Notification No: 541/2023
Date of Award: 10-07-2023

Name of the Scholar: GAURAV JAMWAL
Name of the Supervisor: Dr. ASAD NIAZI
Name of the Co-Supervisor: Prof. K. ASOKAN
Name of the Department/Centre: DEPARTMENT OF PHYSICS

Topic of Research: Study of Physical, Electronic and Thermoelectric Properties of Some Chalcogenide Compounds

FINDING

The world is currently confronted with numerous challenges related to energy supply, consumption, and energy sources. Fossil fuels have been the main source of energy generation so far. Only fossil fuels can meet the world's energy needs. The heavy dependency on fossil fuel may lead to an energy crisis in the near future, as well as several environmental issues such as global warming. Therefore, one of the most urgent problems of the present is to find alternative energy sources that are sustainable and environmentally friendly. This is motivating the search for new thermoelectric (TE) materials and methods, as well as the design of new devices for energy harvesting.

The efficiency of TE materials is evaluated using a dimensionless figure of merit (ZT), given by $ZT = S^2\sigma T/\kappa$, where S = Seebeck coefficient or Thermopower, σ = electrical conductivity, κ = thermal conductivity. Thus, in order to achieve a high ZT, a material must exhibit a large Seebeck coefficient, high electrical conductivity and low thermal conductivity. However, to simultaneously optimize these parameters is difficult because S, σ and κ are strongly interrelated as a function of the band structure, carrier concentration and other factors.

The Ph.D. thesis entitled **'Study of Physical, Electronic and Thermoelectric Properties of Some Chalcogenide Compounds'** is a comprehensive study of bulk materials synthesized by solid state route with spark plasma sintering (SPS). In this work, I have synthesized three types of chalcogenide compounds: $Cu_2ZnSnSe_4$, SnTe and $AgSbTe_2$, and studied the effect of elemental doping on their properties. The crystal structure, morphology, elemental composition,

and thermoelectric properties of the compounds were studied for applications. Doping was found to modify the electrical conductivity by tuning the carrier concentration, and to reduce their thermal conductivity due to phonon scattering, thus leading to enhancement of thermoelectric properties.

The electronic band structure and density of states (DOS) for pure and doped compounds were calculated using DFT and provided important information about the electronic transport properties. Doping was found to produce a variety of effects such as formation of resonant levels around the Fermi level, valence band convergence, carrier concentration tuning, increase in effective mass, and phonon scattering, leading to improved thermoelectric properties of the compounds under study. In order to explore other aspects of energy harvesting, the compound $Cu_2ZnSnSe_4$ was also studied for photovoltaic applications and used to fabricate a solar cell device.