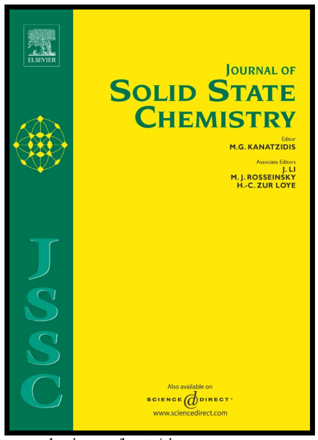

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Emergence of Strain Induced Two Dimensional Metallic State in ReS_2

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Abstract

We present a highly versatile system ReS_2, which transforms from a semiconductor to a two dimensional metal under uni-axial compressive strain along 'a' direction in both bulk and monolayer. The 2D nature is realised from highly flat Fermi surfaces and anisotropic transport properties. Moreover the layer independent electronic structure properties are revisited and thermoelectric properties of ReS_2 in bulk, monolayer and bilayer forms reveal the competing thermoelectric (TE) coefficients in each form. The in-plane power-factor shows an enhancement over '*c*'-axis value as a function of strain, which is almost two orders of magnitude. In addition, strain induced tunable in-plane anisotropy of almost one order has been observed in both bulk and monolayer ReS_2 (around 20%), which further open up the possibility of TE application as nanowires. Our analysis unveils a wide range of application for ReS_2 in the field of thermoelectrics as bulk and thin films for a large temperature range. The magnitude of TE coefficients are comparable with other well established transition metal dichalocogenides.

Keywords: Electronic structure, Thermoelectric properties, Strain

1. Introduction

The realization of two dimensional nature in transition metal dichalcogenide (TMD) has elevated the research pertaining to TMD to the next level[1, 2, 3, 4, 5, 6]. The isolated 2D transition metal dichalcogenide layers have been competing with the two dimensional material like graphene which has several importance in the current technologies. The strong intra layer bonding and weak inter layer bonding in the layered materials is quite interesting, leading to the usage of these materials in the bulk and layered forms[7, 8, 9]. ReS_2 is one of the transition metal dichalcogenides which stands out with very peculiar properties, and has drawn adequate attention in the recent past. Unlike the other layered transition metal dichalcogenides, ReS_2 crystallizes in a triclinic space group. Recent study reveals that the interaction between layers in ReS_2 is negligible implying that the monolayer of ReS_2 might have similar electronic properties as that of bulk, enabling ReS_2 to be the highlight in the last decade[10]. Pressure and strain are the robust tools which can modify the structure and electronic properties of materials, and transition metal dichalcogenides showed considerable response to strain and pressure[11, 12, 13], leading to metallization at high pressure, direct to indirect band gap transitions etc. Optical and electronic properties are also explored for both bulk and layered ReS_2 [14], and this compound has found application in field effect transistors[15, 16]. The inherent structural anisotropy of ReS_2 has further shown an influential response towards pressure and strain, resulting in tuning of in-plane, and through plane anisotropy in several physical properties like resistivity, charge mobility etc, and significant number of studies are dedicated to understand this

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