

Annai Hajira Women's College

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STAFF PUBLICATIONS UNDER UGC CARE LISTED JOURNALS 2021-2022

**Number of research papers in the Journals notified on UGC
CARE list in the year 2021-2022**

Sl.No	Title of paper	Name of the author/s	Department of the teacher	Name of journal	Is it listed in UGC Care list
1	Naan Manikkadikaiyil samooga Ariviyal Sinthanaikal	Dr.S.Uma	Tamil	Modern Tamizh Research	UGC Care Listed
2	Ara noolkalil porul ariviyal	Dr.S.Uma	Tamil	Modern Tamizh Research	UGC Care Listed
3	Vehicle Classification with SVM using cross-correlation	K.M.N.Syed Ali Fathima	Computer Science	Sarah Research Journal	UGC Care Listed
4	Thermal and Mechanical Studies of Nanochitosan incorporated PMMA based composite electrolytes	Dr.N.Ammakutti @ Sridevi	Physics	Journal of Engineering and Applied Science (ISSN: 11101903, 25369512)	UGC Care Listed
5	PVDF/PEO/HNT based hybrid Polymer Gel Electrolyte(HPGE) Membrane for Energy Applications	Dr.R.Anuradha	Chemistry	IONICS	UGC Care Listed
6	Effect of nanostructures on the hydrogen storage properties of MgH ₂ – A first principles study	Dr.R.Lavanya	Physics	Computational Condensed Matter	SCOPUS
7	Deep – Vehicle-Nets: Deep CNN Architectures for Classifying viewpoints using Car Images	K.M.N.Syed Ali Fathima	Computer Science	International journal of Mechanical Engineering	UGC Care Listed

Lajja Datta

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30 பகுதி-3
Part -3

நான்மணிக்கடிகையில் சமூக அறிவியல் சிந்தனைகள்

பா. ஜெயந்தி

முனைவர் பட்ட ஆய்வாளர், பதிவு எண் : 19221174022009, தமிழ் உயராய்வு மையம், ராணி அண்ணா அரசு மகளிர் கல்லூரி, திருநெல்வேலி. (திருநெல்வேலி மனோன்மணியம் சுந்தரனார் பல்கலைக்கழக அங்கீகாரம் பெற்றது), தமிழ்நாடு, இந்தியா.

முனைவர் ச. உமா

நெறியாளர், இணைப்பேராசிரியர், தமிழ்த்துறை, அன்னை ஹாஜிரா பெண்கள் கல்லூரி, மேலப்பாளையம். (திருநெல்வேலி மனோன்மணியம் சுந்தரனார் பல்கலைக்கழக அங்கீகாரம் பெற்றது), தமிழ்நாடு, இந்தியா.

ஆய்வுச்சுருக்கம்:

பழந்தமிழர்கள் அனைத்துத் துறைகளிலும் சிறந்து விளங்கினர். அவர்களின் அறிவியல் அறிவானது நமக்கு மிகவும் தெளிவினைக் கற்றுத்தருவதாக அமைந்திருக்கின்றது. பதினெண் கீழ்க் கணக்கு நூல்களுள் ஒன்றான நான்மணிக்கடிகையில் இடம்பெறுகின்ற சமூக அறிவியல் சிந்தனைகளை விளக்குவதாக இவ்வாய்வு அமைகின்றது. இவ்வாய்வு, கீழ்க்கணக்கு விளக்கம், கீழ்க்கணக்கு நூல்கள், பதினெண்கீழ்க்கணக்கு நூல்களின் வகைப்பாடு, பதினெண்கீழ்க்கணக்கு நூல்களின் காலம், நான்மணிக்கடிகை, சமூக அறிவியல், நான்மணிக்கடிகையில் சமுதாயச் சிந்தனைகள், தமிழ்ச் சமூக மரபும் மாற்றமும், நல்லோரியல்பு, நல்லோரியல்பு, நல்லுணர்வு நெறி, நல்லொழுக்கம், தழிவுநிலை, பெருமை, சிறப்பின் நிலை, நன்மக்கள், மறுமைப்பயன், தொகுப்புரை ஆகிய பக்கத்தலைப்புகளில் விளக்கப்பட்டுள்ளது. அதைத் தொடர்ந்து மேற்கோள் குறிப்புகள் இடம்பெறுகின்றன.

திறவுச் சொற்கள் :

பதினெண் கீழ்க் கணக்கு, அறம், நான்மணிக்கடிகை, சமூகவியல்

முன்னுரை

உலக மக்கள் வாழ்க்கையில் கடைபிடிக்க வேண்டிய நெறிமுறைகளைப் பல இலக்கியங்கள்

சூறியுள்ளன. அவற்றுள் மிகச்சிறந்த இலக்கியங்களாகப் போற்றப்படுவது அரிலக்கியங்களே, அற இலக்கியங்கள் மனிதன் வாழ்க்கையில் கடைபிடிக்க வேண்டிய நன்மை பயக்கும் நெறிகளை வலியுறுத்துகின்றன. நீதி என்பது வழிமுறைகளைத் தெரிவிப்பது எனப் பொருள்படுகிறது. அறம் என்பது மிகப் பழங்காலத்திலிருந்தே தமிழில் வழங்கப்பட்டு வரும் சொல்லாக விளங்குகிறது.

கீழ்க்கணக்கு

பல்வேறு நூல்வகைகளுக்கும் இலக்கணம் கூறும் பாட்டியல் நூல்கள் பிற்காலத்தில் தோன்றின. பன்னிருபாட்டியல் என்பது அவற்றுள் ஒன்று. அது ஆசிரியப்பா, கலிப்பா, பரிபாடல் ஆகிய பாவகைகளில் மிகுதியான அடிகள் கொண்டனவாக ஐம்பது முதல் ஐந்நூறு பாடல்களைத் தொகுத்தமைப்பது மேற்கணக்கு என்று கூறுகின்றது. அதுவே, வெண்பா யாப்பினைப் பயன்படுத்தி, குறைவான அடிகளால் ஐம்பது முதல் ஐந்நூறு பாடல்களைக் கொண்டு விளங்குவது கீழ்க்கணக்கு என்றும் கூறுகிறது. இதனால் பாட்டிலுள்ள அடிகளின் மிகுதியும் குறைவுமே மேல், கீழ் என்ற அடைமொழிகளால் விளக்கப்பட்டன என்பது விளங்கும். இடைக்காலத்தில் எழுந்த நூல்களிலும், உரைகளிலும் - கீழ்க்கணக்கு என்று அடையில்லாமலும், பதினெண்கீழ்க்கணக்கு என்று அடையோடும் இவை குறிக்கப்படுகின்றன.

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அறநூல்களில் பொருளறிவியல்

பா. ஜெயந்தி

முனைவர் பட்ட ஆய்வாளர், பதிவு எண் : 19221174022009, தமிழ் உயராய்வு மையம், ராணி அண்ணா அரசு மகளிர் கல்லூரி, (திருநெல்வேலி மனோன்மணியம் சுந்தரனார் பல்கலைக்கழக அங்கீகாரம் பெற்றது), திருநெல்வேலி, தமிழ்நாடு, இந்தியா.

முனைவர் ச. உமா

நெறியாளர், இணைப்பேராசிரியர், தமிழ்த்துறை, அன்னை ஹாஜிரா பெண்கள் கல்லூரி, மேலப்பாளையம். (திருநெல்வேலி மனோன்மணியம் சுந்தரனார் பல்கலைக்கழக அங்கீகாரம் பெற்றது), தமிழ்நாடு, இந்தியா.

ஆய்வுச் சுருக்கம்:

பொருளறிவியல் என்னும் பகுப்பு பொருளின் தன்மை குறித்ததாக அமைகிறது. இது இயற்பியல் வேதியல் என்னும் அறிவியல் பிரிவுகளை உள்ளடக்கியதாகும். இவ்வாய்வில் அற நூல்கள் குறிப்பிடுகின்ற பொருளறிவியலைப் பற்றி விளக்குவதாக அமைகின்றது. பொருளறிவியல், அளத்தல் அறிவியல், அளக்கும் கோல், நுட்ப அளவுகோல் எடையை எடைக்கொண்டு அளத்தல், இயற்பியல் தராசு, எடை நுட்பம் ஆய்வுக்கூடத் தேவை ஆய்வு வினை-ஆய்வு செய்வதின் மூலம் கிடைக்கும் பயன், இயற்பியல் பொருள் நியூட்டனின் முதல்விதி, நியூட்டனின் இரண்டாம் விதி, வெப்ப ஆற்றல், ஒளி ஆற்றல், ஒலி ஆற்றலின் தன்மை, போன்ற தலைப்புகளில் பொருளறிவியல் பற்றிய கருத்துக்கள் விளக்கப்பட்டுள்ளன. தொகுப்புரை மற்றும் மேற்கோள் குறிப்புகள் ஆகியன தொடர்ந்து இடம்பெற்றுள்ளன.

கலைச் சொற்கள்: பதினெண்கீழ்க்கணக்கு, அறிவியல், பொருளறிவியல், இயற்பியல், வேதியல்

முன்னுரை

தமிழர்கள் மருத்துவம், பொறியியல், உயிரியல், வானியல், நிலவியல் போன்ற பல்வேறு அறிவியல் சிந்தனைகளைக் கொண்டிருந்ததையும், அவற்றை இலக்கியங்களில்

பதிவு செய்துள்ளதையும் பழந்தமிழ் இலக்கியங்கள் காட்டுகின்றன. சங்கம் மருவிய காலத்தில் தோன்றிய பதினெண்கீழ்க்கணக்கில் அறத்தை வலியுறுத்த எழுந்த அற நூல்களில் பொருளறிவியல் பற்றியும், அது தற்கால அறிவியல் வளர்ச்சிக்கு வித்திட்டதையும் ஆராயும் விதத்தில் இக்கட்டுரை அமைகிறது.

பொருளறிவியல்

பொருளறிவியல் என்பது பொருளின் தன்மை மற்றும் அதன் உட்தன்மையை சோதிப்பது ஆகும். இதில் இயற்பியல் மற்றும் வேதியியல் என்று இரு பிரிவுகள் அடங்கும். தாவரவியல் மற்றும் விலங்கியலை உயிரியல் என்ற பிரிவுக்குள் கொண்டு வருவதைப் போன்று இயற்பியல் மற்றும் வேதியியலைப் பொருளறிவியல் என்ற பகுப்புக்குள் அடக்குகின்றனர் அறிஞர்கள்.

அளத்தல் அறிவியல்

இயற்பியலின் இன்றியமையாத பகுதியாகக் கருதப்படுவது, அளப்பது பற்றிய பகுதிதான். பருப்பொருட்களின் பண்புகளை அறிந்து ஏற்ற வகையில் கோட்பாடுகளை வகுக்க முதலில் அளவீடுகள் செய்ய வேண்டுவது இன்றியமையாததாகிறது. அதனால்தான் இயற்பியலை அளத்தல் பற்றிய அறிவியல் என்றும் அறிஞர்கள் கூறியுள்ளனர்.



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VEHICLE CLASSIFICATION WITH SVM USING CROSS-CORRELATION

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ABSTRACT- *Vehicle image classification algorithm an improved vehicle image classification is suggested. Allowing on the way difficulty of the vehicle image, using Convolutional Neural Network in the direction of excerpt the appearance sorts from vehicle's Dataset, to signify an image. As a final point, SVM is recycled to categorize the appearance of the vehicle. The tentative outcomes confirmation that the outmoded pictorial piece of grouping procedure, in this classify the vehicle, pertained on images classification in recent existences, this work offerings a method based on CNN vehicle (car) classification. Through pre-processing the descriptions on the road to make the classical increasingly normal, fractious- association (cross-correlation) methods used for original entrant group are treated in addition to diminishes the treating period, isolate the dataset into various clusters finally formulate and train the model. The precision of the Google net epitome is developed and the classify upshot is improved.*

Keywords: SVM, HOG, Cross-correlation, CBCL, Googlenet.

1. Introduction

Vehicle organization stagnant appearance a little excessive experiments as that the quantity of vehicle period is identical huge and that nearly ascriptions of the vehicle are also adjacent to identify of vehicle. Classification is grouping, solitary to vital undertakings recognition arrangement to the intelligent transportation system. CNN prepared by the appearance of CBCL dataset established aimed at the exposure is produced for the identification and order of on-street

deterrents, such as vehicles. Now this recent work, discourse recognition then identification on road-side substances by a modified Through actual recognition stage, the classify the objects remain sieved such whole scheme is complete to classify individual modules which resemble toward substances, yields to framework remain oblong bouncing cases besides course data articles exist valuable boundaries of movement arranging of the autonomous-drive used transportation.

Section 2 confers the literature review for this work has been done in vehicle classification. Section 3 explains the proposed work which helps to classify the vehicles. The evaluation details are analyzed in Section 4. Section 5 gives the conclusion.

2. Related Work

In past years, much work on image processing and taxonomy has been done with convolutional neural networks (CNNs). The power of CNNs is their capacity for knowledge not only the weights of features but the features themselves as fine. In recent times, these CNNs have attained state of the art precision on general image classification [4, 9]. Wide-ranging usage of CNNs as our crucial architecture of classifiers. Detection of the vehicle can be abused to achieve numerous errands such as calculating the reserves to add the means of transportation[5], which can support the vehicle's user by notice to dawdling down of

RESEARCH

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Thermal and mechanical studies of nanochitosan incorporated polymethyl methacrylate-based composite electrolytes

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Abstract

The composite solid polymer electrolytes based on Polymethyl methacrylate–Lithium triflate with nanochitosan as inert nanofiller were prepared by membrane hot-press method. Nanochitosan was synthesized from shrimp shell. The obtained polymer membrane was subjected to X-ray diffraction and Fourier transform infrared spectroscopy to study the structural behavior. X-ray diffraction studies revealed that the incorporation of nanochitosan in the prepared polymer matrix enhanced the amorphous phase. The complexation behavior of the prepared electrolytes was analyzed by Fourier transform infrared spectroscopy. Thermogravimetric and differential scanning calorimetric studies were carried out to understand the thermal stability of the prepared polymer composite electrode. The incorporation of nanochitosan in the polymer matrix significantly reduces the crystalline temperature of polymethyl methacrylate which was confirmed by differential scanning calorimetric study. Universal testing studies were carried to know the mechanical stability of the prepared solid polymer electrolytes. The ionic conductivity of the prepared composite polymer electrolyte was carried out using electrochemical impedance spectroscopy from ambient to 120 °C.

Keywords: PMMA, Nanochitosan, Structural studies, Thermal stability, Mechanical strength

Introduction

Polymethyl methacrylate (PMMA) is a transparent polymeric material and has many desirable properties such as light weight, high light transmittance, chemical resistance, uncolored, corrosion resistance, and good insulating properties [1]. Also, it has been used as a polymer host due to its high stability at the lithium–electrolyte surface since it is less reactive towards the lithium electrode. In this polymer, a monomer methyl methacrylate (MMA) has a polar functional group in the main polymer chain and has high affinity to lithium ions which are transported. The oxygen atoms in these monomers will form a coordinate bond with the lithium ion which is from the doping salts. Thus, due to the presence of polar functional group in PMMA, the increase in effective ionic transport of PMMA based polymer electrolytes might be achieved. Among various lithium salts, lithium triflate (LiTf, LiCF₃SO₃) is an interesting salt since it decreases the polymer

Authors' contributions

The experiment and analysis of the present study was carried out by the first author. The second author was involving to do the mechanical studies of the prepared samples. Third author gave the ideology to carry out the research work and helped the entire analysis of the submitted article. All authors read and approved the final manuscript.

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Availability of data and materials

The datasets used and/or analyzed during the current study are available from the corresponding author/First author on reasonable request.

Declarations

Competing interests

The authors declare that they have competing interests.

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PVDF/PEO/HNT-based hybrid polymer gel electrolyte (HPGE) membrane for energy applications

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Abstract

In this paper, we present the electrical characteristics and performance of hybrid gel polymer electrolyte (HPGE) based on polyvinylidene fluoride (PVDF)/polyethylene oxide (PEO) blends with various weight percentages of halloysite nanotube (HNT) in addition to liquid electrolyte. The polymer composite membranes were prepared via phase-inversion method (non-solvent-induced phase separation (NIPS)). The polymer composite membranes modified with an additive (40 wt.% of HNT) showed increased porosity and uptake of a large amount of liquid electrolyte (294.9%), which generated a high level of ionic conductivity (4.34 mS cm^{-1}) at room temperature. Moreover, PEO/PVDF with 40 wt.% of HNT-based HPGE has high dielectric constant value and inversely low relaxation time. Based on these results, it is proposed that HNT-based HPGE is a promising electrolyte material to be used in energy storage applications in the near future.

Keywords Hybrid polymer gel electrolyte · Phase inversion method · Ionic conductivity · Dielectric property · PVDF · Halloysite

Introduction

Liquid electrolytes are commonly used for energy storage devices such as batteries and supercapacitors, which suffer from outflow and flammable complications. In particular, the electrode–electrolyte interface (passivating layer) in batteries has dendrite formation, interfacial instability, and increased thermal explosion problems [1–3], which will affect the performance of energy storage devices. Currently, many researchers are working to solve the aforementioned issues by introducing new electrolyte materials such as polymers, composites, and ceramics. Polymer electrolyte is one of the suitable candidates to replace the liquid electrolyte

and to overcome the drainage and flammable complications [4, 5]. Polymer electrolytes usually in a state of solid or gel are a new type of ionic conductor composed of polymer matrix and lithium salt. The solid polymer electrolyte is light in weight, flexible, and possesses high chemical and thermal stability, even though it suffers from low ionic conductivity [6, 7]. Gel polymer electrolytes receive great attention due to their high ionic conductivity compared to the solid polymer electrolytes and free of liquid electrolyte problems [8–10]. Preparation of gel polymer electrolyte is one of the important processes, and concentrating in this issue, the researchers used homogeneous gelation method. In homogeneous gelation process, the polymer host acts as a gelator with liquid electrolyte to form gel polymer electrolyte. But the mechanical properties of polymer electrolyte are severely affected [11, 12] due to dissolving the polymer in solvent, which affects the polymer backbone. Instead, some investigators used liquid electrolyte absorption method, in which the polymer host prepared as a porous membrane uptakes the liquid electrolyte without compromising the mechanical stability of the polymer host [13, 14]. Additionally, the selection of polymer host is an important phenomenon to prepare gel polymer electrolyte, as the polymer host enhances the electrolyte properties like ionic conductivity and mechanical

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stability. A variety of polymer hosts are used to prepare gel polymer electrolyte such as poly (vinylidene fluoride) (PVDF) [15, 16], poly (ethylene oxide) (PEO) [17, 18], poly (methyl methacrylate) (PMMA) [19, 20], and polyacrylonitrile (PAN) [21, 22]. Among all these polymers, PVDF holds excellent mechanical properties and high dielectric constant. PEO has good ionic conductivity, whereas PVDF/PEO blends polymer host shows ionic conductivity [23, 24] in the range 1 mS/cm. Several attempts have been made by the researchers to enhance the ionic conductivity, mechanical stability, and electrochemical properties. The ionic conductivity value of PVDF/PEO blends-based microporous polymer electrolyte is 2 mS/cm, 1.0 mS/cm, and 0.3 mS/cm reported by Xi et al. [25], Patla et al. [26], and Ushakova et al. [27] respectively. In 2022, Y. Xu et al. examined that the electrochemical performance of solid blend polymer electrolyte (PEO/PVDF) with ZnO nano-filler showed the ionic conductivity of 0.34 mS/cm and concluded that adding nano-filler in the composite electrolyte enhances the electrochemical performance and mechanical properties [28].

The present work focuses on enhancing the ionic conductivity of the PVDF/PEO, by the addition of HNT into the polymer electrolyte composite, as the HNT has attracted wide interests for membrane modification due to its advantages such as biocompatibility, low-cost availability, and environmental friendliness. In addition, HNT is composed of aluminol in the inside space of the tubular structure and siloxane (Si–O–Si) groups on the outer surface. This array is helpful to enhance the charge separation in polymer electrolyte. The structural morphology of HNT shows a positively charged inner space of tubular structure and a negatively charged outer space [29–31]. Considering this, as an inorganic nano-filler, can, in fact, improve the performance of the polymer blends. Hence, in this paper, it has been aimed to investigate the effect of HNT in PEO/PVDF polymer blend-based HPGE.

Materials and methods

Preparation of PVDF/PEO/HNT polymer composite membrane

Polyethylene oxide (PEO), polyvinylidene fluoride (PVDF), and halloysite nanotube (HNT) were purchased from Sigma Aldrich, India. Glycerol and dimethylformamide (DMF) were obtained from Merck, India. To obtain polymer solution, appropriate amounts of PEO (0.5 g) and PVDF (0.5 g) were dissolved in DMF (10 ml) solvent and glycerol (1 ml) (non-solvent) and stirred on the magnetic stirrer to get the homogeneous solution. Furthermore, various weight percentages (10, 20, 30, and 40 wt. %) of HNT were added into polymer solution. Then, the solutions were transferred

to the Petri dish and dried in the oven at 60 °C for 12 h, to get the polymer composite membrane (PCM), with the thickness around 200 μm. The prepared polymer composite membranes (PCMs) were soaked in liquid electrolyte (1 mol of LiClO₄/diethyl carbonate (DEC)/ethylene carbonate (EC)) for 1 h. The excess liquid electrolyte was then carefully removed using the tissue paper. The polymer membrane composed of 10, 20, 30, and 40 wt.% HNT with the hybrid polymer gel electrolyte (HGPE) are named (sample code) as PE10, PE20, PE30, and PE40, respectively. The liquid electrolyte uptake percentage, δ (%) of polymer composite membrane was calculated by

$$\delta(\%) = \frac{M - M_0}{M_0} \times 100 \quad (1)$$

where M and M_0 are the mass of wet and dry membranes respectively.

Characterization techniques

Fourier transform infrared (FTIR) spectroscopy (PerkinElmer Spotlight 200i) technique was used to identify the presence of a functional group in HGPE, in the frequency range 4000–400 cm⁻¹. Thermal behavior of the prepared HPGEs was examined by thermogravimetric analysis and differential thermal analysis (STA7200 thermal analyzer). Surface morphology of the prepared HPGEs was explored by OLYMPUS BX53 upright 3 viewer microscope.

Impedance spectroscopy (IS) experiments were carried out by Biologic-VSP300 Multichannel workstation with the frequency range from 7 MHz to 1 Hz. To get the electrical node from HGPE, it was sandwiched between two silver electrodes as blocking electrodes. To calculate the conductivity (σ) and dielectric parameters of HPGE, the following equations are used:

$$\sigma = l/RA \quad (2)$$

where σ conductivity, R resistance from fitting, and A and l are the area and the thickness of the membrane respectively:

$$\epsilon' = -Z' / \omega C (Z'^2 + Z''^2) \quad (3)$$

$$\epsilon'' = Z'' / \omega C (Z'^2 + Z''^2) \quad (4)$$

$$\tan \delta = \frac{\epsilon''}{\epsilon'} \quad (5)$$

$$\tau = \frac{1}{\omega} \quad (6)$$

Table 2 Conductivity parameters of prepared polymer/ceramic composite electrolyte

S. No	Sample code	σ_{dc} (S cm ⁻¹)	τ (s)	D (cm ⁻² s ⁻¹)	μ (cm ⁻² V ⁻¹ s ⁻¹)	n (cm ⁻³)
1	PE10	2.18×10^{-4}	1.38×10^{-4}	3.37×10^{-5}	1.31×10^{-3}	1.00×10^{18}
2	PE20	3.42×10^{-4}	1.04×10^{-5}	3.51×10^{-5}	1.36×10^{-3}	1.58×10^{18}
3	PE30	1.07×10^{-3}	1.59×10^{-6}	4.05×10^{-5}	1.48×10^{-3}	4.26×10^{18}
4	PE40	4.34×10^{-3}	1.81×10^{-7}	4.30×10^{-5}	1.75×10^{-3}	1.62×10^{19}

concentration, which is more reliable with fore mentioned studies.

Conclusion

The porous PVDF/PEO/HNT polymer composite membranes were successfully prepared by phase inversion technique. The porous nature of PVDF/PEO/HNT entraps the large amount of liquid electrolyte resulting in the formation of hybrid polymer gel electrolyte (HPGE). The amount of HNT in the polymer composite significantly enhances the ionic conductivity and dielectric properties. The tubular and surface charge of halloysite nanotube typically increases the number of charge carrier separation in HPGE by reducing resistive behavior of polymer chains. Thus, HPGE shows notable ionic conductivity of 4.34×10^{-3} S/cm for the 40 wt.% of halloysite nanotube in the membrane at room temperature. Likewise, it strengthens the polymer chain flexibility and their segmental motion for the high mobility of lithium ions with low relaxation time to increase the electrical conductivity. Hence, the present method gives a new insight to develop some other porous material for the effective transportation of electrical and ionic conductivity.

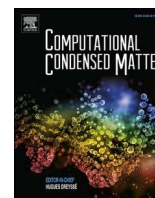
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journal homepage: www.elsevier.com/locate/cocomEffects of nanostructures on the hydrogen storage properties of MgH₂ - A first principles studyK. Iyakutti^{a,*}, V.J. Surya^{a,d}, R. Lavanya^b, V. Vasu^b, R. Rajeswarapalanichamy^c, Y. Kawazoe^{a,d}^a Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur, 603203, Tamil Nadu, India^b School of Physics, Madurai Kamaraj University, Madurai, Tamil Nadu, 625021, India^c Department of Physics, N.M.S.S.V.N. College, Madurai, Tamil Nadu, 625019, India^d New Industry Creation Hatchery Center (NICHe), Tohoku University, Sendai, 980-8579, Japan

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ABSTRACT

Hydrogen storing properties of nanostructured MgH₂ in two phases are investigated through first principles study using density functional theory. It is shown computationally that the hydrogen storage properties of MgH₂ are significantly enhanced by proper engineering of the nanostructure. The nanoparticle clusters of MgH₂ show linear behavior in adsorbing the hydrogen molecules and the binding energy values lie in the range -0.12eV to -0.15eV . The MgH₂ nanowires show non-linearity in hydrogen adsorption. For certain configuration, the hydrogen molecules binding energy values lie in the useful range (-0.15eV \rightarrow -0.27eV). Over all, the nanostructured MgH₂ exhibits good hydrogenation and reduced desorption temperature. Selected configuration of the light metal free standing hydride MgH₂ nanostructure, theoretically shows high hydrogen storage capacity which with suitable substrate is bound to reduce to the useful range of 6.4–8.8 wt%.

1. Introduction

Magnesium hydride (MgH₂) has attracted worldwide attention as solid state hydrogen storage material due to its high theoretical hydrogen capacity, good reversibility, and low cost [1–15].

However, the poor kinetics and thermodynamic properties of hydrogen absorption and desorption seriously hinder the development of this material [16]. The high thermodynamic stability and slow kinetics of MgH₂ has limited its practical application. However, the practical use of MgH₂ as a hydrogen storage medium still needs to overcome great barriers both in the thermodynamics and kinetics [12]. The intrinsic drawbacks of MgH₂ include the undesirable thermodynamic properties and sluggish sorption kinetics [13]. In this respect, nanotechnology plays an important role. It is being investigated by many scientists [6–27] for hydrogen storing application due to its light mass, high energy density and abundance of its raw material in nature. In our earlier research [18], we have found that single walled carbon nanotube (SWCNT) functionalized with magnesium hydride (MgH₂) can be used as practical hydrogen storage medium. However, its hydrogen

sorption performance is greatly hindered by two factors: (1) slow hydrogenation/dehydrogenation kinetics [2–4,20,22] and (2) high operation temperature [4,10]. Investigation on possible ways to overcome these drawbacks has been a subject of interest now-a-days [7–17, 28–35]. Even though MgH₂ has these serious drawbacks which restrict the utilization of such a lightweight system in practical applications, nanocrystalline MgH₂ gives hope in terms of displaying improved hydrogen sorption kinetics [6,7,10,12,13]. One of the most common methods for improving the sorption of hydrogen by magnesium hydrides is ball-milling [4,14,31,33] leading to nanostructured phase. Employing appropriate nanocatalysts [20,28] and nanostructuring for the high-performance hydrogen sorption has been demonstrated to be the effective strategies [28–35]. In nanocrystalline MgH₂, the thermodynamic and kinetic properties would significantly depend on the surface energy of the nanostructure [14]. Researchers have found the onset temperature of hydrogen desorption for MgH₂ nanoparticles below 3 nm occurs at a temperature about 245 K lower than for microcrystalline material [10,15,17]. Zhang et al. observed hydrogen desorption kinetics 5 times faster than that of bulk MgH₂ milled with graphite [14]. The

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changes in thermodynamic properties caused by the nanofabrication of MgH_2 , the load less freestanding nano MgH_2 has received more attention [7]. The motivation for the present study is to use nanoengineering to design different MgH_2 nanostructures and investigate theoretically the improved hydrogen storage properties of MgH_2 [32]. Nanowire and nanoparticle clusters are used as the two model nanostructures. In the past theoretical calculations using Monte Carlo method [36–39] and other computational nanoengineering methods [28,29,35] have been employed to investigate nanowire and nanoparticle structures. We have chosen density functional theory for our computational investigation based on our previous experience [18].

2. Method of calculation

The quantum mechanical first principles calculations are done using density functional theory (DFT) as implemented in Vienna Ab-initio Simulation Package (VASP) [40] code. The plane wave ultrasoft pseudopotentials are used with local density approximation (LDA) [41]. The bond length Mg–H is 1.54 Å. It has 4 valence electrons, which comes from $3s^2$ of Mg atom and $1s^1$ state electrons of H atoms. The super cell dimensions are taken as $30 \times 30 \times 2c$ for the nanowire, where ‘c’ is the repeat distance along ‘z’ axis and $30 \times 30 \times 24 \text{ \AA}^3$ for the nanoparticle model. The dimensions of the super cell along x and y directions are taken as large enough to avoid interactions between the neighboring cells. The $1 \times 1 \times 8$ Monkhorst-Pack k-points scheme has been used to map the Brillouin zone [42]. The convergence threshold is set as 1×10^{-5} eV in energy and 0.5×10^{-3} eV/Å in force. We have considered two sets (8 and 9) of bunches of nanoparticles and nanowires. The H_2 molecules are attached one by one on each MgH_2 molecule with H–H bond length of 0.74 Å. These calculations are continued with more number of hydrogen molecules. The binding energy of H_2 incorporated on MgH_2 structures is calculated by using the formula

$$E_b = E_{(\text{MgH}_2 + \text{H}_2)} - (E_{\text{MgH}_2} + E_{\text{H}_2}) \quad (1)$$

The hydrogen storage capacity is calculated as,

$$\text{Storage Capacity} = \frac{(N_H \times W_H)}{(N_{\text{Mg}} \times W_{\text{Mg}}) + (N_H \times W_H)} \quad (2)$$

where, N represents the number of atoms and W denotes the atomic weight of the atom respectively and the subscripts imply the corresponding atoms.

3. Results and discussion

In the figures the Mg atoms are shown as black solid spheres and the hydrogen atoms are represented by white solid spheres. The hydrogen atoms corresponding to MgH_2 are represented by small white solid spheres. Initially, eight MgH_2 molecules were arranged with space in between them for the 8-nanowires as well as the nanoparticle structures (denoted as 8MgH_2) and both the structures were allowed to undergo relaxation. The relaxed structures of 8MgH_2 nanowire and nanoparticles are presented in Fig. 1. After relaxation in both cases, all the MgH_2 molecules were involved in the dimer formation, where the hydrogen molecules have undergone dissociation. The Mg–H bond lengths are not same in the relaxed structures due to the different repulsive forces present in the dimer. This type of dimer formation was similar to our earlier work associated with MgH_2 functionalized single walled carbon nanotubes [18].

Following that single H_2 molecule was attached in all the MgH_2 molecules of 8MgH_2 nanowires and nanoparticles systems (denoted as $8\text{MgH}_2 + \text{H}_2$) as a trial and it was found that the binding energy per H_2 molecule is very low i.e. 0.15 eV in both the cases. This is beyond the useful limit of binding energy, since the ideal case is where the hydrogens should bind molecularly but with a binding energy value that is intermediate between the physisorption and chemisorption regimes (i.e. 0.2–0.4 eV) [19]. Hence, a new system with nine MgH_2 molecules was built using the same 8MgH_2 structure, where one MgH_2 was attached at the center as shown in Fig. 2(a) and (b) and the structures were allowed to relax. As more number of H_2 are added to MgH_2 and the relaxed 8MgH_2 regroup as $4(2 \text{MgH}_2 + 10\text{H}_2)$ as shown in Fig. 3.

To study the hydrogen adsorption behavior of MgH_2 structures, hydrogen molecules adsorbed 8MgH_2 structures were taken as the base structure as shown in Fig. 3 and one MgH_2 molecule was attached at the center and the structure was allowed to relax. Then, single H_2 molecule was attached on the center MgH_2 and the relaxed structure was denoted as $9\text{MgH}_2 + \text{H}_2$ system: $\{4(2 \text{MgH}_2 + 10\text{H}_2) + \text{MgH}_2\}$. These systems for both nanowires and nanoparticles are shown in Fig. 4. The binding energy per H_2 molecule was the same value as 0.15 eV for the MgH_2 nanoparticle system, whereas it was increased to 0.27 eV for the nanowire.

To further investigate the hydrogen storing properties of 9MgH_2 nanowires as well as the nanoparticle systems, second set of H_2 molecules were attached to the 9th MgH_2 molecule (denoted as $9\text{MgH}_2 + 2\text{H}_2$) and the structures were relaxed. This process is repeated adding increased number of H_2 molecule to the 9th MgH_2 molecule. The systems corresponding to $(9\text{MgH}_2 + 4\text{H}_2)$ is shown in the Fig. 5. Similarly,

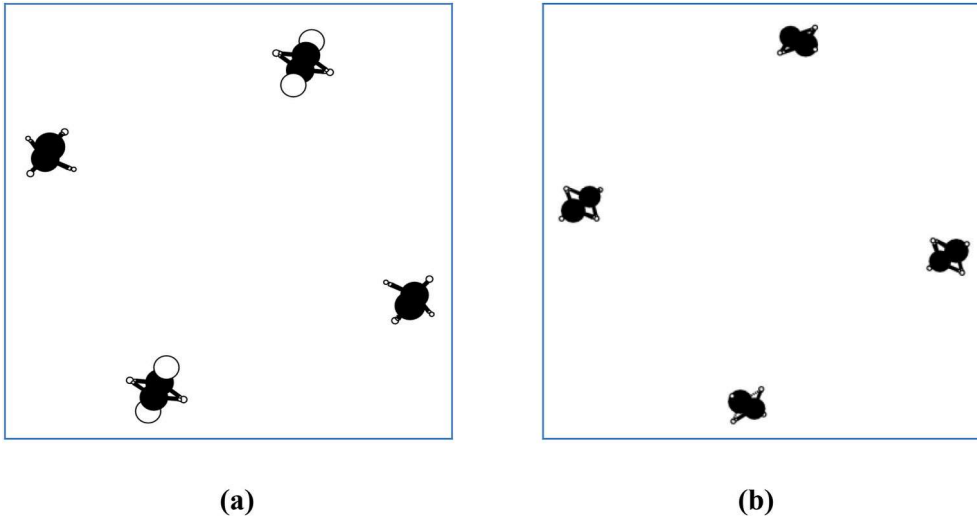


Fig. 1. Relaxed structure of 8MgH_2 (a) nanowires (cross section) (b) nanoparticle.

Table 2

Binding energy per H₂ molecule E_B, desorption temperature (Des.T), hydrogen storage capacity wt% for MgH₂ nanowire.

MgH ₂ nanowire				
S.No.	System	E _B (eV)	Des. T (K)	wt%
1.	8MgH ₂ +H ₂	-0.15	194	31.5
2.	9MgH ₂ +H ₂	-0.27	342	29.0
3.	9MgH ₂ +6H ₂	-0.15	192	31.5
4.	9MgH ₂ +11H ₂	-0.19	243	33.3
5.	9MgH ₂ +12H ₂	-0.20	256	33.8
6.	9MgH ₂ +14H ₂	-0.16	204	34.5
7.	9MgH ₂ +15H ₂	-0.15	192	35.0

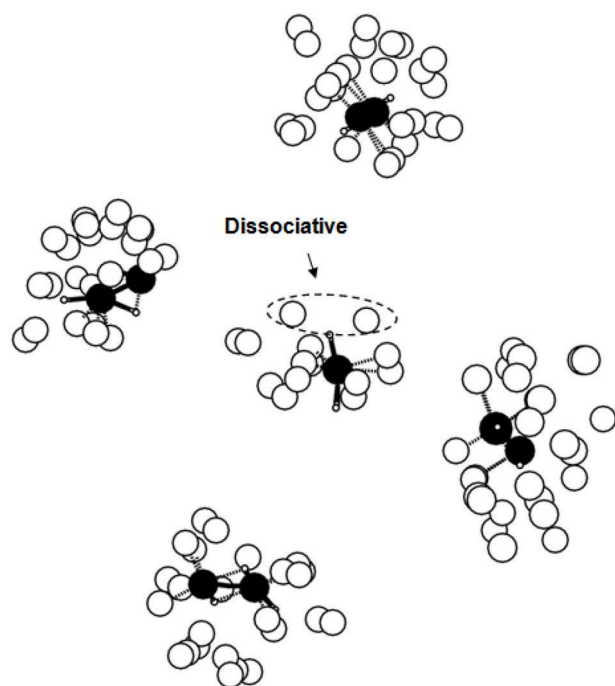


Fig. 6. Relaxed structure of 9MgH₂+7H₂ nanowire (cross section).

Table 3

Binding energy per H₂ molecule E_B, desorption temperature (Des.T), hydrogen storage capacity wt% for MgH₂ nanoparticle.

MgH ₂ nanoparticle				
S.No.	System	E _B (eV)	Des. T (K)	wt%
1.	8MgH ₂ +H ₂	-0.15	194	31.5
2.	9MgH ₂ +H ₂	-0.15	194	29.0
3.	9MgH ₂ +2H ₂	-0.14	188	29.9
4.	9MgH ₂ +4H ₂	-0.13	171	30.7
5.	9MgH ₂ +6H ₂	-0.12	153	33.8

Experimental results by Zhang et al. [14] show that the as-prepared sample with whiskers has a hydrogen storage capacity of 7.14 wt%, but features high thermal stability. Our results for nanowires is in agreement with the results of Sadhasivam et al. [17]. They reported a desorption enthalpy of 34.54 kJ/mol for MgH₂ nanowire, which corresponds to an ambient-close desorption temperature of 264.25 K and concluded that nanostructuring is a good way to achieve practical application of Mg-based hydrogen storage materials [5,17]. Furthermore, for nanowire topology of Mg, a hydrogen enriched state is thermodynamically possible, yielding a hydrogen storage gravimetric density up to 8.8 wt %, which is of interest for hydrogen storage. Also the above nanostructured system exhibits lower desorption

temperatures compared to a bulk MgH₂ [6]. The physical parameters involved in the calculation are binding energy per H₂ molecule, desorption temperature, hydrogen storage capacity for MgH₂. Our investigation clearly brings out improved status of these parameters due to nanoengineering. Based on these physical parameters the systems suitable for practical applications in hydrogen storage are selected.

4. Conclusion

The hydrogen storage capacity of MgH₂ nanostructures, nanowire and nanoparticle, is investigated using density functional theory and the calculated high hydrogen storage capacity values indicate that the system will be a good hydrogen storage medium with suitable support medium. The nanoparticle cluster shows linear behavior in adsorbing the hydrogen molecules and the MgH₂ nanowire shows non-linearity behavior in hydrogen adsorption. Some of the hydrogen adsorbed MgH₂ nanowires/nanoparticles have high volumetric hydrogen storage capacity with binding energies lying in the range -0.15 eV to -0.2 eV. Practically when these free standing systems are supported by suitable substrates, they will turn into good hydrogen storage medium with hydrogen storage capacity around and above 6.6 w%. In view of the changes in thermodynamic properties caused by the nanostructuring of MgH₂, the load less freestanding nano MgH₂ will undoubtedly receive more attention because of the reduced desorption temperatures compared to the bulk MgH₂. Thus the remarkable effects of nanostructures of magnesium hydride, the enhancement of hydrogen storage capacity and reduced desorption temperature, are clearly brought out in this investigation. We hope that our theoretical calculation based on modeling the MgH₂ nanostructures will provide a platform for new experimental investigations.

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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DEEP-VEHICLE-NETS: DEEP CNN ARCHITECTURES FOR CLASSIFYING VIEWPOINTS USING CAR IMAGES

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ABSTRACT:

Popular phase by fast developments in machine visualisation, means of transportation classify the vehicle determines a significant probable to remodel intellectual conveyance schemes. Now the preceding combine of eras, analysis and manipulation of a digitized image, and recognize the pattern -based classify the vehicle edifices obligate remained recycled to improve the efficiency of computerised tax assemblage in highways then stream of transportation managing and controlling schemes. Deep learning enabled Vehicle viewpoint Classification - can classify vehicles viewpoint based on directions or position of the car. The situation is informal in the direction of usage a pre - proficient conv.NeuNET to classify on vehicle metaphors than to physique one since scrape. The finest thing nearby pre-trained CNN is they are fine adjusted then solitary of the greatest prevalent CNNets. This paper presents innovative unfathomable D-CNN designs for mechanized vehicle classification of viewpoints. Current works mainly map RGB images directly to corresponding a consider context information explicitly. The recommended vehicle NETs are intended to afford profligate and correct scrutiny of viewpoints by means of vehicle descriptions for the classification on description of vehicle errands. The designs of VehicleNETs are exploited in an initial tentative training on the CompCars, Stanford dataset and internet sources from vehicle images for vehicle viewpoint focusses structured in a method for three classes. Firstly, train and test the networks to different viewpoints and sizes of the vehicle images and the direction/position of the vehicle. Second, train and test the networks on classification with three different scenarios as Front, back and rear. The experimental results reveal the validity and effectiveness of the planned networks in vehicle viewpoint classification. The recommended representations also outpace the starting point DeePCNN Net designs whereas existence added well-organized.

KEYWORDS : Deep CNN, VehicleNETs, ConvolutionNETs, CompCars, Stanford Cars

1. INTRODUCTION

By means of an exponential construction of vehicles all over the place in this world, vehicle arrangement frameworks can assume a critical part in the advancement of savvy transportation frameworks, i.e., computerized expressway cost assortment, insight into self-driving vehicles, and traffic stream control frameworks. In prior times, laser and circle acceptance sensors-based strategies have been suggested for the vehicle type grouping, information to separate the significant data in regards to vehicles. In any case, the accuracy and security of these techniques are fundamentally affected because of undesired weather patterns and impedance in the street asphalt.vis

In sync with the progression in CV, handling of an image and example acknowledgement based vehicle characterization frameworks. Essentially, a vision-based arrangement framework is a two-venture system; handmade extraction techniques are used to acquire visual highlights from the info visual casings, AI classifiers are prepared on the extricated elements to perform characterization on bunch based information. Hand-made acmes are classified into (i) variable globalized and (ii) region of local elements to portray and address the picture information at the same time. These elements are consolidated in the preparation of customary AI classifiers to perform to classify the object, these strategies are prepared on the restricted carefully assembled highlights extricated from the datasets, while broad earlier information is expected to keep up with precise time climate.

Freshly, DL-based extraction of features and methods of classify the vehicles require remained presented, which established improved usefulness and flexibility than the outdated classify system of the vehicle. CNN constructed classify on the vehicle require attained important exactness scheduled the comprehensive vehicle datasets owed to their erudite manner. However, the progress of the GPU has suggestively improved processing of an image competencies of the calculating machineries. Then the staple of detail is that Convolutional Neural Network established classify the vehicle entails lots of informations to endure accurateness besides confirm simplification. Undecided lately, to the finest of our familiarity, no general standard dataset is obtainable aimed at the

progress then valuation of classify the vehicle. Accordingly, obtainable datasets of classify the vehicles are moderately insignificant, founded taking place partial modules of the precise constituencies, i.e., CCars datasets and SFord cars dataset. Transportation system of these constituencies tin can accomplish important outcomes through these vehicle of datasets; conversely, their enactment is biased in the incidence of regional of other modules. In the direction of statement the beyond declared confines in classification of vehicle systems, must prepared the following supports.

(i) CNN established indiscriminate classification architecture is presented to improve robustness of vehicle classify the system of a vehicle aimed at ITS in viewpoint of their vehicle.

(ii) Dataset of a vehicle involving of 12,450 of a vehicle Images constructed on three classes (i.e., Front, Back and Rear side). The aforementioned is essential to reference that their three classes are exceptional trendy direction and viewpoint, which are not surrounded in the extant means of transportation of their datasets.

(iii) To conclude, a broad learning needs remained passed obtainable amid the planned viewpoint of a vehicle classification methods to found the effectiveness of the scheduled arrangement of a network. Figure. 1. Illustrates whole process of projected system configured.

The recreation of paper is coordinated as follows. In Section 2, profound learning highlights extraction and vehicle perspective order techniques are examined momentarily. In Section 3, network design alongside the pre-handling and dataset assortment has been explained. The outcomes are completed in Section 4. At preceding, the article is padlocked in Section 5.

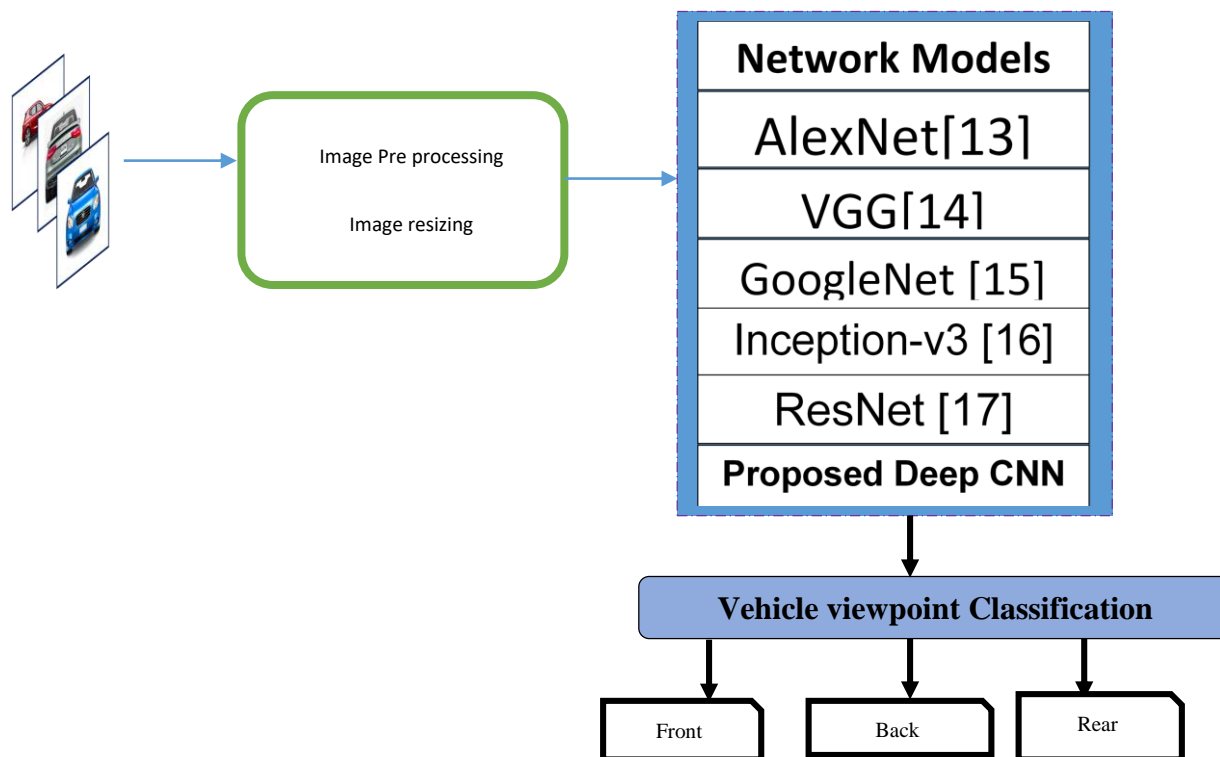


Figure 1. Workflow of DeepVehicleNEts System

2. RELATED WORK

Vision-based vehicle grouping is viewed as a significant component in the discernment module of self-driving vehicles. In the current examination work [5], vision-based vehicle order is arranged into two significant classifications: (I) hand-tailored highlights based and (ii) profound elements based systems. In the early time of PC vision, high-quality highlights in light of vehicle grouping strategies have been projected for canny transportation frameworks. In such a manner, Ng et al. [11] have suggested HOG-SVM based high-quality elements technique to prepare an SVM classifier utilizing HOG highlights with Gaussian part work. The planned classifier has been assessed on a 2800-picture dataset of reconnaissance recordings, which arranged the cruiser, vehicle, and Lorries with 92.3% exactness. In another examination work, Chen et al. [12] have introduced a grouping strategy that separates the surface and HOG elements and orders the vehicles utilizing a fluffy motivated SVM classifier. The introduced classifier has been assessed on the dataset, containing 2000 pictures in which the anticipated frameworks grouped the vehicles, vans, and transports with 92.6% exactness. Matos et al. [8] have offered two-brain networks based joined strategy implanting the elements, i.e., stature, width, and jumping boundaries of the vehicles. Resultantly, the recommended classifier accomplished 69% on the dataset of 100 pictures. Besides, Cui et al. [9] have projected Scale Invariant Feature Transform (SIFT) descriptors and Bad of Words (BoW) based joined model for the extraction of the elements and used SVM to characterize the dataset comprising 340 pictures of vehicles, minibuses, and trucks. In the outcomes, it is shown that the anticipated classifier accomplished 90.2% exactness on the given dataset. Wen et

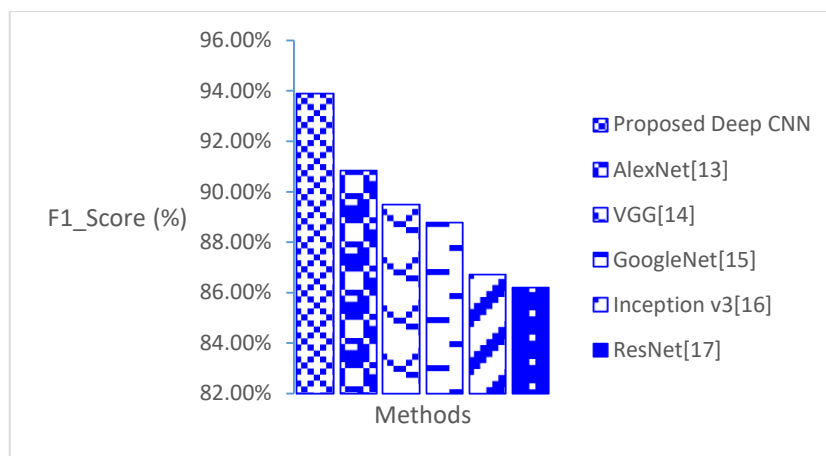


Figure.8. DeepVehicleNEts system of F1-score

The above Figure. 8 configure, the average F1-score value of the DeepVehicleNEts deep CNN method is 3.07%, 4.40%, 5.10%, 7.17%, and 7.71% higher than the methods respectively such as Alexnet, VGG, GoogleNet, inception and Resnet respectively. Even though, the average F1-score of the Alexnet method is close to the DeepVehicleNEts deep CNN method, the DeepVehicleNEts deep CNN method attained 3.07% higher than the Alexnet.

5. CONCLUSION

Now this paper, offered a CNN founded on DeepVehicleNEts for categorising the images on vehicle datasets created on self-constructed dataset keen on three classes of front, back, and rear. Then, recycled open-source datasets that contained 12450 images from internet sources, Stanford and Compcars respectively, separated the training set, in which there were 12450 images (4500 front, 4800 back, 3150 normal). And then designated the amount of to separate class nearly equivalent to per capita added in individual piece consequently that our network also learns viewpoint class characteristics, our training set included 2490 images, and the rest of the images were allocated for evaluating the network and tried to test our model on a large number of images so that our real achieved accuracy would be clear, achieved 95.60% of accuracy, 94.24% of precision, 93.75% of sensitivity, 96.52% of specificity, and 93.89% of F1-score for the viewpoint class. We hope that our trained VehicleNEt model obtainable resolve be supportive for ITS. And similarly confidence that in the imminent, superior benchmark of datasets on vehicles beginning direction or position of the vehicle develop presented, also through consuming them, the accurateness VehicleDeepNEt upsurges promote. After beyond tentative outcomes, dismiss accomplish that the VehicleDeepNEt is actual to means of transportation on classifies the vehicle then stout near the vicissitudes their vehicle viewpoints.

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