$ZnGeSb_2$: A promising thermoelectric material with tunable ultra-high conductivity

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Abstract

First principles calculation predicts the promising thermoelectric material $ZnGeSb_2$ with huge power factor ($S^2\sigma/\tau$) in the order of 3×10^{17} W/mK^2s, due to the ultra-high electrical conductivity scaled by relaxation time around 8.5×10^{25} $\Omega^{-1}m^{-1}s^{-1}$, observed in its massive Dirac state. The observed electrical conductivity is higher than the well-established Dirac materials and almost carrier concentration independent with similar behaviour of both n and p type carriers, which may certainly attract device applications. The low range of thermal conductivity is also evident from the phonon dispersion. Our present study further reports the gradual phase change of ZnGeSb2 from a normal semiconducting state, through massive Dirac states to a topological semimetal. The maximum power factor is observed in massive Dirac states compared to other two states.