Crystal chemistry and crystallography of thermoelectric materials for energy conversion applications

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The growing demand for energy, especially “green” energy, has become one of the more urgent global concerns over the past few decades, resulting in a large increase of relevant research activities. Advances in energy conversion materials, technologies and applications are some of the key areas that can have a significant impact on the worldwide economy and on civilization in general. Energy conversion technologies include thermoelectric (TE) devices, solar cells, fuel cells, batteries, and others. For TE materials, in addition to conventional semiconductors, oxide materials have also been discovered as suitable candidates, particularly due to their stability at high temperatures (Fig 1). In this talk, the background information on TE materials, including the current efforts on the structural characterization, pertinent phase diagrams [1], and property measurements will be discussed. The conversion efficiency of TE materials is characterized by the dimensionless figure-of-merit, $ZT$, which is defined as $S^2\sigma T/\kappa$, where $S$ is the Seebeck coefficient, $\sigma$ is the electrical conductivity, $\kappa$ is the thermal conductivity, and $T$ is the absolute temperature. Optimization of $ZT$, however has been a difficult task due to the inter-dependence of the above properties. Examples of recent research on improving the $ZT$ values will be highlighted [2]. The high-throughput combinatorial process is one of the state-of-the-art approaches for discovery of new materials and for improving material properties; current efforts in high throughput research on TE materials will be summarized [3]. Standard reference materials (SRMs™) are critical for interlaboratory data comparison, and so efforts at NIST on the development and distribution of Seebeck coefficient SRMs [4] will also be discussed.

Figure 1. The unit cell structure of Ca$_3$Co$_4$O$_9+\delta$ showing the alternating subsystems of electrically conductive CoO$_2$ sheets and insulating rock-salt-type Ca$_2$CoO$_3$ layers.