

Rare-Earth Antimony Suboxides as Novel Thermoelectric Materials

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1) RE_3SbO_3 and $RE_8Sb_{3-\delta}O_8$ antimonide oxides (RE is a rare-earth element)

Two families of novel narrow band-gap semiconducting suboxides with the RE_3SbO_3 and $RE_8Sb_{3-\delta}O_8$ compositions (RE = La, Sm, Gd, Ho) have been discovered. Their synthesis was motivated by attempts to open a band gap in the semimetallic *RESb* binaries through a chemical fusion of *RESb* and corresponding insulating RE_2O_3 . This strategy worked for both families of phases as the band gap opened between the valence band dominated by the Sb states and the conduction band composed primarily of the *RE* states.



 RE_3 SbO₃ and RE_8 Sb₃₋₈O₈ contain similar A and B blocks

2) Tuning electron transport mechanism in RE₂SbO₂

The size of rare-earth elements was exploited as a chemical pressure to tune the Sb atomic disorder in the RE_2SbO_2 phases. As a result, RE_2SbO_2 materials with the same structure and charge carrier concentration exhibit a range of transport behaviors. Additionally, the thermoelectric power of these compounds are improved without compromising the electrical conductivity.



 $\textit{RE}_3\textit{SbO}_3$ and $\textit{RE}_8\textit{Sb}_{3\text{-}\delta}\textit{O}_8$ are semiconducting

