Investigating newly synthesized thallium compounds for optoelectronic devices
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The burgeoning field of optoelectronic devices is driving the development of new alkali metal-based chalcogenides with qualities that have to be robustly investigated. The need for efficient optoelectronic devices is growing and hand-in-hand so too is the challenge of discovering new semiconductors with valuable properties. This has spurred significant research in the synthesis and characterization of new alkali metal-based (AM) chalcogenides involving copper, silver and alkali metal with valuable properties like flexibility, high thermal stability, semiconductivity, and photovoltaic effects.

Inspired by the growing demand for new optimum semiconducting materials, a new paper published in EPJ B authored by Abdelmadjid Bouhemadou, Laboratory for Developing New Materials and their Characterizations, Department of Physics, Faculty of Science, University of Ferhat Abbas Setif, Algeria and his co-authors, investigated in detail the structural, elastic, electronic and optical properties of two newly synthesized compounds, namely $\text{Tl}_2\text{CdGeSe}_4$ and $\text{Tl}_2\text{CdSnSe}_4$.

In the paper, the authors describe concerns with AM-based chalcogenides which hinder technological applications, adding that these disadvantages could be overcome by compounds that integrate thallium (TI) including $\text{Tl}_2\text{CdGeSe}_4$ and $\text{Tl}_2\text{CdSnSe}_4$.

The researchers explain that TI is much less electropositive than alkali metals; the electronegativity of TI is much higher than that of any alkali metal. This leads to a less ionic character in TI-based compounds, which may lead to low electrical resistivities and therefore to higher carrier mobilities.

TI is also heavier than any stable alkali metal, which means it has low lattice thermal conductivity improving physical properties requiring low lattice thermal conductivity such as thermoelectric efficiency. TI-containing materials also tend to be less sensitive to air and moisture than AM-based compounds. These and other advantages mean that significant research has been devoted to the exploration of TI-based chalcogenides.

The authors of the paper say that their research revealed that the studied materials exhibit a high absorption in an energy window involving the visible spectrum. In addition to this, the optimized structural parameters of $\text{Tl}_2\text{CdGeSe}_4$ and $\text{Tl}_2\text{CdSnSe}_4$ are in excellent agreement with the experimental counterparts, confirming the reliability of the theoretical method used to predict the physical properties of the title compounds.

This revealed that the studied compounds are soft, ductile, mechanically stable and substantially structurally and elastically anisotropic materials.

**More information:** S. Karkour et al, Structural, elastic, electronic and optical properties of the newly synthesized selenides $\text{Tl}_2\text{CdXSe}_4$ ($X = \text{Ge}$, "$\text{Tl}_2\text{CdSnSe}_4$"