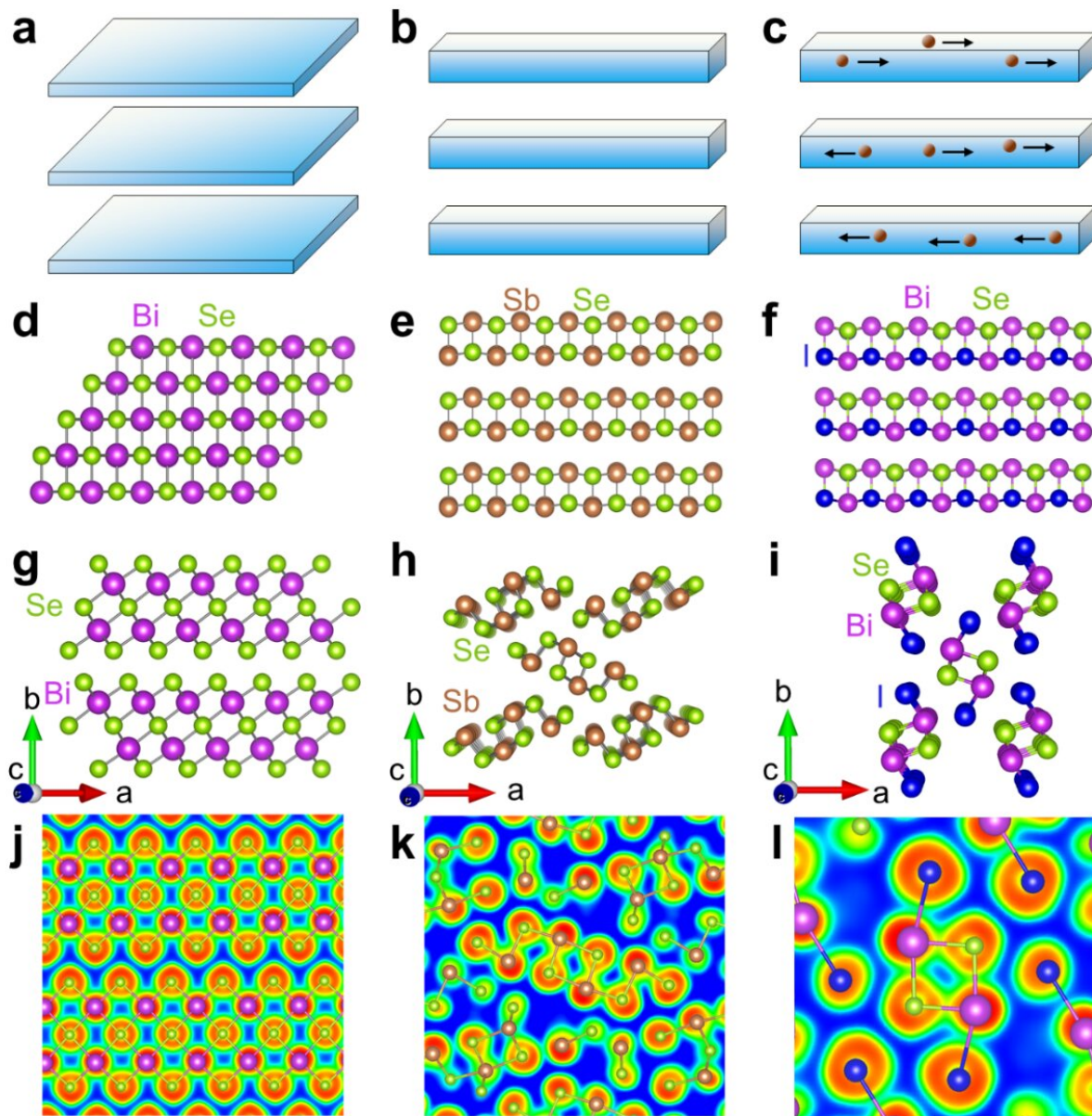
Researchers have reported a new type of simple one-dimensional (1-D) crystal structured bismuth selenohalides (BiSeX, X = Br, I) with extremely low thermal conductivity. Investigations on crystal structure reveal that the ultralow thermal conductivity is due to the weakened chemical bonding in the low-dimensional structure, showing a quasi-0-D

crystal structure. These findings provide a novel selection rule to search low thermal conductivity materials with potential applications in thermoelectrics and thermal barrier coatings.

The low thermal transport properties are important for applications in thermoelectrics and thermal barrier coatings. Today, the strategies to acquire low [thermal conductivity](#) in bulk materials include multi-scale defect (atomic, nano- and meso-scale), heavy molecular weight, complex [crystal structure](#), larger unit cell and strong anharmonicity.

In a recent article in *Science China Materials*, Prof. Li-Dong Zhao from Beihang University and co-workers proposed a new strategy to search intrinsically low thermal conductivity in one-dimensional crystal structure. By using the first-principles calculations and experimental synthesis, they found a type of material with extremely low thermal conductivity, BiSeX (X= Br, I) with a one-dimensional chain structure. The mechanisms behind the low thermal conductivity were revealed from the aspect of crystal structure by neutron powder-diffraction measurements and temperature tunable aberration-corrected scanning transmission electron microscopy (STEM).

To elucidate the origins of ultralow thermal conductivity, the authors made comparisons with several analogs that exhibit cubic- (3-D), layer- (2-D) and chain-like (1-D) crystal structures, and found that the thermal conductivity showed a decreasing trend from 3-D, 2-D to 1-D due to the [chemical bonding](#) strength between the low-dimensional structure becoming progressively weaker and weaker.



Schematic crystal structures and electronic localization functions (ELFs) of 2D, 1D, and soft 1D Bi_2Se_3 , Sb_2Se_3 and BiSeI , respectively. Schematic diagrams and corresponding crystal structures of (a, d) 2D slabs in Bi_2Se_3 , (b, e) 1D chain in Sb_2Se_3 and (c, f) 1D chain with migration of halogens in BiSeI . The crystal structures of Bi_2Se_3 , Sb_2Se_3 and BiSeI viewed along the c direction are given in (g-i), respectively. (j-l) The projected ELF along the chain. The isosurface level of ELF is 0.9. Credit: ©Science China Press

"Based on these guidelines, we found that the chemical bonding along the chain further weakened with added halogen atoms," said Prof. Zhao. Therefore, the chemical bondings of BiSeX along all three crystallographic directions are weaker than in other compounds, showing a quasi-0-D crystal structure.

Different from the ultrahigh thermal conductivity diamond ($> 2000 \text{ W m}^{-1} \text{ K}^{-1}$) with strong covalent bonds between [carbon atoms](#), the phonon transport in bismuth selenohalides was significantly suppressed. As a result, they exhibit extremely low thermal conductivity. "The thermal [conductivity](#) of BiSeI at 573 K reaches $\sim 0.27 \text{ W m}^{-1} \text{ K}^{-1}$, which is close to the theoretical minimum value," said Prof. Zhao.

These findings open up the prospect of achieving [low thermal conductivity](#) materials in a one-dimensional chain-containing bulk structure with potential applications in the fields of thermal barrier coatings, thermoelectric materials, etc.

More information: Dongyang Wang et al, Extremely low thermal conductivity from bismuth selenohalides with 1D soft crystal structure, *Science China Materials* (2020). [DOI: 10.1007/s40843-020-1407-x](https://doi.org/10.1007/s40843-020-1407-x)

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