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Title:	Metavalent bonding in GeSe leads to high thermoelectric performance.
Authors:	Vasdev, Aastha (/jspui/browse?type=author&value=Vasdev%2C+Aastha) Sheet, Goutam (/jspui/browse?type=author&value=Sheet%2C+Goutam)
Keywords:	Thermoelectrics Metavalent Bonding
Issue Date:	2021
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Citation:	Angewandte Chemie - International Edition, 60(18), 10350-10358.
Abstract:	Orthorhombic GeSe is a promising thermoelectric material. However, large band gap and strong covalent bonding result in a low thermoelectric figure of merit, $zT \approx 0.2$ . Here, we demonstrate a maximum $zT \approx 1.35$ at 627 K in p-type polycrystalline rhombohedral $(\text{GeSe})_{0.9}(\text{AgBiTe}_2)_{0.1}$ , which is the highest value reported among GeSe based materials. The rhombohedral phase is stable in ambient conditions for $x=0.8-0.29$ in $(\text{GeSe})_{1-x}(\text{AgBiTe}_2)_x$ . The structural transformation accompanies change from covalent bonding in orthorhombic GeSe to metavalent bonding in rhombohedral $(\text{GeSe})_{1-x}(\text{AgBiTe}_2)_x$ . $(\text{GeSe})_{0.9}(\text{AgBiTe}_2)_{0.1}$ has closely lying primary and secondary valence bands (within 0.25–0.30 eV), which results in high power factor $12.8 \mu\text{W cm}^{-1} \text{K}^{-2}$ at 627 K. It also exhibits intrinsically low lattice thermal conductivity ( $0.38 \text{ W m}^{-1} \text{K}^{-1}$ at 578 K). Theoretical phonon dispersion calculations reveal vicinity of a ferroelectric instability, with large anomalous Born effective charges and high optical dielectric constant, which, in concurrence with high effective coordination number, low band gap and moderate electrical conductivity, corroborate metavalent bonding in $(\text{GeSe})_{0.9}(\text{AgBiTe}_2)_{0.1}$ . We confirmed the presence of low energy phonon modes and local ferroelectric domains using heat capacity measurement (3–30 K) and switching spectroscopy in piezoresponse force microscopy, respectively.
Description:	Only IISER Mohali authors are available in the record
URI:	<a href="https://doi.org/10.1002/anie.202101283">https://doi.org/10.1002/anie.202101283</a> ( <a href="https://doi.org/10.1002/anie.202101283">https://doi.org/10.1002/anie.202101283</a> ) <a href="http://hdl.handle.net/123456789/4545">http://hdl.handle.net/123456789/4545</a> ( <a href="http://hdl.handle.net/123456789/4545">http://hdl.handle.net/123456789/4545</a> )
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