Electronic Structure

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TOPICAL REVIEW

Computational prediction of thermoelectric properties of 2D materials

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Abstract

In low dimensional materials, the conversion of thermal to electrical energy via thermoelectric devices gained much more attention when a ZT > 5 was reported in metastable $Fe_2V_{0.8}W_{0.2}Al$ thin film (2019 *Nature* **576** 85). In this brief review, we tried to describe the underlying physics of nanostructured thermoelectric materials accompanied by the introduction to enhance the efficiency of energy conversion from one form to another. From this determination, we select the two dimensional (AB type) materials such as Sc*X* (*X* = P, As), Si*X* (*X* = S, Se, N, P, As, Sb, Bi), Ge*X* (*X* = S, Se, Te), Sn*X* (*X* = S, Se, Te) and B*X* (*X* = S, Se, Te) etc. Different theoretical methods have also been mentioned to study the intrinsic thermoelectric properties which might help in searching experimentally the new and promising thermoelectric materials. We explore the thermoelectric parameters such as Seebeck coefficient, electrical conductivity and thermal conductivity by using density functional theory, Boltzmann transport theory with constant relaxation time approximation and non-equilibrium Green's function approach. Reduced dimensions potentially expand the thermoelectric efficiency by enhancing the Seebeck coefficient and decrease the thermal conductivity. Theoretical calculations thus recommend the stimulation of the two-dimensional (2D) materials with experimental capabilities in designing and improving the thermoelectric performances.

1. Introduction

From the last few years, the simultaneous global energy consumption and the demand for its reduction has increased persistently. Global warming phenomenon is the main beneficiary of the excessive use of natural energy reserves. Statistics reveal that 84% of the total energy consumed in the world is met by burning fossil fuels; the rest 3% and 13% comes from nuclear and renewable sources of energy, respectively. This kind of dependence on non-renewable sources has led to man-made climate change. Being a part of the scientific community, there exists a major drive toward finding greener and renewable energy solutions with lower carbon footprints. These solutions may be in the form of new energy sources or new ways to improve the utilization of available energy sources. Therefore, it is really important to look into the energy technologies that have flourished to accommodate this energy consumption explosion. Generally, in all the scientific and technical fields many kinds of energy losses are heat, sound, flux and the eddy currents etc, and among all these effluents about 70% of energy is lost as heat. In the field of solid state or semiconductor electronic devices, heat generation in the chips is 100 W cm^{-2} [1] due to dense packaging and advancement in semiconductor lithography. The 1989 report of US air force showed that more than 50% electronic failures are due to the temperature issues [2]. In the case of internal combustion engines, 30% fuel is wasted in engine coolant, 40% is dissipated in exhaust gas, 5% is lost as friction and radiation and only 25% is useable for vehicle mobility [3, 4]. Only in US, annually