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Thermoelectric Properties of 2D Sn_2SSe Monolayer

Baljinder Kaur, Heena, Shakeel Ahmad Khandy, Syed Rashid Ahmad, Munirah D Albaqami, Marutheeswaran Srinivasan, Lokanath Patra, Shobhna Dhiman, and Kulwinder Kaur**

2D Janus materials have drawn great interest in recent years due to their energy applications including thermoelectricity (TE) and photocatalysis. In this work, density functional theory and Boltzmann transport equations are coupled to look into the thermoelectric properties of Sn_2SeS monolayer. Sn_2SeS is an indirect bandgap semiconductor with a bandgap of 0.88 eV. This monolayer is chemically as well as dynamically stable. The thermoelectric parameters such as the Seebeck coefficient, electrical conductivity, and thermal conductivity due to electrons and phonons are explored along the zigzag and armchair orientation. The high value of electrical conductivity and low-value lattice thermal conductivity along the zigzag orientation yields the high value of ZT = 1.93.

1. Introduction

Thermoelectricity is a very important subject when it comes to concern for the environment because it can convert heat into electricity and be used for various applications such as recovering waste heat and solid-state cooling. For nations like India, where smog and fog have become major health concerns, this phenomenon plays a very crucial role[1] in dealing with this type of issue. The dimensionless figure of merit (ZT) can be used to assess the efficiency of thermoelectric materials.[2] In order to create high-performance thermoelectric materials, various methods have been used. Nevertheless, there is still a need to discover an effective, environmentally friendly, and cost-effective method that can be used for large-scale production of these materials.[3–6] Despite the fact that it is challenging to regulate the aforementioned variables separately due to their intricate interrelationships, thermoelectric performance records have been consistently broken over the past 10 years.

Two dimensional (2D) materials offer an amazing opportunity to unravel the physics of electronic, optical, and magnetic properties.[7,8] Nanostructures are regularly used for heat-carrying applications in electronics. Other applications include plasmonics, dielectrics, or magnetic materials where the electrons live in 2D-restricted geometries due to the quantum confinement effect.[9,10] 2D materials are well known for developing high-performance thermoelectric (TE) devices. Due to the unique quantum effects that have a remarkable influence on their thermal and electric properties at small scales. Thermoelectric behavior in 2D materials has gained plenty of attention since the discovery of graphene. A novel class of 2D materials, including monolayer tin sulfide (SnS) and arsenene (a single layer of arsenic), have been discovered in recent years.[11] They have orthorhombic puckered structures and semiconducting bandgaps and showed anisotropy in the physical properties. Hu et al. used ab initio density functional theory to investigate the energetic and thermoelectric characteristics of four monolayer phases of SnSe in conjunction with α-SnSe.[12] They projected that ZT value for the SnSe phase is 2.06 at 300 K, which indicates that this material is promising for new thermoelectric applications. Vu et al. discovered the piezoelectricity and carrier mobility of Janus $\gamma - Sn_2XY$ (X/Y = S, Se, Te) monolayers using first principle.[13] These materials exhibit strong piezoelectric properties and high electron mobility, particularly in the out-of-plane direction. Janus SnSSe monolayer exhibits remarkably low thermal conductivity,

B. Kaur, S. Dhiman
Department of Physics
Punjab Engineering College (Deemed to be University
Sector 12, Chandigarh 160012, India
Heena, S. R. Ahmad
Department of Physics
Jamia Millia Islamia
New Delhi 110025, India
S. A. Khandy
ZJU-Hangzhou Global Scientific and Technological Innovation Center
School of Micro-Nano Electronics, Zhejiang University
Hangzhou 311200, China
E-mail: shakeelkhandy11@gmail.com
M. D Albaqami
Department of Chemistry
College of Science, King Saud University
Riyadh 11451, Saudi Arabia
M. Srinivasan
School of Physical Sciences
Amrita Vishwa Vidyapeetham
Mysure 570026, India
L. Patra
Department of Mechanical Engineering
University of California
Santa Barbar, CA 93106, USA
K. Kaur
Department of Physics
Mehr Chand Mahajan DAV College for Women
Sector 36, Chandigarh 160036, India
E-mail: kulwinderphysics@gmail.com
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