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THE RU IMPURITY EFFECT ON ELECTRONIC, OPTICAL AND THERMOELECTRIC PROPERTIES OF MoS_2 NANO-SHEET: A DFT STUDY

The electronic, optical and thermoelectric properties of MoS_2 nano-sheet in presence of the Ru impurity have been calculated by density functional theory framework with Generalized Gradient approximation. The $MoRuS_2$ nano-sheet electronic structure was changed to the n-type semiconductor by 1.3 eV energy gap. The optical coefficients were shown that the loosing optical energy occurred in the higher ultraviolet region, so this compound is a promising candidate for optical sensing in the infrared and visible range. The thermoelectric behaviors were implied to the good merit parameter in the 100K range and room temperatures and also has high amount of power factor in 600K which made it for power generators applications.

Keywords: MoS_2Ru nano-sheet, DFT, Electronic properties, Optical properties, Thermoelectric Properties

1. Introduction

The physical properties of two-dimension (2D) materials have been opened the new windows in the material sciences [1-4]. Transition-metal dichalcogenides (TMDs), have been more attractive due to their electronic, optical and thermoelectric properties, which are originated in the quantum effects by the atomic-layer of TMD crystals. The two-dimensional (2D) transitions metals as MoX_2 (X = S, Se and Te) have been attractive for science and industry based on their electronic, mechanical, thermoelectric, sensors and photo-detectors properties [5-7] as a surrogate for silicon or organic semiconductors. The MoX_2 2D structures have a Mo layer which is sandwiched with two X layers. Several physical properties of MoX_2 have been investigated in the bulk, film and 2D forms, experimentally and theoretically [8-11]. The MoS_2 nano-sheet is synthesized by mechanical exfoliation technique [12], liquid exfoliation [13] and chemical vapor deposition (CVD) [14,15], physical vapor deposition (PVD) [16] etc.

The experimental efforts were reported that the MoS_2 bulk has an indirect band gap by 1.29 eV, meanwhile, its monolayer with 0.65 nm thickness has the 1.8 eV p-type direct gap [17], which is referred to contribute to low-power electronics, thermoelectric and flexible optoelectronic applications [18-21]. Moreover, this compound is used for energy conversion [22], energy storage [23], and hydrogen evolution [24]. The electronic and optical properties of MoS_2 2D are depended on the same conditions as thickness, defects and impurities, and then need to be understood in detail for the suitable design of devices and their functions [8].

The photoresponsivity of MoS_2 mono-layer was reported as 880 $A.W^{-1}$ for incident light at a wavelength of 561 nm with photoresponse in the 400-680 nm range [25], which can be applied in the ultra-sensitive phototransistors. The photoluminescence and absorption capacity of MoS_2 mono-layer [26] in the ultraviolet area, makes it a promising composition for the ultraviolet detectors [27] and absorber layer in low-cost film solar cells [28-29] and light-emitting diodes (LEDs) [30-34].

Some works have investigated the thermoelectric behaviors of MoS_2 nano-sheet [35-39] to solve energy issues. The efficiency of thermoelectric material is shown by the figure of merit (ZT), which is related to the Seebeck (S), electronic conductivity (σ) and thermal conductivity (K). The ZT of MoS_2 2D lies between 0.02 to 0.53 [40], and some experiment efforts have been shown that this composition is a good thermoelectric material with a large S parameter [41]. Some studies have been shown the effect of the vacancy, defects and doping impurities on the thermoelectric efficiency of MoS_2 2D. The good thermoelectric

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