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Effect of electronic alteration on hydrogen storage and optical response in $NaMgF_3$ using DFT approach

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Abstract

Due to the depletion of non-renewable fossil fuels, energy production and storage is a matter of concern for scientific community. Hydrogen being environmental friendly was presented by the scientists a fruitful replacement of fossil fuel, but the storage of hydrogen is still a matter of concern. Safety concerns are associated with hydrogen as an alternative fuel because it is difficult to store and transport. Perovskite materials have attracted researchers as new materials for solid hydrogen storage. In this present work, Density Functional Theory (DFT) calculations have been performed for perovskite NaMg $\mathbf{F_{3-x}H_x}$ with the GGA-PBE formalism as implemented in the CASTEP code. The aim of the work is to investigate the structural, electronic and optical properties of NaMg $\mathbf{F_{3-x}H_x}$ perovskite hydride material for hydrogen storage applications with varying substituent concentrations (x=0, 0.3, 0.6, 0.9, 1.2). The formation enthalpy of the studied material for each concentration reveals that these compounds are stable and synthesizable experimentally. The hydrogen inclusion in pristine material affects the electronic states significantly which is elaborated using band structure and density of states plots. After Hydrogen inclusion, change in density of states has been observed and the band gap is decreased from $\mathbf{5.74\ eV}$ to $\mathbf{3.311\ eV}$. The alteration of electronic band gap directly influences the optical behavior of the material, thus optical response such as dielectric function, absorption and refractive index was also calculated. For hydrogen storage application,

gravimetric storage capacity ($C_{wt\%}$) was calculated for all concentrations of hydrogen inclusion. The value varied from 0.30% to 1.87%, indicating that the presented material is an efficient material not only for opto-electronic applications but also for the hydrogen storage applications.

Introduction

With consequently rise in the world's population, researchers are focusing on two main factors energy and non-polluting environment for improving overall progress. Serious energy crisis is rising due to rapid consumption of fossil fuels on a global scale [1]. Hydrogen is named renewable energy source having properties that are environment friendly, high-energy-density, lightweight, and no harmful product produced in combustion. In 1792, manmade machine first time worked for humans when steam engine was invented by Thomas Newcomen. Mineral coal is utilized as an energy source for this steam engine. In 1860, 5×10^{12} Kilowatts per year was average consumption of energy and increased to 1.28×10^{14}kW per hour. Nowadays $\mathbf{5\ kw/person}$ and $\mathbf{10\ kw/person}$ is normal routine power consumption in Europe and USA. Demand for energy supply based on limited reserves of fossil fuels on earth will exceed in the future [2]. So we can estimate that the energy consumption would be doubled in next half century. To generate energy and water, hydrogen and oxygen undergo a combustion reaction $\mathbf{2H_2 + O_2 \rightarrow 2H_2O}$ and energy $\mathbf{\Delta H = 120\ KJg^{-1}}$. This reaction is environment friendly, as no carbon produces in reaction. As hydrogen is carbon-free energy carrier, the maximum energy density is produced during reaction. In case of methane combustion $\mathbf{CH_4 + O_2 \rightarrow CO_2 + H_2O}$ contribution of energy from hydrogen and carbon is $\mathbf{120\ kjg^{-1}}$ and $\mathbf{30\ kjg^{-1}}$.Hydrocarbon fuel energy density scale varies with ratio of hydrogen to carbon [3,4] (see Fig.1, Fig.2).

For onboard applications, hydrogen storage is much more complicated compared to stationary applications, but for developed hydrogen economy for both purposes, hydrogen storage is used [5]. A sufficient hydrogen amount is mandatory to cover an appropriate distance in case of onboard storage without refueling the vehicle [5]. A highly accurate storage technique is needed that gives both high volumetric and gravimetric energy density. These are seven techniques used for hydrogen storage cryo-compressed hydrogen, metal hydrides, liquid organic hydrides, physically absorbed hydrogen, compressed hydrogen, and liquefied hydrogen [[5], [6], [7]]. At high-pressure compress, hydrogen technique is mostly used for hydrogen storage. A high rate of filling and releasing hydrogen is obtained by this technique and for releasing hydrogen no extra energy is required, so considering compressed hydrogen is an advanced technique. Volumetric energy density is enhanced to a wide scale as higher density is present in cryogenic or liquid from hydrogen [8]. Achieved energy density is $\mathbf{8\ MJ/LH_2}$ when density of liquid hydrogen approached to $\mathbf{71\ g/L}$ at $\mathbf{-253^{\circ}C}$ [9]. Compare to mechanical storage technique high volumetric and gravimetric density is obtained. No high temperatures and pressure required for the operation of metal hydrides in fuel cell vehicles, and perfect range is between $\mathbf{1-10\ atm}$ and $\mathbf{25-293\ k}$ for PEMFC [10]. Metal hydrides are synthesized by adding/doping hydrogen in the metal [11]. After Thomas Graham's experiment of hydrogen absorption onto palladium scientists start investigating metal hydrides at a large scale. Intermetallic and binary halides are two basic types of metal hydrides [12,13]. While binary has only one metal and intermetallic halides have two or more metals compared to hydrogen. When hydrogen attached to metal is partially covalently bounded with a polyatomic anion is called as complex as complex metal hydrides. Nitrogen and boron-containing hydrides are a major category of complex metal hydrides and they give higher gravimetric storage compared to simple hydrides [8]. For evolution of new practical material, scientists focused on specific material properties of Mg-based hydrides. Perovskite structure has been observed in some Mg-based hydrides like $\mathbf{AMgH_3}$ (where A is alkali element). $\mathbf{NaMgH_3}$ is an insulator according to Vajeeston etal.Volumetric density of $\mathbf{NaMgH_3}$ is $\rho_v = 88\%$ and gravimetric density is $\rho_c = 6\%$ [[14], [15], [16]]. Further research is required to improve hydrogen storage capacity by using a suitable catalyst and through

quenching. Work should be done on the synthesis of $NaMgF_{3-X}H_X$ that presents a high potential for hydrogen storage to evaluate its practical application in onboard hydrogen vehicle. Transport parameters and electron-phonon coupling aspects must also be studied in the future to realize it for purposes of fuel cell applications.

The predicted hydrogen storage capacity of presented material $NaMgF_{3-x}H_X$ (1.87 wt%) is greater than reported storage capacity of complex alloys $Ti_{0.15}Zr_{0.85}La_{0.03}Ni_{1.2}Mn_{0.7}V_{0.12}Fe_{0.12}$ (1.54 wt%), $La_{0.64}Sm_{0.07}Nd_{0.08}Mg_{0.21}Ni_{3.57}Al_{0.10}$ (1.45 wt%) and $(La, Mg)_2Ni_7$ (1.437 wt%) after high annealing [[17], [18], [19]]. Stability of the compound can be checked by negative formation enthalpy, $NaMgF_{3-x}H_x$ is more stable compound then reported $LaMgNi_4$ [20]. Suggested material is not only useful for hydrogen storage, in pure form but also be used as anti-reflecting coating material due to low reflectivity [21]. It could also be used in photonic crystal, data storage and waveguide optical devices [22].

In this work band gap and density of the state $\boldsymbol{NaMgF_{3-X}H_X}$ is calculated by using density functional theory (DFT) with general gradient approximation (GGA) (Fig. 1). In Computational Details computational detail and technique used for investigation are discussed. While in Results and Discussion hydrogen storage of $\boldsymbol{NaMgF_{3-X}H_X}$ is calculated and finally optoelectronic properties are discussed. In the last section, results are deliberated in detail.

Section snippets

Computational details

By using density functional theory in configuration of CASTEP (Cambridge Sequential Total Energy Package) physical properties of $\boldsymbol{NaMgF_{3-X}H_X}$ (X=0, 0.3, 0.6, 0.9, 1.2) was calculated. Plane-wave pseudopotential technique is used to execute all these calculations and basis cut-off energy is 400 eV [[23], [24], [25]]. This technique performs calculations faster without altering efficiency [26,27]. Cubic unit cell of $\boldsymbol{NaMgF_3}$ belonged to space group $\boldsymbol{Pm-3m}$. Wyckoff fractional position for sodium,…

Geometry optimization

By using GGA-PBE in first step, the $\boldsymbol{2\times2\times1}$ supercell of cubic perovskites $\boldsymbol{NaMgF_3}$ geometrically optimized. Murnaghen state equation is used to approximate lattice parameter to maintain overall energy of crystal low and at a certain volume, energy is minimum known as optimized unit cell volume [22]. Lattice parameter optimized from this geometry is $\boldsymbol{a=b=c=0.4\ nm}$ and reported one in other papers is $\boldsymbol{a=b=c=0.39\ nm\ and\ 3.87}$, also compared these lattice parameter [34,35]. After substituting hydrogen it…

Conclusion

In this paper, electronic and optical characteristics of H-incorporated and pristine have been analyzed by the first principle using density functional theory. Cubic structure of $\boldsymbol{NaMgF_3}$ is changed into a tetragonal structure with hydrogen doping. Change lattice parameters indicate the effect of hydrogen doping because the ionic radius of hydrogen and fluorine is different, while volume is increased up to 254.2 nm when concentration increased up to $\boldsymbol{X=0.6}$ and, on further increase in hydrogen…

Data and code availability

This article includes all data generated and analyzed during the study. However, the data made available subject to the approval from journal's editorial board.…

Ethical approval

This work does not involve any kind of human testing or chemical involved to test on humans.…

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.…

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