UNIVERSITI TEKNOLOGI MARA

FIRST-PRINCINPLES STUDY OF THERMOELECTRIC PERFORMANCE OF PURE AND Ni-DOPED Bi_2Se_3 AND Bi_2Te_3 USING DENSITY FUNCTIONAL THEORY

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ABSTRACT

First principles study-based density functional theory on structural, electronic and thermoelectric properties of Bi2Se3 and Bi2Te3 materials was conducted using CASTEP and WIEN2K computer code within the exchange-correlation of local density approximation (LDA). Calculations of electronic properties were carried out with spin-orbit coupling (SOC). The thermoelectric properties were calculated using Boltzmann transport theory that implemented in BoltzTraP with the inclusion of SOC. The effect of SOC on electronic properties and thermoelectric properties were analysed and found that SOC gives a significant contribution. The band gap result showed that spin-orbit coupling is necessary for the calculation to show the true nature of Bi2Se3 and Bi2Te3 that verified by the experimental studies. Bi2Se3 depicts band gap 0.23 eV which is higher than Bi2Te3 with band gap 0.15 eV. Based on the calculated figure of merit, Bi2Te3 shows a better thermoelectric performance of 0.3 compared with the Bi2Se3 which has performance 0.07 at room temperature. The performance of Bi2Se3 increases from temperature 300K to 500K. While, the performance of Bi2Te3 decreases. Then, thermoelectric properties are calculated based on the Fermi level range from -1.0 eV to 1.0 eV to prove that tailoring Fermi level could optimize thermoelectric performance for both Bi2Se3 and Bi2Te3. Thermal conductivity is undesirable for the performance, however it cannot be reduced without reducing electrical conductivity. Adjusting Fermi level could alter the performance of Bi2Se3 and Bi2Te3. It is found that Bi2Se3 has higher ideal thermoelectric performance which possesses figure of merit 0.88, while Bi2Te3 has figure of merit of 0.66. Nickel has reduced band gap of both Bi2Se3 and Bi2Te3, improving electrical conductivity. Ni-doped Bi2Se3 has a slightly better performance with figure of merit 0.335 at 300 K compared with the Ni-doped Bi2Te3 that has figure of merit 0.316.

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