Publications

LIST OF PUBLICATIONS

1. Utilization of biowaste as an eco-friendly biodegradable corrosion inhibitor for mild steel in 1 mol/L HCl solution,Venkatesan Hemapriya, Mayakrishnan Prabakaran, Subramanian Chitra, **Manoharan Swathika**, Seung-Hyun Kim, Ill-Min Chung, Arabian Journal of Chemistry, Volume **30**,Year **2020.**

2. Structural, optical, thermal, biological and molecular docking studies of guanidine based naphthoate metal complexes, N Arunadevi, **M Swathika**, B Prabha Devi, P Kanchana, S Shanmuga Sundari, S Jone Kirubavathy, P Subhapriya, E Ranjith Kumar, *Surfaces and Interfaces.,* 24, **2021**,101094.

3. New epoxy-Nano metal oxide-based coatings for enhanced corrosion protection, N. Arunadevi, **M. Swathika**, M. Mehala, E. Ranjith Kumar, Tahani M. Bawazeer, Moataz Morad, Kholood Alkhamis, Samar Y. Al-nami, Nashwa M. El-Metwaly, *Journal of Molecular Structure*., 6:34,**2021**.

4. Design and synergistic effect of nano-sized epoxy-NiCo2O4 nanocomposites for anticorrosion applications, **M. Swathika**, Kshitij RB Singh, M. Mehala, Sadanand Pandey, Jay Singh, Ravindra Pratap Singh and Arunadevi Natarajan, *RSC Adv*.,12, **2022**, 14888.

5. Recent Advances in Hydrogen Evolution Reaction Using First-Row Transition Metal Complexes as Catalyst, **Swathika M** and Arunadevi Natarajan, *ECS Trans.,* 107, **2022**, 5763.

6. Synthesis and photometric properties of efficient white-emitting phosphor of M-AMG transition metal complexes for OLED applications, **Manoharan Swathika**, Arunadevi Natarajan, *Luminescence*., **2022**,1-14.

7. A two-step strategy to synthesis new aminoguanidinium complexes: cytotoxic effect and perspectives,Natarajan Arunadevi, Ponnusamy Kanchana, Venkatesan Hemapriya, Mayilsamy Mehala, **Manoharan Swathika**, Ill-Min Chung, Mayakrishnan Prabakaran, Taylor & Francis, Year **2022.**

8. Designing an Enhanced Self-Supported Transition Metal Complexes Based on Electrocatalysts for Hydrogen Evolution Reaction, **M. Swathika** and N. Arunadevi, *ECS*, **2023.**
9. Symbiotic study of N-bridged metal complexes as electrocatalysts for hydrogen evolution reaction, Arunadevi Natarajan, **M. Swathika**, Kshitij RB Singh, Ranjana Verma, Shyam S. Pandey, Jay Singh, *International Journal of Hydrogen Energy*, **2023.**

CONFERENCE ATTENDED

Best poster presentation

- First International Conference on Technologies, Sustainable Development Goals and Academia 2022 (ICTSGA-1) was awarded a **'Best Poster Presentation'** for the paper entitled **"Designing an enhanced self-supported transition metal complexes based electrocatalysts for hydrogen evolution reaction"** in July -**2021.**
- International Conference on "Influence of Chemistry in the Transition towards Green Economy" organized by Post Graduate & Research Department of Chemistry, PSGR Krishnammal College for Women, was awarded a **'Best Poster Presentation'** Presented paper "**Synthesis And Crystal Structure Of Guanidinium Salts: Characterization And Crystallographic Studies"** at Mar **2023.**

Paper presented

- International Conference on Multidisciplinary Aspects in Chemistry (ICMAC-2023) organized by the Department of Chemistry, Sri Ramakrishna College of Arts & Science, Coimbatore, for presenting the paper entitled **"Transition metal complexes of guanidine-antioxidant, molecular docking, and beast cancer cell line"** at Feb **2023.**
- International Virtual Conference on "Chemistry – Frontiers & Challenges (ICCFC – 2022)" organized by PG & Research Department of Chemistry PSGR Krishnammal College for Women, presented a paper entitled **"Synthesis, Characterization with Theoretical Study for Ni (II), Co (II) and Cu (II) Complexes of 1-naphthoic acid with guanidine"** at Jan **2022**
- International Conference on Futuristic Materials in Science and Technology (ICFMST-2022)" organized by the Department of Chemistry, Bannari Amman Institute of Technology, has presented a paper entitled **"Design, spectral characterization, and biological studies of alkaline metal(II) complexes with aminoguanidine-based naphthoate"** at Dec **2022.**

- International Virtual Conference on Frontiers in Chemical Research - ICFCR'21 at Bishop Heber College, Trichy, Presented a paper titled "**Synthesis and Thermal Characterization of Transistion Metal Complexes of Benzoic Acid and Aminoguanidine as Ligands"** in Feb **2021.**
- International Conference on Technologies for Smart Green Connected Societies- at the ICTSGS-1 conference led by Yamagata University Japan, Presented a Paper Titled **"Recent Advances In Hydrogen Evolution Reaction Using First-Row Transistion Metal Complexes As Catalyst"** a**t**, Nov-**2021.**
- International Conference on Smart Materials and their Applications in Recent Technologies (SMART 2020), presented a paper entitled **"New aminoguanidinium complexe-cytotoxic effect and their perspectives"** in March **2020.**
- International Conference on Chemical and Environmental Research (ICCER-2020), organized by PG and Research Chemistry, Jamal Mohamed College, Trichy Presented a paper entitled **"Transition Metal Complexes with Guanidine"** in Jan **2020.**

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Structural, optical, thermal, biological and molecular docking studies of guanidine based naphthoate metal complexes

N. Arunadevi [a], M. Swathika [a], B. Prabha Devi [a], P. Kanchana [a], S. Shanmuga Sundari [a], S. Jone Kirubavathy [a], P. Subhapriya [b], E. Ranjith Kumar [c,*]

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Molecular docking

ABSTRACT

The present work reports the complexation of few d-block metals with 3-hydroxy-2-naphthoic acid and guanidine which yields corresponding mononuclear complex bis(guaninium) 3-hydroxy-2-naphthoate metal (II) dihydrate of the type $M(CN_3H_5)_2\{C_{10}H_6(3\text{-}O)(2\text{-}COO)\}].2H_2O$, where M= form Mn(II), Fe(II), Co(II), Ni(II), Cu (II), Zn(II), Cd(II), Pb(II) and Ca(II) of ratio 1:2:4 – metal: acid: base. Characterization of the complexes were done by elemental analysis, IR spectra, UV-Visible spectroscopy, TG-DTA, powder XRD. TG-DTA study reveals various decomposition pattern and thermal stability of the metal complexes. Crystalline nature of the metal complexes is confirmed form powder XRD measurement. SEM coupled with EDAX and AFM confirms the presence of nano-sized metal oxides. Antibacterial studies of the metal complex prove that they are active against *Bacillus subtilis* and *Escherichia coli*. Furthermore, molecular docking was carried out for a study of physico-chemical properties and to show the binding energy of ligands with proteins.

1. Introduction

Guanidine is a high alkalinity crystalline compound formed by guanine oxidation. It is an essential molecule containing 'CN_3' – core with wide range of interesting properties. It was first synthesized by degradation of an aromatic neutral product guanine, by Strecker in 1861 [1-3]. It is neutral, nitrogen- containing compounds extensively used as strong bases in organic chemistry [4, 5]. Guanidinesare the set of compounds with great chemical and biological importance and the hydrophilic nature of guanidine plays an significant role in the stabilization of protein conformations via hydrogen bonding [6]. The main functionalities of the guanidine salts was broadly found in natural products, pharmaceutically active compounds and in the molecules employed for supramolecular study [7,8]. Guanidinium salts have been briefly studied for their structural properties and nature of hydrogen bonding [9]. There are various structural phase transformations of the coordinating composites made up of guanidinium cation using different inorganic acids or salts, some being ferroelectric substances.

Guanidine considered as a versatile ligand which is capable of bonding to the metal centres in a variety of coordination modes. It is most commonly known neutral donor ligand or as a monoanions [10]. From earlier studies on new metal complexes using guanidine with acetic, trichloroacetic and trifluoracetic acids were reported by Drozd [11]. There was a report on the Gold complexes of guanidine [12]. Guanidines are found as counter cations, as chelate guanidinate and as neutral guanidine ligands with various metals in coordination chemistry [13-18].

3-hydroxy-2-naphthoic acid is having great coordination ability of –OH and –COOH groups with metal and assists complex formation. It is a hydrazide derivative highly used in many biological activities [19-23]. The Kolbe – Schmitt reaction is generally used for producing 3-hydroxy-2-napthoic acid. It acts as an important intermediate for synthesis of dyes, medicine, organic pigments. It has naphthalene-based colour intermediate, so it is used in paint, waterproofing agents and photosensitive materials and they frequently used in chelating agents [24-27]. Hydroxy naphthoic acids develop coloured chelates when react with metal ions. This is characteristic to the presence of phenolic hydroxyl and carboxylic acid groups in the adjacent sides. Derivatives of 3-hydroxy-2-naphtoic acid show significant anti-microbial activity against Bacillus thuringiensis, Escherichia coli, Bacillus cereus,

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RSC Advances

PAPER

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Design and synergistic effect of nano-sized epoxy-$NiCo_2O_4$ nanocomposites for anticorrosion applications†

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In the present work, we evaluated the corrosion inhibition properties of a ligand and mixed metal oxide nanocomposite. The ligand and mixed nickel–cobalt complex were synthesized using 1-naphthoic acid and aminoguanidine with the formulae $[C_{11}H_7O_2(CN_4H_5)(CN_4H_6)]\cdot H_2O$ and {Ni–Co $[(CH_5N_4)_2(C_{11}H_7O_2)_2]\}\cdot H_2O$, respectively. After their synthesis, physicochemical techniques such as CHNS analysis, infrared and UV-visible spectroscopy, thermal analysis, and X-ray diffraction (XRD) were employed to characterize both the synthesized ligand and nickel–cobalt complex. The metal oxide prepared from the decomposition of the metal complex was also characterized using several techniques to confirm its bonding and structure. In addition, the corrosion inhibition efficiency of the epoxy-ligand and epoxy-$NiCo_2O_4$ nanocomposite on mild steel (MS) in 3 M hydrochloric acid (HCl), 1.5 M sulfuric acid (H_2SO_4), and 0.5 M phosphoric acid (H_3PO_4) solution was examined and compared using weight loss measurements, Tafel plots, isotherms and electrochemical impedance spectroscopy (EIS). The results from the electrochemical studies disclosed that the epoxy coating of mixed metal oxides with 0.8 ppm concentration yielded excellent corrosion protection. The SEM images of mild steel and mild steel coated with epoxy-ligand/epoxy-$NiCo_2O_4$ in HCl confirmed the anti-corrosive behavior of the synthesized compounds. Hence, the as-prepared material can be a next-generation tool for sustainable anti-corrosive coatings.

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1. Introduction

Aminoguanidine is a hydrazine derivative and a bifunctional molecule, and the salts prepared from aminoguanidine are anticipated to resemble the hydrazine moiety. The nitrogen constituent and asymmetric bifunctional nature of aminoguanidine are responsible for its enhanced thermal and chemical reactivity. Thus, its salts are employed to prepare metal complexes with important physical properties such as ferroelectricity (pyroelectricity and piezoelectricity) and second harmonic generation.[1,2] It is also an excellent chelating ligand and forms monodentate or bidentate complexes with metal ions. Due to the presence of carbon with four nitrogen atoms, aminoguanidine acts as an outstanding starting material in cyclization processes. Specifically, the four nitrogen atoms in aminoguanidine undergo coordination in various modes to form different types of complexes.[3,4] However, in the free state, aminoguanidine is unstable, while in the solid state, it exists as a mono (+1) or di (+2) cation. In the solid form, its extreme nitrogen atom has hydrazine moiety in the sp^3 hybridized state and the extra non-hydrogen atoms are in the sp^2 hybridized state.[5,6]

Further, 1-naphthoic acid (1-naphthalene carboxylic acid) and its derivatives have attracted great attention from researchers because they possess an extensive range of biological and chemical applications in medicine, photochemicals, organic pigments, pesticides, photosensitive materials, dyes, cosmetic preparations, *etc.* Complexes of naphthalene derivatives have been examined since the 1960s, when 1-naphthoic acid was compiled from a planar dimer unit. It was mainly used to synthesize highly economical and effective herbicides, and it also acts as a plant growth regulator, thermal testimony material, and photosensitive object. Some materials prepared from 1-naphthoic acid have the resistivity of plasticizers and solvents, and these significant features led to the detailed spectral examination of 1-naphthoic acid, where one of the best

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Symbiotic study of N-bridged metal complexes as electrocatalysts for hydrogen evolution reaction

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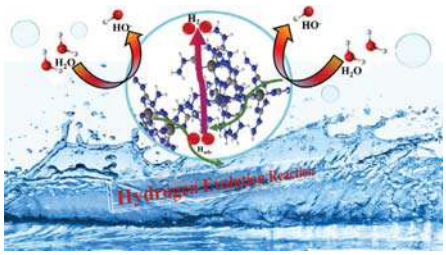
HIGHLIGHTS

- Fabrication of non-noble metal catalyst.
- Low-cost and effective electro-catalyst for HER.
- Lithium catalyst excellent activity through Heyrovsky-Volmer mechanism.
- Highly active and porous nature of the catalyst with enhanced absorption.
- Comparison of alkaline and alkali metal catalyst.

GRAPHICAL ABSTRACT



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ABSTRACT

Design and fabrication of non-noble metal catalysts for the extensive generation of H_2 (hydrogen) gas by water splitting is the upsurging field aiming towards the sustainable environment and need the future clean and green energy. However, scheming and understanding the basic principle regulating the activity of the catalyst is still inexplicable. Although Pt is currently the material of choice owing to its high electrocatalytic activities but need for its high loading and high cost is an intriguing issue needing amicable solution. The hybrid structures of heteroatom-based transition metal complexes are more effective and are cost effective electrocatalysts for hydrogen production. In this proposed work, the electrocatalytic behaviour of alkali (Li^+, Na^+, K^+) and alkaline metal (Ca^{2+}, Sr^{2+}, Ba^{2+}) was figured out along with their synthetic procedure and characterization. Owing to their high complexing ability, ring formation, and bidentate nature, substituted naphthoic acid and aminoguanidine were chosen as bridging ligands. The thermodynamic stability and best catalytic behaviour of synthesized alkali and alkaline earth metals were compared and

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Recent Advances in Hydrogen Evolution Reaction Using First-Row Transition Metal Complexes as Catalyst

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ABSTRACT

The precise use of an electrocatalyst for the HER reaction mainly depends on synthesis cost, durability and over potential. Recently there is promising research for electrocatalyst synthesis using first row transition metals. Working towards this herein we present, synthesis, physio-chemical characterization and hydrogen evolution activity of amino guanidium metal naphthoate complexes. The obtained electrocatalysts were characterized by element analysis, IR spectra, UV-Visible spectroscopy, TG-DTA, and powder-XRD. The thermal behavior of these compounds has been studied by simultaneous TG-DTA techniques. The isomorphic nature of the metal complexes is evident from powder-XRD data.
Key Words: HER, electrocatalyst, cyclic voltammetry, aminoguanidine

1. INTRODUCTION

Hydrogen gas is a perfect, clean and pollution free fuel for the future generation. Production of hydrogen in recent era is mostly attained from burning of fossil fuels. But the main draw back in this method is evolution of large amount of greenhouse gases. The hydrogen production is also possible by means of electro, photo electrocatalytic, and water splitting process but it requires more efficient catalyst (1, 2) . Noble metals like platinum, iridium, and ruthenium exhibit a good catalytic activity but it is too expensive (3,4). Many metal oxide semiconductors like titanium oxide, nickel oxide and zinc oxide were extensively used as catalyst for both HER and OER (5-10). The high band gap energy and formation of free radicals in presence of UV light are considered as main disadvantage of these metal oxides (11,12). We found from literature that the conversion of dative bond to sigma bond between metal and nitrogen atom will increase the metal complex stability and thereby increases hydrogen evolution (13,14). Hence, it is extremely needed to synthesis a simple, low-cost metal complexes as catalyst to increase the evolution of hydrogen. The present work focused on synthesis of new transition metal complexes as electrocatalyst for hydrogen evolution.

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SPECIAL ISSUE ARTICLE

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Synthesis and photometric properties of efficient white-emitting phosphor of M-AMG transition metal complexes for OLED applications

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Abstract

Progression in lighting sources mainly depended on new, robust energy-efficient diodes due to their advanced photometric properties. All organic light-emitting sources are constant energy-efficient devices and will be the light of the future. We explore the potential of transition metal complexes by focusing on cobalt(II), nickel(II), and copper (II) with aminoguanidine naphthoate as white phosphors in organic light-emitting diodes (OLEDs). The phosphors synthesized at optimized temperature were characterized structurally and thermally by spectral, thermal, and diffraction techniques. The photophysical studies of the target compound in several organic solvents having divergent polarity were also studied, and the results were exhibited. Photometric properties of the complexes were studied using photoluminescence, CIE (Commission internationale de l'éclairage) chromaticity coordinates, correlated color temperature, color purity, Duv, and TLCI (Television Lighting Consistency Index) to verify the applicability of complexes as phosphors. Excellent luminescence property with a high coloring index for (Cu(2NA-AMG-2H_2O)) opens the advanced avenue for light sources and serves as vital constituents for light-emitting diodes.

KEYWORDS
CIE, color purity, color rendering index, energy-efficient diodes, OLEDs, transition metal complexes

1 | INTRODUCTION

Transition metal complexes attract many researchers due to their fascinating photophysical and chemical properties.[1] Last few decades, plenty of research has been carried out to stabilize the chemical structure of complexes to get efficient photoluminescent properties. In the latest lighting technology, white light-emitting diodes (WLEDs) are frequently used due to their life span, efficiency, different range of color availability, and good stability.[2–5] Phosphor-WLEDs with tricolor or near-ultraviolet (n-UV)/blue chips are widely utilized as solid-state lighting sources due to their outstanding performance.[6,7] WLED produced by using n-UV region was found to be good for living beings and will not create environmental problems. The main limitation is blending two or more phosphors with a diode.

Moreover, it will have a high rendering index but poor luminous efficiency because of re-emission. The single solid light emitting diode will solve this problem and have enhanced properties like low cost, high efficiency, nil reabsorption, and numerous color options. Hence, more attention has been devoted to exploring the novel single phosphors working in n-UV regions.

Usually, phosphors have two essential components like activators and hosts. In WLED, the activators may be transition metal rare-earth metals. The color variation due to metal doping into the base component may result from 4f–4f, d–d, 4f–5d transitions or charge transfer

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New epoxy-Nano metal oxide-based coatings for enhanced corrosion protection

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ABSTRACT

Aminoguanidium-1-naphthoate and its Ni(II) and Co(II) complexes were synthesized and characterized by spectral, thermal and structural methods. By using these compounds as precursors, epoxy coated ligand, NiO and CoO has been prepared by Sol-gel method in order to protect the corrosion on mild steel substrate. Resistance and protection against corrosion of the synthesized sample was studied in 3 M HCl, 1.5 M H_2SO_4, and 0.5 M H_3PO_4 by weight loss measurements, potentiodynamic polarization and electrochemical impedance spectroscopy (EIS). The surface and structural morphological studies of epoxy-metal oxides were investigated using powder XRD and SEM analysis. The corrosion protection efficiency of epoxy -NiO and epoxy -CoO nanoparticles film on mild steel is high than epoxy-L. The molecular docking study against 3T88 and 1Y2T protein with synthesized compound was performed to study the interactions responsible for anti-bacterial activity against S. aureus and E. coli.

1. Introduction

Aminoguanidine, a derivative of hydrazine, is a diacidic base, forming aminoguanidinium (+1) and aminoguanidinium (+2) salts with minerals, carboxylic acids, or both. Because of their manufacturing methodologies and physical features, aminoguanidine and related salts have recently attained more interest. In acidic conditions, it forms salts with both aromatic and aliphatic carboxylic acids, and undergoes condensation reaction with acids to yield hydrazides [1,2].

Naphthoic acid is an aromatic compound having two fused benzene rings with COOH as functional group [3,4]. It is mainly used as an intermediate in the preparation of dye and the photosensitive material [5]. Hydroxy naphthoic acid is a very good bidentate ligand and coordinate through carboxylate and hydroxyl oxygen [6,7]. It is used as a lithographic printing plate and produces color for various dyes [8,9].

Corrosion causes major problems in many industries, particularly in the petroleum industry, where acids are employed to dissolve impurities. The sulphate, nitrate, and phosphate salts have lower solubility in aqueous media than hydrochloric acid (HCl), hydrofluoric acid (HF), and formic acid [10,11].Phosphoric acid is frequently used in food industry, acid pickling, acid cleaning, and acid descaling. Though the corrosion problem in industry is unavoidable, we should find an appropriate solution to solve it. The corrosion process requires an efficient corrosion inhibitor to control damage in mixing tanks and other metallic surfaces [12,13].One of the most important revolution in corrosion science is the use of organic substances as inhibitors [14]. The chemical structure of the inhibitor, the chemical composition of the solution, the nature of the metal surface, and the electrochemical potential of the metal–solution interface all influence the modes of adsorption. The inhibitor is chosen based on two primary considerations namely inexpensive ingredient and increased adsorption. In general, a strong coordination bond provides greater protection efficiency, and the protection efficiency increases as the sequence oxygen<nitrogen<sulfur<phosphate [15,16].

According to the literature, nitrogen- heterocyclic compounds such as triazole, pyrazole, pyridinete, and trazole derivatives are act as very good inhibitors [17–20]. The objective of this work is to study the corrosion protection of durable epoxy film with metal

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Designing an Enhanced Self-Supported Transition Metal Complexes Based on Electrocatalysts for Hydrogen Evolution Reaction

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Abstract

Progressing efficient and low-cost catalysts to reduce overpotential within the hydrogen evolution reaction (HER) in large-scale production is highly desirable in the present era. The catalysts are accustomed to initiating an excellent approach to optimizing the electronic characteristics employed to boost their electrocatalytic production. In this article, we described the activity of transition-metal complexes with the nitrogenous analog of carbonic acid and naphthalene ring containing monocarboxylic acid to study hydrogen evolution reactions. The HER activity in transition metal complexes was varied through physicochemical and electrochemical properties. Density function theory (DFT) was calculated using the B3LYP hybrid functional and the basis set of 6-311 + G (d,p) to deliver the relevant frontier orbitals.

Keywords: HER, naphthoic acid, guanidium, DFT, TG-DTA, Electrocatalyst

Introduction

The development of current technologies for clean and sustainable hydrogen energy has drawn increasing attention over the past few years; hydrogen is hailed as a promising energy source to reduce our necessity for fossil fuels and benefit the atmosphere by reducing the emissions of greenhouse and other toxic gases also. To this end, an effective and promising method is used for the electrolysis of hydrogen production. Hydrogen evolution reaction (HER) of electrocatalytic preferably determined by solar energy produces a desirable methodology for these requirements, making it efficient, low-cost, and environmentally friendly (Du and Eisenberg, 2012; Natarajan Arunadevi et al., 2021; Jain et al., 2018 we report the electrocatalytic behavior of the neutral, monomeric Ni(II).

In this HER reaction, the significant role was played by the H^+ ion, the nature of the catalyst, and the electron produced by the catalyst. The catalyst not only adsorbs the free H^+ ion in acidic electrolytes but breaks the H-O-H bonding in the electrolytes before adsorbing the H^+ ion. So, the acidic electrolytes are preferred in hydrogen production due to their enough H^+ ions in the electrolyte to react with the electrode surface. Hydroxide conducting polymeric material is also used as an electrolyte still in its initial technological