CHAPTER 5

CONCLUSION

The objective of this thesis is to predict the thermoelectric properties of CNTs–added $CaMnO_3$ by first calculating its electronic structure and assessing its thermal properties. This chapter provides a conclusion to the research that was performed with a view to satisfying this objective.

Electronics structure

The clusters under examination were comprised of a CMO cubic structure, CMO orthorhombic structure, CNTs–added CMO, and C–substitute CMO.

The CMO cubic structure exhibited a particular distance for each order and this tended to be consistent with the ideal structure of CMO. The orthorhombic structure exhibited strong bonding as well as indicating good electrical conductivity at the a–, and c–axes. The CNTs–added CMO exhibited C residing closely in the unit cell. The C–substitute CMO exhibited strong bonding of Mn–, Ca–, and O–C.

The DOS of CMO with two structures presented Ca 4p, Ca 4s, Mn 4p, Mn 4s, O 2p and O 2s orbitals, respectively. The case added and substitute C exhibited C 2s and C 2p orbitals, respectively. The DOS of C–substitute CMO exhibited an energy intensity increase greater than the DOS of CMO. Each DOS exhibits characteristics typical of *n*–type thermoelectric material. The energy level shows the orbitals as having the same values as those derived using the DOS. The energy gap was derived from the energy level. The CMO cubic structure has an energy gap of 0.5 eV which agrees with the literature (Cardoso et al., 2008, p.035202).

The CMO orthorhombic structure has an energy gap of 0.7 eV which also agrees with the literature (Zhang et al. 2011, pp. 542–245; pp. 4171–4175; pp. 1258–1262; Seetawan, 2014, pp. 9–14; Zhang et al., 2015, pp. 1–5). The CNTs–added CMO has an energy gap of 0.19 eV. The C–substitute CMO has an energy gap of 0.03–0.04 eV.

The Fermi energy of the CMO cubic structure was different to that of the orthorhombic structure. It presented as 0.24 eV for the cubic and 0.34 eV for the orthorhombic structure at 300 K. The CNTs–added CMO exhibited a Fermi energy value of 0.089 eV at 300 K. The Fermi energy of C–substitute CMO was observed as 0.14–0.24 eV.

Thermal properties

The cluster atoms model of CMO cubic used a total of 320 atoms (Ca 64, Mn 64, O 192), CMO orthorhombic used a total of 240 atoms (Ca 52, Mn 60, O 128) and CNTs–added CMO used a total of 247 atoms (Ca 64, Mn 27, O 108). These cluster atoms models were designed to calculate thermal properties by MXDORTO.

The thermal properties consisted of the lattice parameter, compressibility and linear thermal expansion coefficient. These materials were seen to expand with increasing temperature. The rate of expansion was significantly greater for CNTs–added CMO and C–substitute CMO. The heat capacity was well calculated and showed agreement with Dulong–Petit law at 600 K, indicating also that thermal conductivity tends towards a constant value. The auto–correlation function showed quick decay to zero with increasing temperature. At 700 K the CNTs–added CMO displayed a greater heat flux auto–correlation function than had been calculated by the research team. In addition, the thermal conductivity at various times decreased in value as the temperature increased.

Thermoelectric properties

The thermoelectric properties examined for this research paper were the Seebeck coefficient, electrical conductivity, power factor, thermal conductivity, and Dimensionless Figure of Merit. The results for CMO showed agreement with the experimental data and the literature. The CNTs–added CMO displayed the Seebeck coefficient as reduced by 50%, electrical conductivity enhanced by 86%, thermal conductivity enhanced by 40% and PF enhanced by 73%. The C–substitute CMO displayed the Seebeck coefficient as reduced by 41%, electrical conductivity enhanced by 68–71%, thermal conductivity enhanced by 41% and the power factor enhanced by 75%.

The CNTs–added CMO exhibited good ZT at 300–560 K. The C–substitute CMO exhibited good ZT at 560–700 K. The probability of the ZT value of CNTs–added CMO is between 0.055 – 0.195 at 700 K.

Suggestion

The computer simulation should be administered at high speed. It had the wrong power outage and should be used with a computer powered through a UPS. The equation should be derived before evaluating or predicting thermoelectric properties