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Tuning the Bandgap of Bulk Molybdenum Disulphide using Defects

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Abstract

This report highlights the use defects to changes the electronic properties of bulk molybdenum disulphide (MoS2). The defects introduced also have significant effects on the thermal properties. We further demonstrate how altering the atom arrangement or introducing other atoms in the lattice, affects the electronic properties of MoS2 and other metal dichalcogenides. Pristine MoS2 is p-type semiconductor and it can also be turned into an n-type semiconductor, depending the choice of impurity introduced. This has been demonstrated by use of plots of Seebeck coefficients against chemical potential. The high Seebeck coefficients observed suggest that defect modified MoS2 is a potential candidate for thermoelectric applications. The anisotropic nature of the electronic properties of MoS2 is demonstrated for the thermal conductivity and electronic conductivity as a function of chemical potential. The induced defects lead to bandgap reductions ranging between 10.7% and 100%, relative to the pristine MoS2.

For bulk MoS2 a supercell of 2x2x2 totaling to 48 atoms was used. From these, an atom was either added into the interstitial sites or removed from the lattice. Quantum ESPRESSO code was used and its output was taken as the input for BoltzTrap code. The calculations were spread on 24 cores adopting MPI program using CHPC facility.

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