Preface

Energy is playing an important role in human survival and society. Today, the demand of energy in the world has been covered by fossil fuels. Fossil fuels are expected to supply huge portion of the demand even in future. The need for light-weight, high capacity energy stores is determined by the essential for a more sustainable approach to reducing the global dependency on fossil fuels. The recent studies show that the hydrogen storage in solids is a better option compared to the storage in gaseous or liquid state, because storage in solids is safer and requires less space. For the same alkali metal hydrides are best alternatives.

As the topic of the present thesis suggest, we have to study possibilities to store hydrogen atoms in alkali metal hydrides along with extra added hydrogen atoms that is \( \text{XH}_n \text{H}_2 \) \((\text{X}=\text{Li}, \text{Na}, \text{K}; n=0, 1, 3, 4)\). Therefore first we have to establish the structural stability of these series. The whole computational work is done using the density functional theory (DFT) based on full potential linearized augmented plane wave method (FPLAPW). In computation the exchange-correlation energy is obtained generalized gradient approximation (GGA). The present thesis is organized as follows:

Chapter 1 starts with a brief introduction of the energy problems in future, the probable alternatives of energy and their overall aspects as an energy source. It is followed by a brief discussion of the concept of hydrogen as energy carrier and a source of energy alternative of future, the production of hydrogen from the available sources and the possible ways to store hydrogen. In the end of this chapter, motivation and objective of the present work is mentioned.

Chapter 2 described various methods and assumptions that have been used to perform the calculations related to structural, electronic and optical properties of compounds. Density Functional Theory (DFT) has become one of the most important tool for ab-initio calculations in materials science. Density Functional formalism based on the fundamental theorems of Hohenberg and Kohn, and Kohn and Sham (KS) has demonstrated a large predictive power in the study of the ground states properties of real materials. A brief discussion about DFT along with Wien2k code is also presented in this chapter.

Chapter 3 begins with an introduction to the alkali metals hydride materials. It starts with the current interest in compounds \( \text{XH} \) \((\text{X}=\text{Li}, \text{Na}, \text{K})\). Calculations have
been carried out for XH (X=Li, Na, K) with added extra hydrogen compounds \( \text{LiH} \cdot n\text{H}_2 \), \( \text{NaH} \cdot n\text{H}_2 \) and \( \text{KH} \cdot n\text{H}_2 \) where \( n=1, 3, 4 \) residing in interstitial region. The crystal structure, cohesive energy and electronic properties at ambient conditions have been studied.

**Chapter 4** compiles the elastic properties of XH\(_n\text{H}_2\) (X=Li, Na, K; \( n=0, 1, 3, 4 \)) in cubic structure. Elastic properties are calculated by the ‘cubic elastic’ package which is interfaced to the “wien2k” code. Obtained elastic constants obey the conventional mechanical stability criteria for all these compounds in series. Obtained elastic constants are used to drive the other elastic parameters such as bulk modulus, anisotropy factor, shear modulus, Young’s modulus, Poisson’s ratio and B/G ratio. Results are listed in the form of table and discussed to draw conclusions.

**Chapter 5** summarizes the study of optical properties of XH\(_n\text{H}_2\) (X=Li, Na, K; \( n=0, 1, 3, 4 \)) using the optic program of WIEN-2k code. The obtained results of dielectric constant, refractive index, optical absorption, extinction coefficient, optical conductivity, energy loss function and reflectivity with in energy range 0-30eV have been discussed in detail. The calculated results are presented in the form of tables and figures.

**Chapter 6** is the concluding part of the thesis. In this chapter, we have summarized the studies done in the thesis along with the future scope of the work.

In the end of each chapter references are included.