Sustainable thermoelectric materials fabricated using high entropy perovskite oxynitride nanoparticles as building blocks

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Thermoelectric (TE) materials, which can convert temperature differences directly into electric current, are seen as promising materials for sustainable energy systems, but many practical high-performance materials make use of toxic or rare elements. Perovskite-type oxides consist of non-toxic, abundant elements and have high temperature stability.[1] However, their TE performance is limited by their low electrical conductivity (resulting from a low carrier concentration and large band gap) and high thermal conductivity.[2]

For the development of practical, sustainable TE materials we chemically synthesized high entropy perovskite oxynitride nanoparticles containing multiple alloying elements using a simple solvothermal method and confirmed the cationic composition by STEM-EDS (Fig. 1a), while the presence of N was indicated by changes in the band gap. We then investigated the TE properties of their sintered bodies. The use of nanoparticles to create grain boundaries within the material significantly reduced the thermal conductivity, which was further reduced by the high entropy effect as additional elements were added (Fig 1b).[3] Sustainable elements (Ca, Mn, Nb, Ta, and N) were chosen and the effects of each element's inclusion on the TE properties was investigated. Mn and N inclusion reduced the energy band gap, while Nb and Ta increased the carrier concentration, resulting in a significant increase in electrical conductivity compared to the undoped perovskite sample. In this presentation we will discuss the correlation between the structures and their electronic/thermal transport properties.

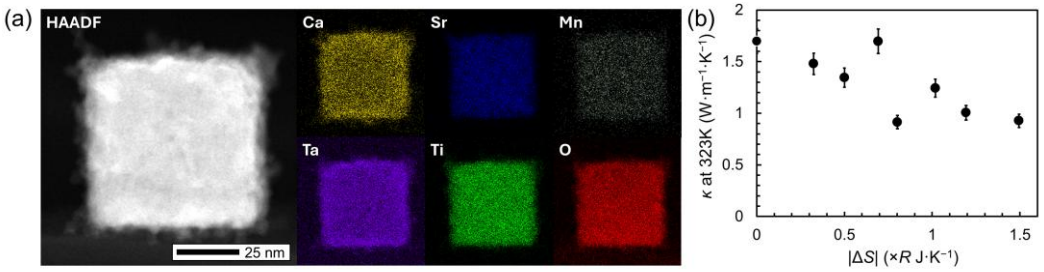

Fig. 1. (a) STEM HAADF image of multi-alloyed perovskite $(Ca_{0.5}Sr_{0.5})(Mn_{0.1}Ti_{0.9})O_3$ NPs and EDS mapping images. In order: Ca K-line (Yellow), Sr K-line (blue), Mn K-line (grey), Ta L-line (purple), Ti K-line (green), and O K-line (red). (b) Plot of thermal conductivity, κ, at 323 K against configurational entropy, $|\Delta S|$, for all samples.

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