The layered compounds of group VI like molybdenum disulphide and molybdenum diselenide have recently attracted many researchers because of their fascinating properties and have thus gained a new impetus. The study of their interesting anisotropic behaviour in the past few years have become an intensively investigated field in the study of the solid state research. The single crystals of most of these substances can be successfully grown has made it possible to apply new techniques of investigation of these materials.

Their Physics and Chemistry has therefore rapidly progressed. An excellent survey of the existing information on the layer compounds has been reported by D.Reidel publishing Company in a series “Physics and Chemistry of Materials with Layered structures”

Although number of layered materials such as silicate (mica, clays,) organic compounds, ternary inorganic compounds and intercalation compounds exist, the present work is limited to the transition metal dichalcogenides of the type MX$_2$, where M is one of the transitions metals and X is a chalcogenide atom. The structure of these compounds resemble a stacking of sandwiches in each of which a plane of hexagonally arrange metal atom lies between two planes of similarly arranged chalcogen atoms. The bonding within each sandwich is essentially covalent while the sandwiches are held together by much weaker van der Waals bonding. This has led to considerable anisotropy in their physical properties. Even more interesting is the enhancement in the two dimensional nature of the materials which can be achieved by intercalating large organic molecules and effectively isolating the layers from one another.
Under normal conditions solids exhibit a particular crystal structure for which total energy is minimum. However, on application of high pressure, the atomic arrangement in solid changes resulting in changes in interatomic distances and crystal structure. These changes in solid can be studied in greater detail to reveal several new features of the interatomic forces which are of great importance to visualize the mechanism governing the structural changes and to reveal solid state properties associated with different structures. In this context, the behavior of the molybdenum disulphides and molybdenum diselenids single crystals under pressure up to 6.5 GPa, has been studied.

A comparison of liquid junction photoelectrochemical (PEC) solar cells with conventional photovoltaic devices indicates that in the fabrication of PEC devices many processing steps required for conventional solid state solar cells (e.g. p-n junction) are either simplified or completely eliminated. This leads to a significant reduction in cost for the fabrication of a PEC device relative to solid state solar cells. In addition, PEC devices can also be used to store energy locked up in conventional fuels. Significant optical to electrical/chemical conversion efficiencies has been obtained in solid state photovoltaic and PEC solar cells. Author made an attempt to use tin monoselenide in the fabrication of a PEC solar cell.

The work presented in the thesis has been divided into ten chapters. As the thesis essentially deals with the growth and characterization of molybdenum disulphides and molybdenum diselenides single crystals, all the existing information on molybdenum disulphides and molybdenum diselenides is outlined in Chapter 1.
The Chapter 2 of the thesis contains the complete methodical description of the growth of molybdenum disulphide and molybdenum diselenide single crystals. The important features of the Chemical Vapor Transport Technique (CVT) have been thoroughly explained. Details of the experimental set-up, furnace construction, temperature controller circuit and method have also been explained.

The structural characterization of both crystals using X-ray diffraction techniques and the elemental analysis using the Energy Dispersive Analysis by X-rays (EDAX) and a study of microstructures on the growth surface has been carried out to explain the mechanism of growth of these crystals is included in Chapter 3.

The optical band gap of semiconductor plays a vital role in deciding its effectiveness in thermoelectric devices. The detail study of this parameter is extremely desirable therefore. A complete study on its determination for molybdenum disulphides and molybdenum diselenides single crystals and therefore been made by optical absorption. The results thus obtained are presented in Chapter 4.

The various physical properties such as room temperature resistivity, high temperature resistivity (perpendicular to c-axis), anisotropy, low temperature resistivity (77 K to room temperature), Hall effect measurements, thermoelectric power measurements, were carried out and the results obtained have been systematically represented in Chapter 5.

Chapter 6 reviews the techniques of high pressure generation and describes the measurements of high pressure of the order of Kbar.
Chapter 7 explains the effect of pressure on electrical resistance of the grown crystals. The results obtained are presented.

Chapter 8 contains the description of necessary introduction to PEC solar cells. The solar cells of different types are explained and discussed. The advantage of PEC solar cells over the sold state photovoltaic cells have also been thoroughly discussed.

The Photoelectrochemical study carried out by the author on the grown crystals has been presented in the Chapter 9.

Finally the far reaching conclusion of the work described in the thesis and the scope for the future work are precisely explained in Chapter 10.