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Applications of Heterocyclic Compounds in the Material Sciences: An Overview

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Abstract: Heterocyclic compounds are essential in the material sciences due to their distinctive structure, which provides them with various adjustable electrical and physicochemical properties. Researchers develop materials with specific characteristics for various innovative uses by modifying the type and positioning of heteroatoms. In material science, heterocyclic compounds are used in several applications, such as fluorescent markers for imaging and diagnostics, polymers and copolymers for their structural and electrical characteristics, and dyes and pigments for their coloring capabilities. They can also be used as corrosion inhibitors, developers, antioxidants, and parts of photovoltaic cells and light-emitting diodes (LEDs) because of their special structural and chemical characteristics.

Keywords: *Heterocyclic compounds, organic electronics, dyes, pigments, polymers, corrosion inhibitors*

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I.INTRODUCTION:

In the 19th century important significance of heterocyclic compounds in modern medicine, biochemistry, and material science is intricately linked to the greater history of organic chemistry. The identification and description of basic heterocycles, development of synthetic methods and study of its biological value in molecules such as DNA, vitamins, and colors are important stages [1-3]. Heterocyclic compounds contain rings with at least one atom other than carbon, such as nitrogen, oxygen, or sulfur are among the most important and widely studied classes of compounds in chemistry. While their significance in pharmaceuticals and agrochemicals is well known, heterocyclic compounds have also emerged as key building blocks in material sciences, owing to their diverse chemical and physical properties [4-6]. In the twenty-first century, the use of heterocyclic compounds increased despite their conventional applications. These compounds have structural flexibility, electronic tunability, and thermal stability, making them ideal candidates for a wide range of advanced material applications [7-8]. Their adaptability electrical properties have made them important for advanced materials. Their ability to participate in π-conjugated systems, interact with light, and conduct electricity has led to their extensive use in organic electronics such as OLEDs and OPVs, where heterocycles are utilized as emitting and semiconducting materials [9-11], along with this it used in solar cells, sensors, corrosion-resistant coatings, and functional polymers. Modern uses for heterocyclic compounds involve molecular probes for bioimaging, high-performance polymers, and new catalysts [12-14]. The field is very active, with ongoing studies into innovative synthetic methods and the exploration of new applications. In the course of ongoing research, new heterocyclic compounds that display distinctive properties are being discovered, which in turn expands the range of possible applications for these compounds. It is anticipated that advancements will be made in fields ranging from materials science to medicinal chemistry as researchers continue to investigate their unique properties.

II. Applications of Heterocyclic Compounds in the Material Sciences:

Organic electronics:

Anthony, John E. described importance and performance of Heteroacenes and Functional Acenes for Organic Electronics [15]. Jiang, Wei, Yan Li, and Zhaohui Wang, provided recent approaches toward realizing high performance p-channel field effect transistors based on heteroacenes and heteroatom annulated polycyclic aromatics (PAHs) as key functional components [16]. Wang, Chengliang, et al. explored n Organic Electronics Material through Field-Effect Transistors with Semiconducting π-Conjugated Systems [17]. Allard, Nicolas, et al. synthesized and characterized new heterofluorene derivatives based on germanium. These germafluorene monomers have been polymerized with different aromatic comonomers and resulting homopolymers and alternating copolymers poly[2,7-(9,9-di-n-octylgermafluorene)-alt-5,5-(4′,7′-di-2-thienyl-2′,1′,3′-benzothiadiazole)] tested in field-effect transistors and bulk heterojunction photovoltaic cells which shows a hole mobility up to 0.04 cm2 (V·s)−1 with an Ion/Ioff ratio of 1.0 × 106 and the best photovoltaic results were obtained with a power conversion efficiency (PCE) of 2.8% [18]. Figueira-Duarte summarized briefly Materials Using Pyrene in Organic Electronic [19]. Brunetti, Fulvio G., et al. presented features and properties of 9,10-di(1,3-dithiol-2-ylidene)-9,10-dihydroanthracene (exTTF) in molecular electronics which has remarkable applications in several fields of interest comprising covalent and supramolecular ensembles, molecular wires, artificial photosynthetic systems as well as photovoltaic devices [20]. Schipper, Derek J., and Keith Fagnou.reported direct arylation as a synthetic technique for the fabrication of Organic Electronic Materials based on Thiophene [21]. Patra, Asit, Michael Bendikov, and Suresh Chand reported derivatives of Poly(3,4-ethylenedioxyselenophene) showed various electronic applications as high conductivity, a reduced band gap, rigidity, multicolor electrochromism, and quick redox switching made them innovative Organic Electronic Substances [22]. Balan, Abidin,et al informed conjugated polymers with benzotriazole for a variety of organic electronic applications due to their good solubility, optical and electrical properties, and synthetic availability [23].Hu, Yunbin, et al. reported Sulfur Heterocycle-Fused Core which expanded Naphthalene Diimides with electron-withdrawing groups at the end for air-stable solution-processed n-channel organic thin film transistors [24]. Neto, Brenno AD, et al., described synthesis, characteristics, reactions, and a few instances of light technology applications of 2, 1, 3-Benzothiadiazole and derivatives [25].

Dyes, pigments:

Shams, Hoda Zaki, et al. synthesized new azo dye precursors and polyfunctionalized acyclic and heterocyclic dye precursors based on conjugate enaminones and enaminonitrile moieties.In order to disperse color nylon, acetate, and polyester textiles, dyes were applied at a depth of 5% [26]. Şener, Izzet, and Gulşah Aydin reported hetaryl tetrakisazobenzidine based dyes which were derived from heterocyclic amines in nitrosylsulphuric acid and reacted with 2 equivalent coupling components in KOH/H2O [27]. The use of heterocyclic compounds based on 1,2,3,4-tetrahydroquinoline and 2,3-dihydroindole as precursors for blue oxidative dyes, particularly on human hair, has been studied by Li, D., Y. Huang, and J. Su. [28]. An article by Henary,Maged t al. that focuses on the synthesis and particular uses of different benzothiazole cyanine dyes [29]. Shindy, Hassan Abazied. reported different classes of six membered heterocyclic cyanine dyes viz. styryl cyanine dyes, bis styryl cyanine dyes, cyclic mero cyanine dyes, trimethine cyanine dyes, pentamethine cyanine dyes, undecamethine cyanine dyes, meso substituted methine cyanine dyes, bridged cyanine dyes and zwitterionic bridged cyanine dyes [30]. Kaur, Matinder, and Dong Hoon Choi reported fluorescent probes based on diketopyrrolopyrrole, an intense red pigment dye, and its uses in identifying biologically significant species such as anions, cations, reactive oxygen species, thiols, and gases [31]. Son, Young-A., et.al .assessed the photochromic and electro chromic properties of a hetero-bifunctional chromic dye [32].Using ab initio Hartree-Foc and density functional theory, Ucun, Fatih, et al. developed tautomeric forms of a heterocyclic disazo dye [5-(3-methyl-4-phenylazo-1H-pyrazole-5-ylazo) barbituric acid] [33]. Baf, Mozhgan Mazloum Farsi et al. synthesized blue-violet dye 2-(3-hydroxyimino-2,3-dihydroimidazo [1,2-a]pyridin-2-yliden)-2-(2-thienyl) acetonitrile and investigated its electrochemical properties and antibacterial activity [34]. Cyclic voltammetry studies and DFT computations of heterocycl ic green dyes 2-arylacetonitriles of 5-hydroxyimino 1-alkyl-4,5-dihydro-1H-4-indazolyliden reported by Pordel, Mehdi et al [35].

High-performance polymers

By casting chloroform or N-methylpyrrolidone solutions of polyimides or poly (imide-amide)s with silicon and phenylquinoxaline units in the main chain onto glass plates, thin films polymer formed reported by Hamciuc, Corneliu, et al. [36]. BRUMĂ, Maria synthesized polyphenyl quinoxalines with silarylene units. Aromatic diamines with phenylquinoxaline rings and a dianhydride or diacid chloride with silarylene units undertook a polycondensation reaction to create these polymers. These polymers have mostly been researched for use in advanced microelectronics and optoelectronics as high-performance thin films or coatings [37].McCulloch, Iain, et al. designed Semiconducting Indacenodithiophene Polymers through optimization process with an aromatic backbone skeleton rich in electrons from indacenodithiophene. These polymers used in Solar Cells and High-Performance Transistors [38]. Dippold, Alexander A. et al. reported N-Oxides are used in the design of high-performance insensitive energetic materials 3,3′-dinitro-5,5′-bis-1,2,4-triazole-1,1′-diol [39]. Cheng, Lin, et al. reported with an N-C coupling reaction, a variety of unsymmetrical, twist, and noncoplanar phthalazinone-containing monomers and an activated difluoro monomer were easily transformed into a number of new heterocyclic polymer material poly(arylene ether ketone)s [40]. S Kushwaha et al. tested effective electrolyte for high temperature polymer electrolyte membrane fuel cells is acid-doped polybenzimidazole membranes [41]. Agag, Tarek, et al. reported newly synthesized benzoxazine resins as precursors to produce more thermally stable cross-linked polybenzoxazole polymer via a novel approach [42]. Chang, Chia-Ming, and Ying-Ling Liu demonstrated functionalization of multi-walled carbon nanotubes through the use of four polymers: poly(vinylidene fluoride) (PVDF), polysulfone (PSF), poly(2,6-dimethylphenylene oxide), and poly(phthalazinone ether ketone) [43].Mallakpour et al. studied heterocyclic polyamides 4-(4-dimethylaminophenyl)-1,2,4-triazolidine-3,5-dione, it was polycondensed with a variety of aliphatic diacid chlorides in the presence of room-temperature ionic liquids and molten tetrabutylammonium bromide as an IL to create heterocyclic polyamides in a simple and effective manner [44]. Sadeghipour, Hojjatolah, et.al synthesized heterocyclic polyimide/titania nanocomposite thin films. In the incorporation of soluble poly(amic acid) precursors, 3,5-diamino-1,2,4-triazole was polycondensed with four dianhydrides (3,3′,4,4′-benzophenonetetracarboxylic dianhydride,1,2,4,5-benzenetetracarboxylic-1,2,4,5-dianhydride,

4,4′-(hexaflouroisopropylidene) diphthalic anhydride and 1,4,5,8-naphthalenetetracarboxylic dianhydride). Heterocyclic polyimide /titania nanocomposite thin films were then created by thermally integrating titania (TiO2) nanoparticles into the polyimide matrix [45].

Corrosion inhibitors

The effects on nitrogen heterocyclic compounds, 2-mercaptobenzimidazole,2mercapto,benzoxazole, 2 mercaptobenz othiazole, on the inhibition of copper corrosion in 0.5 M sulfuric acid was investigated by Shahrabi, T. et al **[45]**. Şahin, M., et al. has been studied 3-amino-1,2,4-triazole, 4-hydroxy-2H-1-

benzopyran-2-one, and 4-hydroxy-3-(1H-1,2,4-triazole-3-ylazo) compounds' efficiency-2H-1-benzopyran-2-one-using Tafel extrapolation and linear polarization techniques as steel corrosion inhibitors in 3.5%NaCl **[46]**.Lashgari, Mohsenexamined the corrosion inhibition capabilities of 3-mercapto1,2,4 triazole, benzotriazole,thiophene, and tetra hydrothiophene) in Cu/H3PO4 media using polarized Continuum and gravimetric methods **[47]**. Carbon steel corrosion inhibition using heterocyclic compounds 2-styrylbenzo(d)oxazole, 4((E)-2-(benzo(d) oxazol-2yl)vinyl)-N,N-dimethyl benzenamine &4-((E)-2-(benzo(d)thiazol-2yl) vinyl)-N,N-dimethyl benzenamine in hydrochloric acid solutions reported by Fouda, A. S., et al **[48]**. Diazoles 3-amino-1H-isoindole, indazole, imidazole, 4-bromoimidazole, 4-methylimidazole, pyrazole, 4-nitropyrazole, and 4-sulfopyrazole compounds were examined by Babic-Samardzija, Ksenija, et al. employing ac and dc techniques as corrosion inhibitors of iron in 1 M HCl **[49]**. Hnini, Khadija, et al. demonstrated that the compounds [(4-Hydroxy-6-methyl-2-oxo-2H-pyran-3yl)-phenyl-methyl]urea and [(4-Hydroxy-6-methyl-2-oxo-2H-pyran3-yl)-(4-methoxy-phenyl)-methyl]urea function as cathodic inhibitors against stainless steel in polluted phosphoric acid, using electrochemical resistance and potentiodynamics measurements **[50]**. 5-(4-methoxyphenyl)-1,3,4-oxadiazole-2-thiol and 5-(4-nitrophenyl)-1,3,4-oxadiazole-2-thiol were investigated by Gapil, Shelly, et al. as corrosion inhibitors for nickel metal **[51]**. Shaban, Abdul et al. tested thiazole derivatives as copper corrosion inhibitors in acidic conditions using piezogravimetric analysis method **[52]**. Halambek, Jasna, et al. prepared 4-(methoxymethyl)-1,6-dimethyl-2-oxo-1,2- dihydropyridine-3-carbonitrile and 4-amino-3,5-bis [6-(methoxymethyl)-3,4-dimethyl-2-oxo-1,2-dihydropyridine-1-yl]-1,2,4-triazole-2(H) compounds and investigated its Al-3Mg alloy corrosion inhibition in 0.5 M and 1 M HCl which was studied by weight loss and potentiodynamic polarization measurements **[53]**. Ameer, M. A., et al., reported steel corrosion in an alkaline medium containing chloride is inhibited by heterocyclic organic compounds used of electrochemical and hydrogen evolution techniques **[54]**.

III. CONCLUSION:

Heterocyclic compounds have adaptive molecular frameworks makes them important building parts for advanced materials in many different high-tech industries like electronics, energy, and bio-applications. They are essential when developing materials with specific functions for organic electronics, high-performance polymers, photovoltaic devices, sensors and new colors because of their capacity to be precisely modified using synthetic chemistry. This field has the potential for future expansion with the combination of modern and sustainable synthesis methods promising that heterocyclic compounds will continue to be at the center of developments in energy, electronics, and nanomaterials, with an essential role in the development of next-generation materials that are useful. These technological advances could result in improvements in device performance and energy efficiency, providing up the window to more advanced technology and sustainable methods. The integration of these materials into common technologies could transform fields as electronic devices and renewable energy as discoveries are made.

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Declaration:

- Conflict of interest: The author declares that, there is no conflict of interests regarding the publication of this paper.
- Ethical approval: This has not been published elsewhere and is not currently under consideration for publication elsewhere.

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