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Thermoelectric Properties of Li-Intercalated $ZrSe_2$ Single Crystals

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Zirconium diselenide ($ZrSe_2$) is one of many members of the layer-structured transition-metal dichalcogenide family. The structure of these materials features a weakly bonded van der Waals gap between covalently bonded CdI_2-type atomic layers that may host a wide range of intercalants. Intercalation can profoundly affect the structural, thermal, and electronic properties of such materials. While the thermoelectric potential of layer-structured transition-metal dichalcogenides has been formerly studied by several groups, to our best knowledge, neither the thermoelectric properties of $ZrSe_2$ nor the impact of intercalation on its thermoelectric properties have been reported (specifically, the full evaluation of the dimensionless figure of merit, ZT, which includes the thermal conductivity). In this proof-of-principle study, $ZrSe_2$ single crystals have been synthesized using an iodine-assisted vapor transport method, followed by a wet-chemistry lithium intercalation process. The results of resistivity, thermopower, and thermal conductivity measurements between 10 K and 300 K show that Li intercalation induced additional charge carriers and structural disorder that favorably affected the thermoelectric properties of the material. As a result, a dimensionless figure of merit $ZT \approx 0.26$ has been attained at room temperature in a Li-intercalated sample, representing nearly a factor of three improvement compared with the pristine sample. These improvements, along with the abundance, relatively low toxicity, and low cost of such materials, merit further thermoelectric investigations of intercalated zirconium diselenide, especially in conjunction with a substitutional doping approach.

Key words: Thermoelectric, transition metal, dichalcogenide, intercalation, lithium, zirconium diselenide

INTRODUCTION

Thermoelectricity is the simplest technology applicable for direct thermal–electrical energy conversion. Thermoelectric (TE) devices can directly convert heat to clean electricity or work in “reverse” as a heat pump, without any noise, hazardous liquids, or greenhouse-gas emissions. The conversion efficiency of a TE device is largely determined by the dimensionless figure of merit $ZT = \alpha^2\sigma T/\kappa$ of the TE material of which it is made, where α, σ, T, and κ are the thermopower, electrical conductivity, absolute temperature, and thermal conductivity, respectively. The past couple of decades have witnessed renewed interest in developing higher-ZT materials due to the ecological, economic, and political drive for renewable energy sources. While many advances have been made in improving the ZT values of various TE materials, this has often come with certain disadvantages in terms of scalability due to the high cost of materials or methods necessary to

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