Summary

A renewable and clean source of energy is required to change the current energy scenario which is based on carbon-based fossil fuels technologies. Renewable energy sources like solar, wind, water, biomass etc. have received a lot of attention in this regard to reduce the carbon emission. Hydrogen could be an appropriate alternative in terms of clean energy technologies as the only by-product of hydrogen fuel-cell is non-polluting water vapour. At the same time it is one of the abundant sources of energy and has a high energy content in unit mass. In past decade, intensive research has been done to store the hydrogen and to utilize it as a fuel in our daily life. Storing hydrogen is one of the major issues due to low density of hydrogen gas at ambient conditions. Hydrogen can be stored in a safe and energy efficient manner in terms of physisorption of hydrogen gas molecules on solid adsorbent. In this context, single-walled carbon naotube (SWCNT) is the promising one to adsorb hydrogen gas molecules into its unique curved hollow structure above the storage target defined by the U.S Department of Energy (DOE). Here, this thesis presents hydrogen storage in single-walled carbon nanotube by incorporating several structural changes by state of the art molecular dynamics simulation and density functional theory. At the beginning of the thesis a preliminary study based on pure SWCNT is conducted to optimize the diameter and chirality of nanotubes and to find optimum operating conditions for hydrogen storage. Literature says the storage goal in terms of physisorption, can only be reached at cryogenic temperatures. Thus my main objective of Ph.D work is to tune the structure of the nanotubes to make it suitable to store hydrogen above the DOE goal at room temperature. At the time of synthesis of nanotube several topological defects form on nanotube's surface. Thus the consensus which indicates several discrepancies in

storage target of SWCNT, can be attributed to nature of structural defects present in nanotube's surface. Binding energies of defective rings present on nanotube's surface plays a crucial role for hydrogen adsorption. Stone-Wales 5,8 defective nanotube can enhance the storage capacity whereas all the other types of defective nanotubes decrease the capacity. Moreover, when nanotubes are arranged in a specified lattice, number of adsorption sites increases. At an increased value of lattice constant, number of captured hydrogen in groove volume and interstitial volume increases. Thus single-walled nanotubes arranged in a square lattice show better storage capacity at room temperature compared to isolated one. The next two parts of my thesis is devoted to dope foreign atoms on nanotubes. We find a new technique to dope titanium atom on nanotube structure, which reaches the storage capacity of 7.75 wt% above the DOE goal at room temperature. We have also studied hydrogen storage in lightweight alkaline metal, beryllium doped defective nanotubes. Due to light weight of beryllium it increases gravimetric storage capacity of nanotubes significantly. Lastly, in contrast to arranged structure of nanotube, we studied hydrogen storage in completely amorphous structure, formed from melting of nanotube and other carbonaceous materials above their melting point. We find that there is a significant effect of starting structure on hydrogen storage. In summary, hydrogen storage depends on defect, doping of foreign atoms and several structural changes present in adsorbent and by doping metal on defective single-walled carbon nanotube high storage capacity above the target could be reached even at room temperature and moderate pressure. This theoretical approach and all the novel findings could be an appropriate guideline to start an experiment.