

# High-Temperature Thermoelectric Properties of Compounds in the System $\text{Zn}_x\text{In}_y\text{O}_{x+1.5y}$

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Based on results obtained utilizing combinatorial chemistry techniques to screen the thermoelectric power factor of materials in the system  $\text{Zn}_x\text{In}_y\text{O}_{x+1.5y}$ , several multiphase candidates were down-selected and investigated in terms of their thermoelectric response from room temperature to 1050°C. While the screening experiments suggested that peaks in the power factor occur at relatively high indium oxide content, only the thermoelectric properties of zinc-oxide-rich homologous layered phases in the system  $(\text{In}_2\text{O}_3)(\text{ZnO})_k$  have been well documented, since the phases where  $k < 3$  cannot be easily formed. In the present study, indium-oxide-rich materials in the system  $\text{In}_2\text{O}_3-(\text{In}_2\text{O}_3)(\text{ZnO})_3$  were fabricated and their figures of merit were determined. The results suggest that the indium-oxide-rich phases have improved figures of merit, especially at elevated temperatures, relative to the best performing  $k$  phases by combining the high power factor of  $\text{In}_2\text{O}_3$  and the low thermal conductivity of  $(\text{In}_2\text{O}_3)(\text{ZnO})_k$ .

**Key words:**  $\text{In}_2\text{O}_3$ ,  $\text{ZnO}$ ,  $(\text{In}_2\text{O}_3)(\text{ZnO})_k$ , thermoelectrics, oxides

## INTRODUCTION

Recently, semiconducting oxides have received significant attention for mid- to high-temperature-range thermoelectric energy harvesting and power generation applications. Compared with more conventional narrow-bandgap thermoelectric materials, oxides offer dramatically improved stability when operating in air. However, these materials have not been fully investigated, and significant work must still be done to improve their performance before they can be used in commercial devices. Thermoelectric materials are characterized by their dimensionless figure of merit  $ZT$ , which is defined according to Eq. 1 as

$$ZT = \frac{S^2\sigma}{\kappa}T, \quad (1)$$

where  $S$  is the Seebeck coefficient,  $\sigma$  is the electrical conductivity,  $\kappa$  is the thermal conductivity, and  $T$  is

the absolute temperature. The power factor  $\xi = S^2\sigma$ , is also frequently used to characterize thermoelectric materials, and it has recently been suggested as a more meaningful measure of efficiency, since in many potential energy harvesting applications, thermoelectric devices are utilized under fixed thermal gradients.<sup>1</sup> Unfortunately, all of these material properties are strongly correlated, since the Seebeck coefficient typically decreases with increasing charge carrier concentration and the electrical conductivity typically increases with increasing charge carrier concentration. Also, the thermal conductivity can be broken down into contributions both from phonon and electron scattering. To reduce the thermal conductivity without sacrificing electrical conductivity, phonon scattering must be selectively increased.

Typically, better efficiencies should be achieved at higher temperatures, since the figure of merit is proportional to temperature. However, this has not been observed in the majority of thermoelectric materials such as bismuth and lead telluride as well as  $\text{Si}_x\text{Ge}_{1-x}$  alloys.<sup>2,3</sup> The reason is that these

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