JUNE, 2025

Academic Research in Science and Mathematics

Editors

Prof. Hüsniye Sağlıker, Ph.D.
Assoc. Mine Sulak, Ph.D.

DOI: 10.5281/zenodo.15772888

Academic Research in Science and Mathematics

Editors

Prof. Hüsniye Sağlıker

Assoc. Prof. Mine Sulak

Publisher
Platanus Publishing®

Editor in Chief
Prof. Hüsniye Sağlıker, Ph.D & Assoc. Prof. Mine Sulak, Ph.D.

Cover & Interior Design
Platanus Publishing®

The First Edition
June, 2025

ISBN

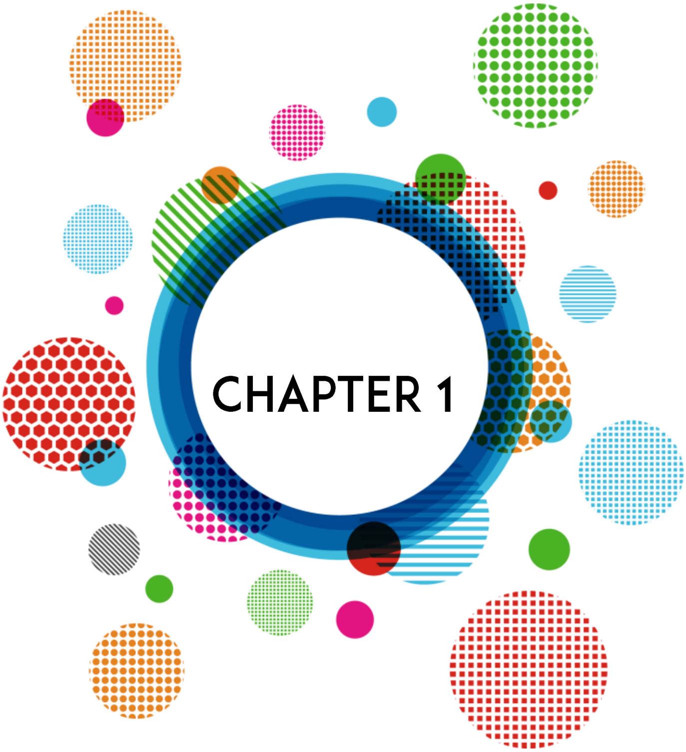
979-829-0144-44-3

Platanus Publishing®
Address: Natoyolu Cad. Fahri Korutürk Mah. 157/B, 06480, Mamak, Ankara, Turkey.

Phone: +90 312 390 1 118
web: www.platanuspublishing.com
e-mail: platanuskitap@gmail.com

Platanus Publishing®

CONTENTS



CHAPTER 1

Development and Applications of Pva/Borax-Based Flexible Solid-State Capacitors

Serkan Demirel[1]

---

[1] Assoc. Prof. Iğdır University, Electricity and Energy Department, Iğdır-Türkiye
ORCID: 0000-0003-1158-4956

Introduction

The global transition towards sustainable energy technologies has markedly increased the demand for efficient and environmentally benign energy storage systems. Renewable energy sources, such as solar and wind, are inherently intermittent, necessitating the development of reliable storage solutions to ensure a steady and controllable power supply [1,2]. Consequently, the advancement of energy storage devices has become a cornerstone in the progress of modern technologies, ranging from smart grids and electric vehicles to wearable electronics devices [3].

Among various energy storage devices, capacitors have garnered considerable attention due to their ability to deliver high power density, rapid charge-discharge capabilities, and long cycle life [4]. Unlike conventional batteries, which store energy through slow faradaic reactions, capacitors operate via non-faradaic processes, enabling them to respond almost instantaneously to energy demands. In recent years, the focus has shifted towards developing advanced capacitor systems—particularly supercapacitors and solid-state capacitors (SSCs)—that combine high performance with flexibility (Figure-1) and environmental sustainability [5].

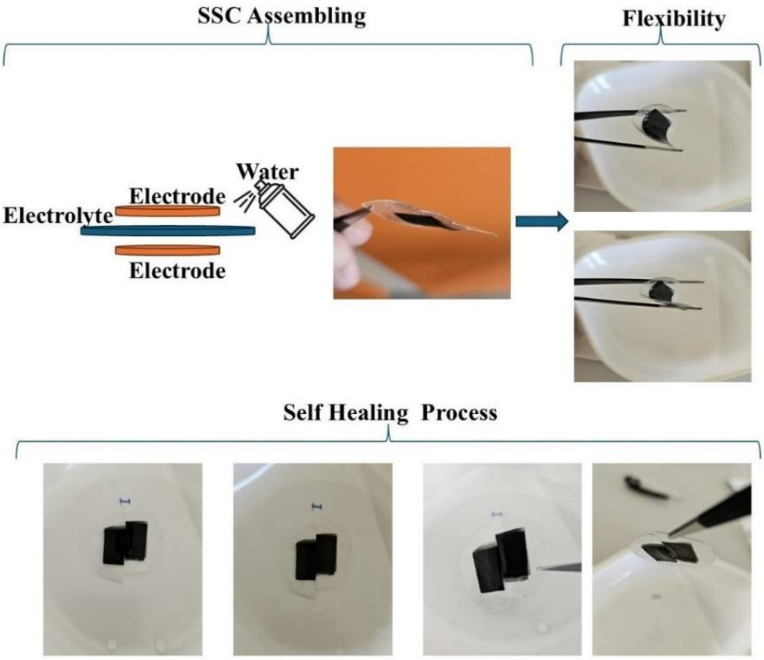


Figure 1. PVA/borax based SSC with filexibility and self-healing features.

Solid-state capacitors, in particular, represent a promising direction for next-generation energy storage due to their inherent safety, mechanical stability, and compatibility with flexible and miniaturized electronic systems [5]. Unlike traditional capacitors that often use liquid electrolytes prone to leakage, flammability, or environmental toxicity, SSCs employ solid or gel-like electrolytes that offer enhanced safety and device integrity [6]. Additionally, their adaptable form factor makes them especially suitable for integration into flexible substrates and portable technologies.

Among the various materials used in SSCs, polyvinyl alcohol (PVA) has emerged as a versatile and environmentally friendly polymer. PVA is water-soluble, biodegradable, and capable of forming robust, transparent films with good mechanical properties [7]. When crosslinked with borax (sodium tetraborate), PVA forms a physically crosslinked network through hydrogen bonding and dynamic diol-borate interactions, resulting in a flexible and ion-conductive hydrogel-like structure [8]. This PVA/borax matrix (Figure 1) not only maintains mechanical flexibility but also facilitates ionic mobility, making it an attractive candidate for solid polymer electrolytes in green capacitor technologies.

Recent studies have demonstrated that PVA/borax-based SSCs exhibit promising electrochemical characteristics, such as high capacitance retention, low internal resistance, and excellent cycling stability [9]. Furthermore, their low cost, non-toxicity, and ease of processing via solution-based methods make them viable for large-scale and disposable electronics applications [10]. These advantages align well with the broader movement toward sustainable, safe, and low-carbon electronic materials.

This study aims to investigate the synthesis, structural characterization, and electrochemical performance of PVA/borax-based solid-state capacitors. By exploring the interaction mechanisms within the polymer matrix and evaluating their comparative advantages over conventional capacitors and batteries, this work seeks to shed light on the role of such biopolymer-based systems in the future of sustainable energy storage. Additionally, the potential applications of these SSCs in emerging Technologies particularly in wearable electronics and low-power devices will be discussed to contextualize their practical relevance.

History of Capacitors

The development of capacitors over nearly three centuries mirrors the broader trajectory of scientific and technological advancements in energy storage. The inception of capacitor technology can be traced to the invention of the Leyden jar in 1745, one of the earliest devices capable of storing static electricity. Named after the city of Leiden in the Netherlands, the Leyden jar comprised a glass container partially filled with water and coated internally and externally with metal foil, effectively functioning as a rudimentary form of the parallel-plate capacitor [11]. Although primitive by today's standards, it laid down the basic principles of electrostatic energy storage and accelerated research into electricity.

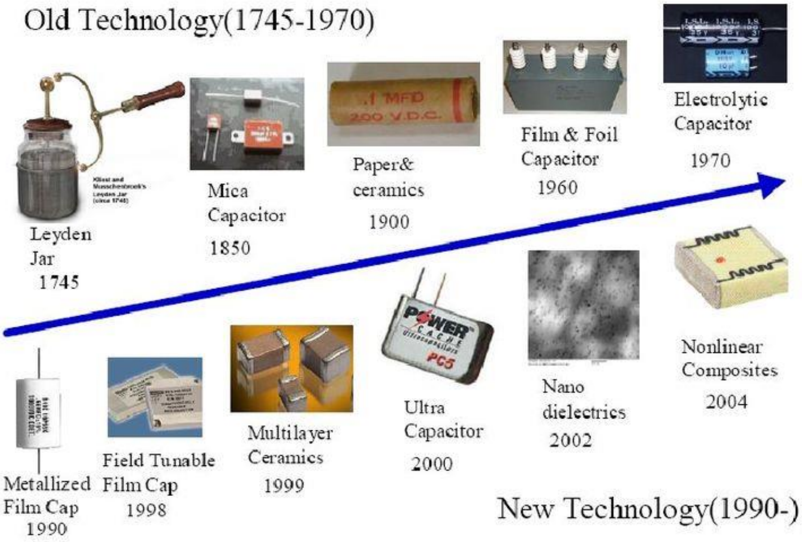


Figure 2. Evolution of the Capacitor technology with timeline [12].

As seen in the Figure 2, throughout the 19th and early 20th centuries, capacitor designs evolved in tandem with advances in materials science and electromagnetism. The development of metal foil and paper dielectric capacitors enhanced energy density and reliability, rendering them suitable for early telecommunication and radio technologies [13]. The introduction of electrolytic capacitors in the 1920s, which utilized an oxide layer as a dielectric, marked a significant advancement in compact energy storage. These components offered substantially higher capacitance in smaller volumes, facilitating the miniaturization of electronic circuits [13].

The post-World War II era witnessed rapid innovation in ceramic capacitors, film capacitors, and tantalum capacitors—each offering specific advantages in terms of thermal stability, dielectric strength, or longevity. This diversification of capacitor types paralleled the proliferation of consumer electronics, computing, and industrial automation technologies during the latter half of the 20th century [14,15]. However, traditional capacitors remained constrained by relatively low energy densities, rendering them unsuitable for applications requiring both high energy and high power.

To address this limitation, the late 20th century saw the emergence of electrochemical capacitors, commonly referred to as supercapacitors or ultracapacitors. These devices combined the charge storage mechanisms of conventional capacitors and batteries, employing electric double-layer capacitance and pseudocapacitance to achieve higher energy densities while retaining rapid charge-discharge capabilities [13–15]. Supercapacitors initially found applications in memory backup systems, but their utility quickly expanded to renewable energy buffering, electric vehicles, and regenerative braking systems.

More recently, solid-state capacitors (SSCs) have gained prominence in response to the growing demand for safer, smaller, and more flexible energy storage systems. Unlike their liquid-based electrolytic counterparts, SSCs utilize solid or gel polymer electrolytes, eliminating leakage risks and enhancing operational stability across a broader temperature range [6, 16]. This advancement has opened new pathways for integrating capacitors into emerging technologies such as wearable devices, flexible electronics, and bio-integrated systems.

Thus, the historical trajectory of capacitor technology reveals a continuous trend toward higher performance, miniaturization, and environmental sustainability. From the Leyden jar to contemporary biopolymer-based SSCs, capacitors have evolved from basic scientific curiosities into indispensable components in modern energy infrastructure.

Comparative Analysis of Energy Storage Technologies

Understanding the comparative performance of energy storage technologies is essential for identifying niche applications where solid-state capacitors (SSCs), particularly those based on PVA/borax systems, can offer distinct advantages. Conventional capacitors, supercapacitors, and batteries each operate based on unique electrochemical mechanisms, resulting in trade-offs between energy density, power output, charge/discharge rates, and longevity [17].

Capacitors, which rely on the electrostatic accumulation of charge on parallel plates separated by a dielectric, are unparalleled in terms of power density—often exceeding 500 W/kg. This characteristic makes them ideal for short-duration, high-power applications such as pulse power delivery, filtering, and power conditioning [18]. However, their energy storage capacity is extremely limited, typically less than 0.1 Wh/kg, rendering them unsuitable for applications requiring sustained energy supply.

Supercapacitors, or electrochemical capacitors, bridge the performance gap between conventional capacitors and batteries by combining double-layer capacitance and pseudocapacitance. They offer moderate energy densities (1–10

Wh/kg) and power outputs ranging from 500 to 10,000 W/kg, along with charge-discharge times measured in seconds or minutes [18]. This unique profile makes them attractive for load leveling, regenerative braking, and hybrid energy systems.

Batteries, particularly lithium-ion systems, provide the highest energy densities among the three (100–300 Wh/kg for Li-ion), enabling prolonged energy supply for applications such as electric vehicles, smartphones, and grid-level storage. However, batteries exhibit slower charge and discharge rates, often ranging from tens of minutes to several hours, and are limited by finite cycle lives—typically 500 to 3,000 cycles depending on chemistry and use conditions [19].

In contrast, SSCs, especially those based on gel polymer electrolytes like PVA/borax, offer high cycle stability, often exceeding thousands of cycles with minimal capacity fade. Some systems approach quasi-infinite lifespans due to the absence of electrochemical degradation mechanisms found in battery electrodes [20]. These characteristics position SSCs as ideal candidates for applications requiring frequent and rapid charge-discharge cycles, such as wearable electronics, sensors, and backup power systems in microdevices.

Solid-State Capacitors: Advantages and Challenges

Solid-state capacitors (SSCs) represent a significant advancement in capacitor technology by addressing numerous limitations associated with liquid-electrolyte-based systems. The elimination of volatile and potentially hazardous liquid electrolytes results in substantial enhancements in safety, thermal stability, and long-term reliability. SSCs are inherently less susceptible to leakage, corrosion, or combustion, facilitating their application in compact and high-temperature environments (typically 60–110°C or higher, depending on materials)[10].

A primary performance advantage of SSCs is their low equivalent series resistance (ESR), which minimizes energy losses as heat and enhances overall power efficiency. Additionally, the compact and flexible nature of solid or gel electrolytes permits the development of thin, bendable capacitor architectures—features highly desirable in next-generation electronic platforms [21].

However, the performance of SSCs is significantly influenced by the nature of the electrolyte material. While liquid electrolytes provide superior ion mobility and interfacial contact, they often suffer from poor thermal and chemical stability, rendering them unsuitable for long-term or high-temperature applications. In contrast, solid electrolytes offer exceptional mechanical integrity, environmental safety, and long shelf life, but they may encounter challenges such as low ionic conductivity and poor electrode-electrolyte interfacial contact [17].

Gel polymer electrolytes, such as PVA/borax systems, present an attractive compromise between these two extremes. These systems retain the structural robustness and safety of solid-state materials while maintaining sufficient ionic mobility through hydrated or semi-hydrated polymer matrices. Moreover, the use of environmentally benign and non-toxic materials like PVA and borax aligns with the increasing emphasis on green electronics and sustainable manufacturing [9,10].

Nonetheless, challenges persist in optimizing the electrochemical interface, ionic conductivity, and mechanical flexibility of these systems. For instance, the presence of water in hydrogel-based electrolytes may limit their use at elevated temperatures or in sealed environments. Ongoing research focuses on modifying the polymer matrix, incorporating nanofillers, or developing hybrid gel systems to overcome such limitations.

The absence of liquid electrolytes fundamentally reshapes capacitor design philosophy—transitioning from bulky, rigid forms to compact, flexible, and integratable formats. Reliability is improved due to reduced risks of electrolyte leakage, evaporation, and flammability, while the use of solid components supports form-factor innovations in flexible electronics. However, ensuring optimal ion transport and interfacial stability without the benefits of liquid-phase mobility remains a key area for continued research and development.

Material Characteristics of PVA/Borax-based Solid-State Capacitors

Polyvinyl alcohol (PVA) is a water-soluble, biodegradable and highly crystalline synthetic polymer; these properties make it an ideal material for flexible electronic and biomedical applications [9,20]. When combined with borax (sodium tetraborate), dynamic borate-diol bonds are formed between the hydroxyl groups of PVA and borate ions, forming a physically cross-linked, flexible, stretchable and self-healing hydrogel matrix. This hydrogel provides high ionic conductivity due to its water content (typically 10^{-3} to 10^{-2} S/cm, depending on the additives used) and the hydrogen bonds formed by the water molecules between the polymer chains enhance ion mobility [9,20].

The degree of crystallinity of PVA/borax hydrogels varies between 20-40% depending on the polymer concentration and crosslinking density, providing a balance between mechanical strength and flexibility. For example, hydrogels prepared at 10% PVA and 0.5% borax concentration exhibit a tensile strength of about 1-2 MPa and an elongation capacity of up to 300% [22,23]. The self-healing property is due to the reversible nature of borate ester bonds, which can regenerate after mechanical damage and restore up to 90% of the structural integrity of the hydrogel . Furthermore, when additives such as graphene, carbon nanotubes or conducting polymers (e.g., polyniline) are added, the hydrogel can be used as both electrolyte and active electrode material. By increasing the surface area, these additives can increase the capacitance to between 50-200 F/g and improve the electrical conductivity up to 10^{-1} S/cm [22,23].

These properties make PVA/borax systems a safer and environmentally friendly alternative to conventional liquid electrolytes. However, the high water content of the hydrogel can pose a risk of evaporation at high temperatures (>80°C), which can limit stability in long-term applications. To overcome this problem, hybrid systems with additives such as ionic liquids or nanofluids are being developed [10].

Synthesis and Manufacturing Strategies

The synthesis of PVA/borax-based solid-state capacitors is usually carried out using solution casting or in-situ polymerization techniques. The process starts by dissolving PVA in water at 80-90°C, which ensures complete dissolution of the polymer chains. Gelation is then initiated by adding a 0.1-1.0% borax solution. Critical parameters include PVA concentration (5-15%), borax ratio (0.1-0.5% by mass of PVA), pH (usually 7-9) and temperature (25-60°C). For example, higher concentrations of borax (0.5%) improve mechanical strength by increasing crosslinking density, but may decrease ionic conductivity (from 10^{-3} S/cm to 10^{-4} S/cm) .

Electrodes are prepared from materials such as activated carbon, carbon fabric, reduced graphene oxide (rGO) or metal oxides (e.g., MnO_2) and arranged in symmetric or asymmetric configurations[24]. The hydrogel is cast or coated between the electrodes to form a flexible capacitor structure. Electrical properties can be improved by integrating conductive fillers (e.g. carbon nanotubes or PEDOT:PSS) into the hydrogel; for example, 1% graphene doping can increase ionic conductivity by 30%. During the production process, techniques such as drying under vacuum or freeze-drying increase the porosity of the hydrogel, facilitating ion transport [24].

For industrial scale production, methods such as roll-to-roll coating or 3D printing are being investigated. These techniques optimize the homogeneity of the hydrogel and the electrode-electrolyte interface quality while increasing cost-effectiveness. However, challenges remain in large-scale production, such as homogeneous distribution of borax concentration and long-term environmental stability of the hydrogel.

Electrochemical Performance and Stability

PVA/borax-based SSCs perform similar to electrical double layer capacitors (EDLCs) and can exhibit pseudocapacitive behavior with redox-active additives. Capacitance values range from 10-500 F/g depending on the electrode material and hydrogel composition. For example, a symmetric PVA/borax SSC with activated carbon electrode offers a specific capacitance of 50-150 F/g in the potential range of 0.5-1 V, while this value can reach 300-500 F/g when pseudocapacitive materials such as MnO_2 or polianiline are used [9,25].

The electrochemical performance is evaluated by techniques such as cyclic voltammetry (CV), cyclic charge-discharge (CCD) and electrochemical impedance spectroscopy (EIS). EIS measurements reveal the low equivalent series resistance (ESR, typically 0.1-1 Ω) of PVA/borax SSCs, resulting in high power efficiency. Energy density ranges from 1-10 Wh/kg and power density from 500-5000 W/kg, depending on electrode porosity and electrolyte thickness [24,25].

Cycle stability is the most remarkable feature of PVA/borax SSCs; capacitance loss is usually 5-10% even at 100,000 cycles. This is possible due to the reversible ion transport of the hydrogel and the mechanical flexibility of the borate ester bonds. In mechanical deformation tests (e.g., 100% elongation or 90° bending), 90% of the capacitance is retained, which is ideal for wearable devices. However, dehydration of the hydrogel at high temperatures (>60°C) or low humidity can reduce the ionic conductivity by up to 50%. To solve this problem, stability can be increased by adding ionic liquids or moisture retaining agents such as glycerol.

Application Areas and Technological Potential

The flexibility, biocompatibility and environmentally friendly chemistry of PVA/borax-based SSCs offer potential in a wide range of application areas. Wearable Electronics: These capacitors can be used as energy storage in smart textiles (e.g., fabrics with pulse sensors) and flexible displays (e.g., foldable OLED displays). For example, a PVA/borax SSC can operate with a capacitance retention rate of 95% after 1,000 cycles of shrinkage, which increases the durability of wearable devices. Biomedical Applications: Thanks to their biocompatibility, these systems can be used in implantable sensors (e.g. glucose monitoring devices) or soft robotic systems. For example, self-healing PVA/borax hydrogels provide resistance to mechanical damage in skin patch-like devices. Renewable Energy Systems: PVA/borax SSCs can be used as auxiliary energy buffers to store and dissipate short bursts of energy from photovoltaic panels or piezoelectric sensors. For example, in a solar energy system, they can provide a power density of 1000 W/kg to meet sudden power demands. Internet of Things (IoT): In IoT devices with low power requirements (e.g., environmental sensors), these capacitors provide reliable energy with their small size and high cycle stability [26].

However, their low energy density (less than 10 Wh/kg) limits them from being the primary storage in high energy demand applications such as electric vehicles. Instead, they can be an auxiliary component in memory backup, thermal buffering or low power management systems. Environmentally friendly manufacturing processes are in line with sustainability goals, especially in the production of biodegradable electrics.

Conclusion

PVA/borax-based solid-state capacitors offer unique advantages such as safety, flexibility, biocompatibility and low environmental impact, making them an environmentally friendly alternative to conventional energy storage systems. Easy synthesis, cost-effectiveness and scalability make these systems attractive for academic research and commercial pro-totyping. However, low energy density (1-10 Wh/kg) compared to liquid electrolyte supercapacitors or lithium ion batteries and stability issues at high temperatures are the main limitations. Future research should focus on enhancing electrochemical performance through nanostructuring (e.g. graphene or MOF-based composites), doping strategies (e.g. ionic liquids) and electrode-electrolyte interface engineering. For example, it is estimated that the porous structure of MOFs can increase ion transport by 20-30%. Furthermore, for industrial-scale production, innovative methods such as roll-to-roll coating or 3D printing could increase commercial viability by reducing costs. These advances could bring PVA/borax SSCs to a wider range of applications in areas such as wearable electro-technics, biomedical devices and IoT, thus contributing to the development of sustainable and smart energy systems.

Reference

[1] C.L. Benson, C.L. Magee, On improvement rates for renewable energy technologies: Solar PV, wind turbines, capacitors, and batteries, Renew Energy 68 (2014) 745–751. https://doi.org/10.1016/J.RENENE.2014.03.002.

[2] D. Brogioli, Extracting renewable energy from a salinity difference using a capacitor, Phys Rev Lett 103 (2009) 058501. https://doi.org/10.1103/PHYSREVLETT.103.058501/FIGURES/4/THUMBNAIL.

[3] G. Lan, D. Ma, W. Xu, M. Hassan, W. Hu, Capacitor-based Activity Sensing for Kinetic-powered Wearable IoTs, ACM Transactions on Internet of Things 1 (2020). https://doi.org/10.1145/3362124.

[4] T. Zhang, F. Zhang, L. Zhang, Y. Lu, Y. Zhang, X. Yang, Y. Ma, Y. Huang, High energy density Li-ion capacitor assembled with all graphene-based electrodes, Carbon N Y 92 (2015) 106–118. https://doi.org/10.1016/J.CARBON.2015.03.032.

[5] X. Lu, M. Yu, G. Wang, Y. Tong, Y. Li, Flexible solid-state supercapacitors: design, fabrication and applications, Energy Environ Sci 7 (2014) 2160–2181. https://doi.org/10.1039/C4EE00960F.

[6] M. Akin, X. Zhou, Recent advances in solid-state supercapacitors: From emerging materials to advanced applications, Int J Energy Res 46 (2022) 10389–10452. https://doi.org/10.1002/ER.7918.

[7] K. Cicek, S. Demirel, Self-healable PVA–graphite–borax as electrode and electrolyte properties for smart and flexible supercapacitor applications, Journal of Materials Science: Materials in Electronics 32 (2021) 16335–16345. https://doi.org/10.1007/S10854-021-06186-W/TABLES/3.

[8] S. Demirel, R. Topkaya, K. Cicek, Stretchable and self-healable PVA–Nickel–Borax electrodes for supercapacitor applications, Journal of Materials Science: Materials in Electronics 34 (2023) 1–10. https://doi.org/10.1007/S10854-022-09392-2/FIGURES/7.

[9] A. Kockar, S. Demirel, G. Kerimli, Self-healable Mn-doped PVA-borax hydrogel electrodes for supercapacitor applications, J Appl Polym Sci (2024) e56143. https://doi.org/10.1002/APP.56143.

[10] S. Demirel, Temperature Dependent Polarization Effect and Capacitive Performance Enhancement of PVA-Borax Gel Electrolyte, Int J Electrochem Sci 15 (2020) 2439–2448. https://doi.org/10.20964/2020.03.75.

[11] B. Brusso, S. Chaparala, The evolution of capacitors [history], IEEE Industry Applications Magazine 20 (2014) 8–12. https://doi.org/10.1109/MIAS.2014.2342592.

[12] Knowledge Pin. https://in.pinterest.com/pin/414401603183606151/ (accessed May 29, 2025).

[13] J. Both, Electrolytic capacitors, 1890 to 1925: Early history and basic principle, IEEE Electrical Insulation Magazine 31 (2015) 22–29. https://doi.org/10.1109/MEI.2015.6996675.

[14] Y. Liu, P.R. Shearing, G. He, D.J.L. Brett, Supercapacitors: History, Theory, Emerging Technologies, and Applications, Advances in Sustainable Energy: Policy, Materials and Devices (2021) 417–449. https://doi.org/10.1007/978-3-030-74406-9_15.

[15] J. Park, W. Kim, History and Perspectives on Ultrafast Supercapacitors for AC Line Filtering, Adv Energy Mater 11 (2021) 2003306. https://doi.org/10.1002/AENM.202003306.

[16] Y. Liu, P.R. Shearing, G. He, D.J.L. Brett, Supercapacitors: History, Theory, Emerging Technologies, and Applications, Advances in Sustainable Energy: Policy, Materials and Devices (2021) 417–449. https://doi.org/10.1007/978-3-030-74406-9_15.

[17] M. Akin, X. Zhou, Recent advances in solid-state supercapacitors: From emerging materials to advanced applications, Int J Energy Res 46 (2022) 10389–10452. https://doi.org/10.1002/ER.7918.

[18] A. Burke, R&D considerations for the performance and application of electrochemical capacitors, Electrochim Acta 53 (2007) 1083–1091. https://doi.org/10.1016/J.ELECTACTA.2007.01.011.

[19] Z. Yao, W. Tang, X. Wang, C. Wang, C. Yang, C. Fan, Synthesis of 1,4-benzoquinone dimer as a high-capacity (501 mA h g−1) and high-energy-density (>1000 Wh kg−1) organic cathode for organic Li-Ion full batteries, J Power Sources 448 (2020) 227456. https://doi.org/10.1016/J.JPOWSOUR.2019.227456.

[20] S. Demirel, R. Topkaya, K. Cicek, Co-doped PVA-borax anodic supercapacitors with high capacity and self-healability features, Solid State Ion 396 (2023) 116230. https://doi.org/10.1016/J.SSI.2023.116230.

[21] R. Vicentini, L.M. Da Silva, E.P. Cecilio, T.A. Alves, W.G. Nunes, H. Zanin, How to Measure and Calculate Equivalent Series Resistance of Electric Double-Layer Capacitors, Molecules 24 (2019) 1452. https://doi.org/10.3390/MOLECULES24081452.

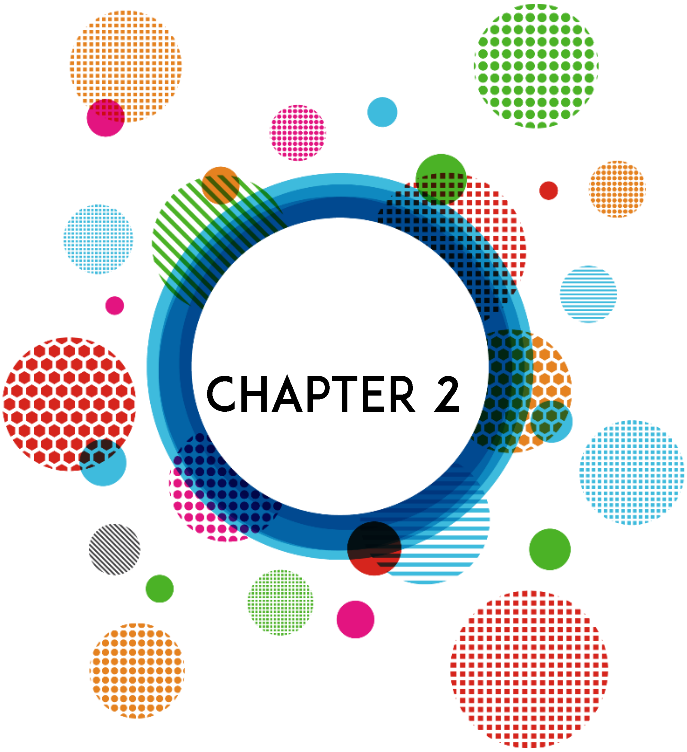
[22] N.Y. Abu-Thabit, A.S. Hamdy Makhlouf, Smart textile supercapacitors coated with conducting polymers for energy storage applications, Industrial Applications for Intelligent Polymers and Coatings (2016) 437–477. https://doi.org/10.1007/978-3-319-26893-4_21.

[23] A.R. Polu, H.W. Rhee, Ionic liquid doped PEO-based solid polymer electrolytes for lithium-ion polymer batteries, Int J Hydrogen Energy 42 (2017) 7212–7219. https://doi.org/10.1016/J.IJHYDENE.2016.04.160.

[24] X. Zhou, A. Rajeev, A. Subramanian, Y. Li, N. Rossetti, G. Natale, G.A. Lodygensky, F. Cicoira, Self-healing, stretchable, and highly adhesive hydrogels for epidermal patch electrodes, Acta Biomater 139 (2022) 296–306. https://doi.org/10.1016/J.ACTBIO.2021.07.069.

[25] F. Seidi, Y. Jin, J. Han, M.R. Saeb, A. Akbari, S.H. Hosseini, M. Shabanian, H. Xiao, Self-healing Polyol/Borax Hydrogels: Fabrications, Properties and Applications, The Chemical Record 20 (2020) 1142–1162. https://doi.org/10.1002/TCR.202000060.

[26] J.N. Liu, Q. He, M.Y. Pan, K. Du, C. Bin Gong, Q. Tang, An energy-saving, bending sensitive, and self-healing PVA-borax-IL ternary hydrogel electrolyte for visual flexible electrochromic strain sensors, J Mater Chem A Mater 10 (2022) 25118–25128. https://doi.org/10.1039/D2TA06667J.



CHAPTER 2

Ethylene Vinyl Acetate (Eva) Polymer: Properties, Processing, and Applications

Yusuf Yılmaz[1]

---

[1] Department of Chemistry Technology, Naci Topçuoğlu Vocational School, Gaziantep University, Gaziantep 27310, Türkiye, Orcid: 0000-0003-4363-0427

1. Definition, History, and Types of EVA Polymer

Ethylene vinyl acetate (EVA) is a widely used copolymer composed of ethylene and vinyl acetate (VA) monomers (Figure 1). This thermoplastic polymer exhibits a unique combination of elasticity, impact resistance, and ease of processing, making it an essential material in various industries.

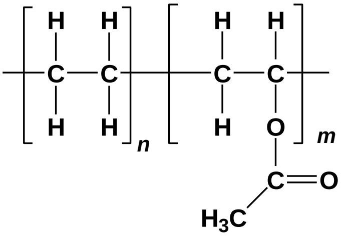


Figure 1. Chemical structure of EVA polymer

EVA is characterized by its lightweight nature, flexibility, and excellent weatherability, which contribute to its extensive use in footwear, packaging, and construction materials (Henderson,1993). Historically, the development of EVA polymers dates back to the mid-20th century when advancements in polymer chemistry enabled the synthesis of new copolymers with tailored properties. The commercialization of EVA gained traction in the 1960s when industries started recognizing its potential for replacing traditional rubbers and plastics (Bidsorkhi et al., 2014). Due to its cost-effectiveness and versatile applications, EVA has become a key material in the polymer industry. EVA polymers are classified based on the VA content, which significantly affects their physical properties:

1.1. Low VA Content EVA (4-10% VA)

This type exhibits greater rigidity and lower flexibility, making it suitable for applications requiring structural integrity, such as laminated films, adhesives, and cable insulation.

1.2. Medium VA Content EVA (10-30% VA)

With enhanced elasticity and durability, this category is commonly used in footwear, foam sheets, and industrial applications where moderate flexibility is required.

1.3. High VA Content EVA (30-50% VA)

This variant resembles rubber and demonstrates exceptional flexibility and resilience. It is frequently employed in sports equipment, soft packaging, and shock-absorbing materials.

The tunability of EVA properties based on VA content makes it an attractive alternative to other elastomers and plastics. Additionally, EVA can be modified with additives to enhance its thermal stability, UV resistance, and mechanical performance, further broadening its industrial applications (Camacho et al., 2017; Spina, 2015; Wilson et al., 2012).

2. Processing Methods of EVA Polymer

The processing of EVA polymers involves several advanced techniques, each tailored to the desired final product. The most commonly employed methods include extrusion, injection molding, blow molding, and foaming.

2.1. Extrusion

Extrusion is one of the primary processing methods for EVA, particularly in film and sheet manufacturing. In this process, EVA granules are melted and forced through a die to obtain continuous profiles. The extruded sheets are widely used in solar panel encapsulation, automotive interiors, and industrial packaging due to their excellent mechanical properties and thermal resistance (Ramírez-Vargas et al., 2009).

2.2. Injection Molding

Injection molding is a preferred method for producing complex EVA components, such as shoe soles, protective gear, and electronic casings. The process involves melting the polymer and injecting it into a mold cavity under high pressure. The rapid cooling and solidification of the material allow for mass production of intricately designed EVA products with high dimensional accuracy (Almeida et al., 2011).

2.3. Blow Molding

This method is utilized in the packaging sector, particularly for producing EVA-based bottles, containers, and flexible films. The molten EVA polymer is extruded into a tube and inflated with compressed air to form a hollow structure. The resulting products exhibit high impact resistance and chemical stability, making them ideal for food and pharmaceutical packaging applications (Spina, 2015).

2.4. Foaming

EVA foams are widely used in footwear, sports equipment, and cushioning materials due to their lightweight and shock-absorbing properties. The foaming process involves the incorporation of blowing agents that create a cellular structure within the polymer matrix. The density and resilience of the foam can be controlled to achieve specific performance characteristics, such as thermal insulation and energy absorption (Wypych, 2022).

Each processing technique offers unique advantages, allowing EVA to be tailored to various industrial needs. Additionally, advancements in processing technologies, such as 3D printing and reactive extrusion, continue to expand the potential applications of EVA in innovative fields (Novriadi et al., 2024).

3. Applications of EVA Polymer

The diverse properties of EVA enable its utilization across multiple industries, including packaging, footwear, construction, electronics, and healthcare.

3.1. Packaging Industry

EVA is extensively used in flexible packaging materials, adhesive films, and sealants. Due to its excellent adhesion properties, it serves as an effective bonding layer in multilayer packaging films, enhancing barrier performance against moisture and gases.

3.2. Footwear and Slippers

EVA is a dominant material in the footwear industry, particularly for producing lightweight and comfortable shoe soles. It offers superior impact resistance and flexibility, making it ideal for athletic footwear, sandals, and orthopedic insoles.

3.3. Construction Materials

In the building sector, EVA-based products are used in insulation panels, waterproof membranes, and soundproofing materials. Its resistance to environmental factors and ease of processing make it a preferred material in modern construction techniques.

3.4. Electronics and Solar Panels

EVA is an essential component in the encapsulation of photovoltaic (PV) solar cells, protecting them from environmental degradation and improving energy efficiency. It is also used in electrical insulation for wiring and cable coatings due to its dielectric properties.

3.5. Medical and Hygiene Products

Due to its non-toxic nature, EVA is used in medical tubing, prosthetics, and hygiene products such as baby mats and flexible containers (Schneider et al., 2017; Das et al., 2009; Sidiqui and Waris Khan, 2024; Badiee et al., 2016; e Dias et al., 2018).

4. Use of EVA Polymer in Footwear and Slipper Industry

The footwear industry extensively relies on EVA due to its outstanding balance of comfort, durability, and cost-effectiveness.

- **Shock Absorption:** EVA soles provide excellent cushioning, reducing impact forces and minimizing foot fatigue.
- **Flexibility and Comfort:** Its soft texture enhances user comfort, making it suitable for long-term wear.
- **Water Resistance:** EVA does not absorb water, making it ideal for beach sandals, shower slippers, and outdoor footwear.
- **Lightweight Nature:** Compared to traditional rubber, EVA soles offer significant weight reduction, enhancing mobility and comfort (Paiva et al., 2016).

5. Recycling of EVA Polymer

The growing environmental concerns surrounding plastic waste have prompted extensive research into EVA recycling. Various recycling techniques have been developed to reduce waste and promote sustainability.

- **Mechanical Recycling:** In this method, post-consumer EVA waste is collected, shredded, and reprocessed into new products. This approach is commonly used for manufacturing recycled shoe soles, foam mats, and industrial components.
- **Chemical Recycling:** This involves depolymerizing EVA into its monomeric components, which can be reused to synthesize new EVA materials. Although promising, this method requires significant energy input and is still under development for large-scale applications.
- **Energy Recovery:** EVA waste can be incinerated to generate energy, but this method raises environmental concerns due to emissions. Research is ongoing to develop cleaner combustion processes that minimize toxic byproducts.

Recent studies have also explored biodegradable EVA alternatives and bio-based copolymers to enhance sustainability. The development of eco-friendly

EVA formulations with improved recyclability remains a priority for researchers and industry professionals (Martínez et al., 2024; Dias et al., 2017; Bohland et al., 1997).

Conclusion

EVA polymer represents an essential class of thermoplastic elastomers with wide-ranging applications in footwear, packaging, electronics, and construction. The advancements in its processing methods and material modifications continue to enhance its properties, making it a preferred alternative to traditional materials. However, the increasing environmental concerns regarding EVA waste necessitate the development of sustainable recycling methods. The ongoing research in mechanical and chemical recycling, along with the potential for bio-based EVA alternatives, highlights the industry's commitment to sustainability. Future innovations in polymer science and green chemistry will play a crucial role in addressing the environmental challenges associated with EVA, ensuring its continued use in a more eco-friendly manner.

Acknowledgements: This study was supported by Naci Topçuoğlu Vocational School Project Coordination Office (PDK). The author also thanks Chemist Fatma Yılmaz for her contribution to this study.

References

Almeida, A., Possemiers, S., Boone, M. N., De Beer, T., Quinten, T., Van Hoorebeke, L., Vervaet, C. (2011). Ethylene vinyl acetate as matrix for oral sustained release dosage forms produced via hot-melt extrusion. *European Journal of Pharmaceutics and Biopharmaceutics*, *77*(2), 297-305.

Badiee, A., Ashcroft, I. A., & Wildman, R. D. (2016). The thermo-mechanical degradation of ethylene vinyl acetate used as a solar panel adhesive and encapsulant. *International Journal of Adhesion and Adhesives*, *68*, 212-218.

Bidsorkhi, H. C., Soheilmoghaddam, M., Pour, R. H., Adelnia, H., & Mohamad, Z. (2014). Mechanical, thermal and flammability properties of ethylene-vinyl acetate (EVA)/sepiolite nanocomposites. *Polymer Testing*, *37*, 117-122.

Bohland, J. R., & Anisimov, I. I. (1997, September). Possibility of recycling silicon PV modules. In *Conference Record of the Twenty Sixth IEEE Photovoltaic Specialists Conference-1997* (pp. 1173-1175). IEEE.

Camacho, J., Díez, E., Díaz, I., & Ovejero, G. (2017). PC-SAFT thermodynamics of EVA copolymer–Solvent systems. *Fluid Phase Equilibria*, *449*, 10-17.

Das, C. K., Kumar, S., & Rath, T. (2009). 17 Vinyl Polymer Applications and Special Uses. Handbook of Vinyl Polymers, 541.

Dias, P., Javimczik, S., Benevit, M., & Veit, H. (2017). Recycling WEEE: Polymer characterization and pyrolysis study for waste of crystalline silicon photovoltaic modules. *Waste Management*, *60*, 716-722.

e Dias, R. B., & Coto, N. P. (2018). Systematic Study of Ethylene-Vinyl Acetate (EVA) in the Manufacturing of Protector Devices for the. *Biomaterials in regenerative medicine*, 319.

Henderson, A. M. (1993). Ethylene-vinyl acetate (EVA) copolymers: a general review. *IEEE Electrical Insulation Magazine*, *9*(1), 30-38.

Martínez, M., Barrueto, Y., Jimenez, Y. P., Vega-Garcia, D., & Jamett, I. (2024). Technological Advancement in Solar Photovoltaic Recycling: A Review. Minerals, 14(7), 638.

Novriadi, D., Muslim, O. F., Farishi, S., Pratama, A., Hakim, A. R., & Yurohman, Y. (2024, February). Comparative study on compressive strength of polyethylene and ethylene vinyl acetate foam mixture using compression and rotational molding method. In *AIP Conference Proceedings* (Vol. 3003, No. 1). AIP Publishing.

Paiva, R. M., Marques, E. A., da Silva, L. F., António, C. A., & Arán-Ais, F. (2016). Adhesives in the footwear industry. *Proceedings of the Institution of*

Mechanical Engineers, Part L: Journal of Materials: Design and Applications, *230*(2), 357-374.

Ramírez-Vargas, E., Valera-Zaragoza, M., Sánchez-Valdes, S., Hernández-Valdez, J. S., & Ibarra-Castillo, F. F. (2009). Effect of processing conditions on the structural morphology of PP–EP/EVA/organoclay ternary nanocomposites. *Polymer bulletin*, *62*, 391-403.

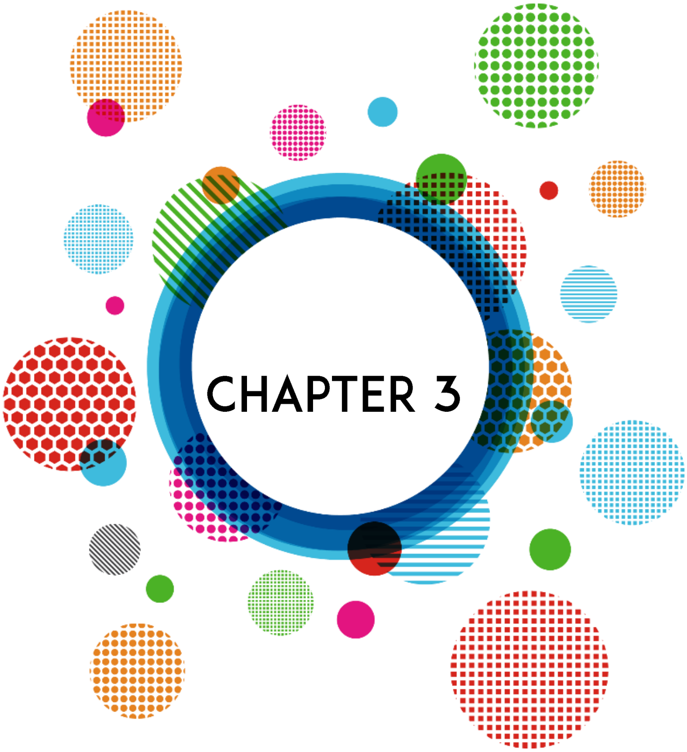
Schneider, C., Langer, R., Loveday, D., & Hair, D. (2017). Applications of ethylene vinyl acetate copolymers (EVA) in drug delivery systems. *Journal of Controlled Release*, *262*, 284-295.

Sidiqui, A. J., & Waris Khan, M. G. (2024). Emerging Trends of Polymer Materials for Footwear Applications in India. *Engineering Headway*, *11*, 17-26.

Spina, R. (2015). Technological characterization of PE/EVA blends for foam injection molding. *Materials & Design*, 84, 64-71.

Wilson, R., Plivelic, T. S., Aprem, A. S., Ranganathaiagh, C., Kumar, S. A., & Thomas, S. (2012). Preparation and characterization of EVA/clay nanocomposites with improved barrier performance. *Journal of applied polymer science*, *123*(6), 3806-3818.

Wypych, G. (2022). *Handbook of foaming and blowing agents*. Elsevier.



CHAPTER 3

Advancing Green Chemistry: Innovations in Chalcone Synthesis

Lütfiye Sirka[1]

---

[1] Assist. Prof., Çankırı Karatekin University Şabanözü Vocational School of Health Services, ORCID: 0000-0003-3973-6675

1 Introduction

Concerns about the environmental impact of human society's growth have become widespread, making sustainability a key priority across all areas of human activity. As a significant contributor to human progress, the chemical industry faces mounting pressure to develop more sustainable practices. In this context, Green Chemistry is defined as the design of chemical products and processes aimed at minimizing or eliminating the use and creation of hazardous substances. It was established through principles intended to guide chemists in their pursuit of greener solutions.

Over the last twenty years Green Chemistry has gradually achieved broad recognition within the scientific community. As it is let the importance of the term green chemistry sink in, it can be imagined what is the field of sustainable chemistry. This is science that operates in a specific area aimed at avoiding or reducing the production of hazardous substances in processes and products. On the ground of the principles articulated by Paul Anastas and John Warner in 1998, green chemistry strives to minimize the environmental and health effects caused by many processes in chemistry and indeed all industries are able to adopt principles of sustainable development. Development of the last three years in this sphere can be characterized as significant especially in such domains as renewable feedstocks, greener solvents and waste minimization tactics [1,2].

1.1. Green Chemistry

The 12 Principles of Green Chemistry are a set of guidelines introduced by Paul Anastas and John Warner in 1998 to help chemists design more environmentally friendly processes and products. Here’s a sorted and clarified version:

Prevention: Emphasize prevent or minimize the generation of waste rather than eliminate it after it has been created.

Atom Economy: Ensure the maximum utilization of reactants by ensuring that all materials used in the process are converted into the product.

Less Hazardous Chemical Syntheses: Design synthetic methods to be as safe as possible, avoid the production of substances that are toxic or hazardous to human health and the environment.

Designing Safer Chemical: Create chemicals that are effective and purpose-driven but not to pose a threat to human health and the environment.

Safer Solvents and Auxiliaries: Minimize or eliminate the use of solvents or auxiliary substances (e.g., separation agents) whenever possible. If necessary, use safe and environmentally friendly solvents.

Design for Energy Efficiency: Optimize processes to consume the least amount of energy. Preferably, use ambient temperature and pressure conditions.

Use of Renewable Feedstocks: Use raw materials that are renewable rather than depleting, such as plant-based chemicals instead of petroleum-based ones.

Reduce Derivatives: Avoid using unnecessary derivatives, such as blocking groups, protecting groups or temporary modifications that require additional reagents and generate waste whenever possible.

Catalysis: Use catalytic reagents instead of stoichiometric ones to enhance efficiency. Catalysts which can be reused are more efficient and reduce waste generation.

Design for Degradation: Design products to break down into harmless substances in the environment. Avoid substances that persist or bioaccumulate.

Real-Time Analysis for Pollution Prevention: Implement monitoring techniques to detect and control hazardous substances during the process. Real-time analysis helps prevent the formation of pollutants and ensures safety.

Inherently Safer Chemistry for Accident Prevention: Design processes to minimize the potential for accidents such as chemical releases, explosions or fires. Use safer chemicals and conditions.

The 12 Principles of Green Chemistry are there to encourage sustainability in chemical processes and reduce the levels of pollution caused by chemical manufacture. A way to identify and measure how far — or close — you are from designing safer, more efficient chemical products that reduce waste, require less energy output or use of hazardous substances offered by the Green Chemistry Principles. In applying these fundamentals, chemists are working to finds way definitely certain work that not only generates the desired chemicals but also takes care of our environment, serving as a balance between technological advance and ecologic preservation. In addition, the principles help direct prupcllrges within the chemical industry to be more sustainable in a way that encourages innovation while protecting human health and environment [1]. The 12 Principles of Green Chemistry have been demonstrated Fig.1.

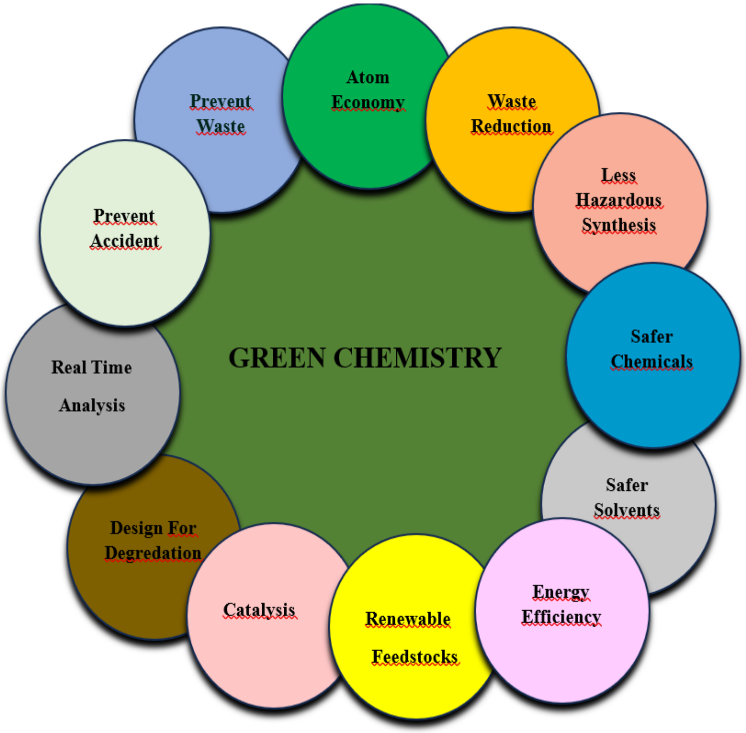


Fig. 1. Twelwe Principle Of Green Chemistry

Over the past ten years, the idea of "Green Chemistry" in relation to "Sustainable Development" has been extensively studied [3]. Sustainable development is defined as progress that fulfills present needs while ensuring future generations can meet their own requirements [4]. Given its focus on pollution concerns and the unsustainable use of natural resources, sustainable development holds particular significance for numerous chemistry-related industries [5]. Key factors for green synthesis of various chemicals include choosing an environmentally friendly solvent (commonly water, ethanol, or their combinations), a non-toxic reducing agent and a safe stabilizing substance. Chemical processes are often highly expensive and require the use of toxic and dangerous substances which pose numerous environmental hazards [6].

The most critical scientific question facing the chemical industry in shaping the future of Earth is determining the character, nature and production methods of synthetic chemicals essential for a sustainable society. Chemistry has a long-standing tradition of creating vital and high-performing products and processes; however, this progress has often been achieved with a limited focus on function, overlooking harmful side effects [7]. Currently the chemical sector operates on a linear model (Fig. 1, left), where finite, mostly fossil-based raw materials are processed through a production chain dependent on reagents that while designed to be highly reactive are frequently also unintentionally persistent and/or toxic. This poses risks for workers and can lead to accidental or intentional releases. Many of these processes generate waste (often toxic, persistent, and bioaccumulative), frequently exceeding the amount of the intended product, especially as product complexity increases (e.g., 5 to 50 times for specialty chemicals and 25 to 100 times for pharmaceuticals) [7]. Additionally, chemical products are typically designed with their intended use in mind, relying on external controls to minimize exposure to hazards that often remain unassessed, likely due to a historical lack of adequate tools and models, as evidenced by numerous unforeseen negative impacts. Given the essential functions provided by chemical industry products, the future question must focus on two objectives: (i) how to maintain and significantly enhance performance improvements, and (ii) how to minimize or eliminate the harmful impacts that jeopardize human and planetary sustainability. Addressing this question is a pressing scientific challenge [8,9]. Substantial progress in "green chemistry" and "green engineering" has demonstrated that chemical products and processes can achieve higher performance and functionality while reducing negative impacts. These achievements need to become systematic rather than isolated examples. To succeed, it is essential not only to change the conditions under which chemical products are made and used but also to redefine the chemical products and reagents themselves throughout the entire value chain from raw materials to application (Fig. 1). This requires redefining "performance" to include both function and sustainability, achievable only through the careful design of the intrinsic properties of molecules and their transformations [10].

Traditional approaches to chemical synthesis generally make use of stoichiometric reagents, hazardous solvents and energy-intensive processes under conditions where very substantial amounts of waste generation and environmental risks are produced. These traditional approaches prioritize efficiency and yield but too often overlook the sustainability of inputs and outputs. On the other hand, green chemical synthesis of the future seeks to surmount such limitations by applying the 12 Principles of Green Chemistry including the design of safer chemicals, atom economy, and reduction of energy use. Green synthesis techniques strive to employ renewable feedstocks, environmentally benign solvents (or no use of solvents at all) and catalytic reactions that would reduce waste and toxicity [1]. Besides, further development of techniques like microwave-assisted synthesis, mechanochemistry and biocatalysis holds out prospects for more efficiency with less environmental impact. In cases where industries are considering going green such replacement of traditional methods of synthesis with green synthesis methods marks one of the important steps toward the goal of making chemical manufacturing compatible with the general philosophy of environmental care and conservation. [Table 1.].

Tradiational Chemistry	**Green Chemistry**
Maximizing Chemical Output to Enhance Profitability.	Optimal Efficiency with Minimal Use of Harmless Materials
Lineer Process	Circular Process
Toxic and Hazardous Chemical Products	Bening Chemical Products
Strong Covalent Bonds	Weak Non-covalent Bonds
Waste Treatment	Waste Utilization
Resource-intensive separation and refinement	Autonomous Separation System
Toxic ad Non-eco-friendly Solvents	Rcyclable,inert eco-friendly solvents
Fossil Raw Materials	Renewable Raw Materials
Large Waste Volume	Minimal Waste Volume
Design Solely for Application Relying on Situational Management	Planned Molecule Design for Full Life Cycle

Table 1. Comparison of Traditional and Green Chemical Sector

One of the principles of green chemistry is the use of safer solvents and auxiliaries, or their complete elimination whenever possible. In recent years, methods for conducting organic syntheses without solvents have been developed and optimized [11].

1. 2. Green Synthesis of Chalcones

The trans-chalcone family, also known as (E)-1,3-diaryl-2-propenone, is a significant subgroup of flavonoids. Chalcones consist of two aromatic rings connected by a three-carbon α,β-unsaturated carbonyl system (Figure 1). These compounds are well-recognized for their wide range of biological and pharmaceutical properties including antiviral, antimalarial, anxiolytic, antioxidant, anticancer, anti-inflammatory, anti-diabetic and anti-mitotic effects [12–18]. Additionally, chalcones serve as key intermediates in the synthesis of various heterocyclic compounds like pyrazolines, flavones, flavanones, flavonols, aurones and more [19-23]. These versatile applications have heightened interest in developing environmentally friendly synthesis methods. Multiple research groups have worked on creating diverse approaches for synthesizing chalcones [24].

The first synthesis of chalcones was achieved by the German chemist Charles Rainer (Carl Rainer) in 1869. He used a simple condensation reaction between an aldehyde and an acetophenone, which is now known as the Claisen-Schmidt condensation. This method forms the basis for the classical synthesis of chalcones and remains widely used today [Fig.2.].

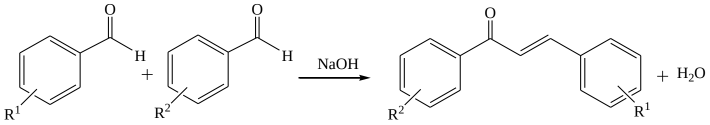


Fig. 2. General Synthesis Method of Chalcones

Chalcones are a group of compounds that have been extensively studied by scientists particularly due to their widespread applications in the healthcare field. For this purpose, green synthesis methods have been developed as alternatives to the Claisen-Schmidt reaction. One of these is a green mechanochemical approach performed by Ma and his team which involves the simple grinding of solid reactants (or a combination of solid and liquid) [25]. In this method, equivalent amounts of the relevant methyl ketones and various aldehydes are mixed in a porcelain mortar, eliminating the need for solvents and utilizing solid sodium hydroxide. After 3 to 5 minutes of grinding, a yellow-colored solid mass is obtained, identified as the desired chalcone. The grinding process is continued for an additional 5 to 10 minutes. The subsequent purification of the crude products is carried out through crystallization from appropriate solvents following their separation by Buchner filtration and washing with cold water [26].

1.2.1. Solvent-Free Methods

One of the principles of green chemistry is the use of safer solvents and auxiliaries or their elimination altogether whenever possible. In recent years, methods have been developed and optimized for conducting organic syntheses without solvents [27].

Synthetic reactions are typically performed in a solvent medium, but this leads to several issues, such as volatile organic compounds (VOCs), solvent loss in effluents, the need to recover and recycle solvents and product contamination. Additionally, multiple reaction steps may require different solvents.[28]. Green chemistry promotes solvent-free or "neat" reaction systems, encouraging synthetic organic chemists to shift towards this approach. The ideal scenario involves conducting reactions in molten states, dry grinding or solid-supported reactions using materials like clay and zeolites. These methods often require nontraditional activation methods like microwaves, ultrasound or visible light. There’s also a need for new separation and purification techniques that don't rely on solvents, presenting innovative challenges for chemists and chemical engineers

The well-established Claisen-Schmidt reaction method has conventionally been one of the most applied methods in the synthesis of chalcone structures due to their wide pharmacological benefits. In recent years, the process has involved including solvent-free and mechanochemical techniques in an effort to fit into the 12 Principles of Green Chemistry. These combinations greatly reduce the ecological footprint compared to traditional methods based on solvents. This approach aims to create more sustainable processes with minimal use of hazardous reagents and at the same time achieving a lower environmental impact [29].

Chemists have developed green synthesis methods for many compound groups. Chalcones are a group of compounds with particularly important applications in the field of health. Today, the use of green synthesis methods developed for the synthesis of these significant compounds has a great importance. In this study, it has been examined the three important green synthesis methods mentioned below.

Grinding or Mechanochemical Synthesis: This method involves grinding the reactants together in the absence of solvents, promoting a solid-state reaction. It has been recognized since the late 1800s that specific chemical compounds react differently when exposed to heat and mechanical energy. Mechanochemistry was subsequently established as a separate discipline within chemistry, thanks to the contributions of Carey Lea. In 1891, Ostwald introduced the term "mechanochemistry" to describe this related area of physical chemistry. Therefore, mechanochemistry should be considered alongside other associated fields such as thermochemistry, electrochemistry, photochemistry, sonochemistry, chemistry under high pressure, shock waves or microwave effects [30].

When organic molecules are subjected to mechanical energy (such as milling or grinding), two surfaces slide against each other, creating a frictional force. The kinetic energy of the contacting materials is transformed into their internal energy through these non-conservative frictional forces. In some instances, friction and other mechanical actions can lead to thermodynamically metastable states by increasing enthalpy. This rise affects both the kinetics of the mechanically activated molecules and their equilibrium state. Consequently, this effect is analogous to the mixing of liquids [31].

One of the mechanochemical methods for chalcone synthesis is high-speed ball milling. This method involves the mechanical milling of reactants at high speeds to synthesize chalcones without the use of solvents [Fig. 3.].

$$\mathrm{RCOCH_2} + \mathrm{R'CHO} \xrightarrow[\text{Grinding}]{\text{NaOH}} \mathrm{RCOCH{=}CHR'}$$

Fig. 3. Mechonochemical Synthesis of Chalcones

Microwave-Assisted Synthesis: In synthetic chemistry, 1986 marked a significant milestone for the adoption of microwave devices. Since then, numerous laboratory-scale syntheses using microwaves have been conducted. This approach frequently leads to a substantial decrease in reaction times while maintaining similar product yields compared to traditional energy input methods. Additionally, microwaves can often minimize unwanted side reactions and eliminate the need for solvents. The use of microwave irradiation in the synthesis of chalcones was notably pioneered by *Richard Gedye* and his team in the mid-1980s. Richard Gedye is credited with one of the first reports on microwave-assisted organic synthesis. His work demonstrated how microwaves could accelerate chemical reactions, including the synthesis of chalcones, which are compounds formed by the Claisen-Schmidt condensation of an aromatic aldehyde and an aromatic ketone [29]. Utilizes microwave irradiation to heat the reaction mixture, significantly speeding up the reaction and improving yields. The microwave-assisted synthesis of chalcone derivatives has emerged as a preferred method due to its ability to provide uniform heating and yield high product quantities within shorter reaction times. This microwave approach is particularly intriguing for a range of reactions, including cycloaddition, condensation, and coupling reactions, facilitating the production of diverse heterocyclic compounds [32].

The unique features of microwave radiation (short reaction times, higher product purity and yield) have recently attracted interest from chemical scientists. It represents an interesting complementary choice to allow a more convenient access for the synthesis of some organic molecules and it is far simpler in terms of operational procedures, reaction conditions between other criteria. Such methods when used for synthesis in open vessels were accompanied with a solvent-free approach by Varma [33]. Considering these results, simple and effective strategies can be defined for the preparation of chalcones under solvent-free microwave irradiation conditions.These advantages make the microwave synthesis quite attractive to prepare chalcones or indeed other organic compounds [Fig. 4.].

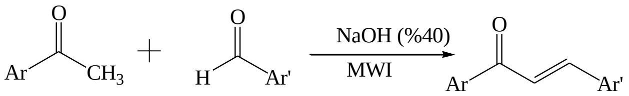


Fig.4. Ultasonic Synthesis of Chalcones

Ultrasound-Assisted Synthesis: Ultrasound is a highly effective and relatively harmless method used in synthetic chemistry for many years, with varying levels of success. This high-energy input not only amplifies mechanical effects in heterogeneous reactions but can also trigger new chemical transformations, resulting in the formation of novel compounds. What sets sonochemistry apart is the phenomenon of cavitation, a process that has become a key focus of research due to its intriguing and promising findings [34]. Employs ultrasonic waves to enhance reaction rates and improve product yields, often in solvent-free conditions. Ultrasound synthesis is a powerful and increasingly utilized technique for accelerating organic reactions, recognized as a green synthetic approach. Ultrasonication offers advantages over conventional methods, including higher yields, shorter reaction times, greater selectivity, and minimal side reactions. It has been effectively applied to synthesize various organic frameworks, from simple carbocyclic compounds to complex biologically active heterocyclic structures. The technique has proven environmentally friendly and effective, especially for synthesizing 5-7 membered heterocyclic rings containing one to three heteroatoms. Additionally, it provides excellent yields under mild conditions without requiring complex purification processes [35]. Despite all these methods, the use of solvents may be necessary under certain conditions. In such cases, green chemists prefer to use environmentally friendly solvents like water or ethanol, either alone or in combination, to reduce toxicity and environmental impact.

These methods highlight the move toward more sustainable practices in the synthesis of chalcones, emphasizing efficiency and reduced environmental impact.

2. Conclusions

Green synthesis of chalcone represents one step forward compared with classical methodologies by employing principles of green chemistry. The use of environmentally benign catalysis-or the condition free from solvent or renewable solvents-reduces the environmental impact and generation of hazardous wastes to a minimum. Enhanced reaction efficiency, reduction in energy consumption and the use of nontoxic reagents add to the overall sustainability of the process. It therefore follows that green chalcone syntheses not only provide a workable route for large-scale production but also set a standard against which future development in sustainable organic chemistry will need to be measured. Thus, it has to do with the future dealing with optimization of methods and finding their application in several other synthetic pathways so that the impact and applicability may broaden.

3. References

Bhagwat, G., Gray, K., Wilson, S. P., Muniyasamy, S., Vincent, S. G. T., Bush, R., & Palanisami, T. (2020). Benchmarking bioplastics: A natural step towards a sustainable future. Journal of Polymers and the Environment, 28, 3055-3075.

Döhler, N., Wellenreuther, C., & Wolf, A. (2022). Market dynamics of biodegradable bio-based plastics: Projections and linkages to European policies. *EFB Bioeconomy Journal*, *2*, 100028.

Anastas, P. T., & Zimmerman, J. B. (2003). Peer reviewed: design through the 12 principles of green engineering.

Keijer, T., Bakker, V., & Slootweg, J. C. (2019). Circular chemistry to enable a circular economy. *Nature chemistry*, *11*(3), 190-195.

Robertson, J. C., Coote, M. L., & Bissember, A. C. (2019). Synthetic applications of light, electricity, mechanical force and flow. *Nature Reviews Chemistry*, *3*(5), 290-304.

Cannavacciuolo, C., Pagliari, S., Frigerio, J., Giustra, C. M., Labra, M., & Campone, L. (2022). Natural deep eutectic solvents (NADESs) combined with sustainable extraction techniques: a review of the green chemistry approach in food analysis. *Foods*, *12*(1), 56.

Sheldon, R. A. (2017). The E factor 25 years on: the rise of green chemistry and sustainability. *Green Chemistry*, *19*(1), 18-43.

Anastas, P. T., & Warner, J. C. (2000). *Green chemistry: theory and practice*. Oxford university press.

Erythropel, H. C., Zimmerman, J. B., de Winter, T. M., Petitjean, L., Melnikov, F., Lam, C. H., ... & Anastas, P. T. (2018). The Green ChemisTREE: 20 years after taking root with the 12 principles. *Green chemistry*, *20*(9), 1929-1961.

Zimmerman, J. B., Anastas, P. T., Erythropel, H. C., & Leitner, W. (2020). Designing for a green chemistry future. *Science*, *367*(6476), 397-400.

Tanaka, K., & Toda, F. J. C. R. (2000). Solvent-free organic synthesis. *Chemical Reviews*, *100*(3), 1025-1074.

Li, Z., Zhao, H., Han, H., Liu, Y., Song, J., Guo, W., ... & Sun, Z. (2017). Graphene-supported ZnO nanoparticles: An efficient heterogeneous catalyst for the Claisen-Schmidt condensation reaction without additional base. *Tetrahedron Letters*, *58*(42), 3984-3988.

Domínguez, J. N., León, C., Rodrigues, J., Gamboa de Domínguez, N., Gut, J., & Rosenthal, P. J. (2005). Synthesis and evaluation of new antimalarial phenylurenyl chalcone derivatives. *Journal of Medicinal Chemistry*, *48*(10), 3654-3658.M.

Marder and A. C. Paladini, “GABA(A)-Receptor Ligands of Flavonoid Structure,” Current Topics inMedicinal Chemistry 2, no. 8 (2002): 853–67.

Orallo, F. (2008). Trans-resveratrol: a magical elixir of eternal youth?. *Current medicinal chemistry*, *15*(19), 1887-1898.

Modzelewska, A., Pettit, C., Achanta, G., Davidson, N. E., Huang, P., & Khan, S. R. (2006). Anticancer activities of novel chalcone and bis-chalcone derivatives. *Bioorganic & medicinal chemistry*, *14*(10), 3491-3495.

Kunimasa, K., Kuranuki, S., Matsuura, N., Iwasaki, N., Ikeda, M., Ito, A., ... & Oikawa, T. (2009). Identification of nobiletin, a polymethoxyflavonoid, as an enhancer of adiponectin secretion. *Bioorganic & Medicinal Chemistry Letters*, *19*(7), 2062-2064.

Kawai, M., Hirano, T., Arimitsu, J., Higa, S., Kuwahara, Y., Hagihara, K.,& Tanaka, T. (2009). Effect of enzymatically modified isoquercitrin, a flavonoid, onsymptoms of Japanese cedar pollinosis: a randomized double-blind placebo-controlled trial. *International archives of allergy and immunology*, *149*(4), 359-368.

Reddy, G. V., Maitraie, D., Narsaiah, B., Rambabu, Y., & Rao, P. S. (2001). Microwave assisted Knoevenagel condensation: a facile method for the synthesis of chalcones. *Synthetic Communications*, *31*(18), 2881-2884.

Lakshmi Kantam, M., Veda Prakash, B., & Venkat Reddy, C. (2005). Efficient synthesis of chalcones by a solid base catalyst. *Synthetic communications*, *35*(14), 1971-1978.

Drexler, M. T., & Amiridis, M. D. (2003). The effect of solvents on the heterogeneous synthesis of flavanone over MgO. *Journal of Catalysis*, *214*(1), 136-145.

Choudary, B. M., Ranganath, K. V. S., Yadav, J., & Kantam, M. L. (2005). Synthesis of flavanones using nanocrystalline MgO. *Tetrahedron Letters*, *46*(8), 1369-1371.

Kumar, S., Lamba, M. S., & Makrandi, J. K. (2008). An efficient green procedure for the synthesis of chalcones using C-200 as solid support under grinding conditions. *Green Chemistry Letters and Reviews*, *1*(2), 123-125.

Tanpure, S., Ghanwat, V., Shinde, B., Tanpure, K., & Lawande, S. (2022). The eggshell waste transformed green and efficient synthesis of K-Ca (OH) 2 catalyst for room temperature synthesis of chalcones. *Polycyclic Aromatic Compounds*, *42*(4), 1322-1340.

Ma, W., Liu, Y., Yu, N., & Yan, K. (2021). Solvent-free mechanochemical diaza-Cope rearrangement. *ACS Sustainable Chemistry & Engineering*, *9*(48), 16092-16102.

Friščić, T., Mottillo, C., & Titi, H. M. (2020). Mechanochemistry for synthesis. *Angewandte Chemie*, *132*(3), 1030-1041.

Neelam, V. D., & Neelam, A. K. N. (2023). Solvent-free Mechanochemical synthesis of organic compounds. *Journal of Pharma Insights and Research*, *1*(2), 007-014.

Ma, X., Lim, G. K., Harris, K. D., Apperley, D. C., Horton, P. N., Hursthouse, M. B., & James, S. L. (2012). Efficient, scalable, and solvent-free mechanochemical synthesis of the OLED material Alq3 (q= 8-Hydroxyquinolinate). *Crystal growth & design*, *12*(12), 5869-5872.

Gedye, R. N., Smith, F. E., & Westaway, K. C. (1988). The rapid synthesis of organic compounds in microwave ovens. *Canadian Journal of Chemistry*, *66*(1), 17-26.

Muñoz-Batista, M. J., Rodriguez-Padron, D., Puente-Santiago, A. R., & Luque, R. (2018). Mechanochemistry: toward sustainable design of advanced nanomaterials for electrochemical energy storage and catalytic applications.

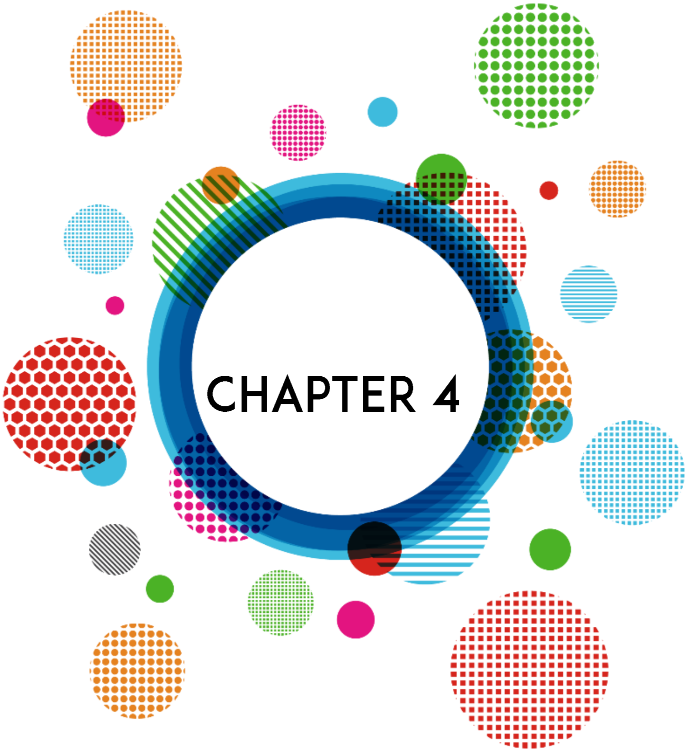
Beyer, M. K., & Clausen-Schaumann, H. (2005). Mechanochemistry: the mechanical activation of covalent bonds. *Chemical reviews*, *105*(8), 2921-2948.

Hosseinzadeh, Z., Razzaghi-Asl, N., Ramazani, A., & Aghahosseini, H. (2020). Synthesis, cytotoxic assessment, and molecular docking studies of2, 6-diaryl-substituted pyridine and 3, 4-dihydropyrimidine-2 (1H)-one scaffolds. *Turkish Journal of Chemistry*, *44*(1), 194-213.

Varma, R. S. (1999). Solvent-free organic syntheses on mineral supports using microwave irradiation. *Clean Products and Processes*, *1*(2), 132-147.

Doble, M., Rollins, K., & Kumar, A. (2010). *Green chemistry and engineering*. Academic Press.

Shabir, G., Shafique, I., & Saeed, A. (2022). Ultrasound assisted synthesis of 5–7 membered heterocyclic rings in organic molecules. *Journal of Heterocyclic Chemistry*, *59*(10), 1669-1702.



CHAPTER 4

On Some Biperiodic Leonardo Numbers

Sule Curuk[1] & Serpil Halici[2]

---

[1] Dr., Pamukkale University, Science Faculty, Turkey, ORCID: 0000-0002-4514-6156
[2] Prof. Dr., Pamukkale University, Science Faculty, Turkey,
ORCID: 0000-0002-8071-0437

1. Introduction

For the natural numbers $n \geq 2$ and non-zero real numbers a, b biperiodic Fibonacci numbers are defined by the following relation

$$q_n = \begin{cases} a\, q_{n-1} + q_{n-2}\,, & n \text{ is even} \\ b q_{n-1} + q_{n-2}\,, & n \text{ is odd} \end{cases} \tag{1}$$

The initial conditions are $q_0 = 0\,, q_1 = 1$ and when $a = b = 1$, this sequence reduces to the classical Fibonacci sequence. The nth term of this sequence, $\lfloor n \rfloor$ where n is the floor function of n, is

$$q_n = \frac{a^{1-\delta(n)}}{(ab)^{\lfloor \frac{n}{2} \rfloor}} \left(\frac{{g_1}^n - {g_2}^n}{g_1 - g_2} \right), \tag{2}$$

where $\delta(n)$ is the parity function. The values g_1 , g_2 in the last formula are determined with the help of the formula below [10].

$$g_1 = \frac{ab - \sqrt{a^2 + b^2 + 4ab}}{2} \text{ and } g_2 = \frac{ab - \sqrt{a^2 + b^2 + 4ab}}{2}. \tag{3}$$

In [4], the biperiodic Lucas number sequence with initial conditions $\ell_0 = 2\,, \ell_1 = a$ is defined as

$$\ell_n = \begin{cases} b\ell_{n-1} + \ell_{n-2}\,, & n \text{ even} \\ a\ell_{n-1} + \ell_{n-2}, & n \text{ odd} \end{cases} . \tag{4}$$

In the case $a = b = 1$, in the last formula above, this sequence is reduced to the well known Lucas sequence $\{\ell_n\}_{n \geq 0}$.

$$\ell_n = \frac{a^{\delta(n)}}{(ab)^{\lfloor \frac{n+1}{2} \rfloor}} \left({g_1}^n + {g_2}^n \right). \tag{5}$$

We can give some equations exist between the roots of in the relation (3) and the coefficients a, b. And these numbers will be used throughout the study as follows.

$$g_1 - g_2 = \sqrt{a^2 b^2 + 4ab}. \tag{6}$$

$$g_1 + g_2 = ab. \tag{7}$$

$$g_1 g_2 = -ab. \tag{8}$$

$$(g_1+1)(g_2+1)=1. \tag{9}$$

$${g_1}^2+{g_2}^2=ab(ab+2). \tag{10}$$

$$g_1(g_2+1)=-g_2,\quad g_2(g_1+1)=-g_1. \tag{11}$$

2. Leonardo, Biperiodic Leonardo Numbers and Some Related Identities

Leonardo numbers are defined by

$$Le_n=Le_{n-1}+Le_{n-2}+1,\ n\geq 2 \tag{12}$$

with the initial values $Le_0=Le_1=1$ [9]. In 2012, Kocer discussed Leonardo numbers and their relationship with Fibonacci numbers [2]. In 2019, Catarino and Borges studied Leonardo numbers [5]. The same authors defined and studied incomplete Leonardo numbers in 2020 [6]. In 2021, Soykan discussed generalized Leonardo numbers. In 2021, Alp and Koçer defined Hybrid Leoonardo numbers and discussed some of their properties [1]. In 2021, Kürüz and others discussed Leonardo Pisano Hybrinomials [17]. In 2022, Karakus and his colleagues defined Hyper dual Leonardo numbers [14]. In 2022, Karatas defined complex Leonardo numbers and gave the Binet formula of these numbers [15]. In 2022, Shattuck gave combinatory identities by considering generalized Leonardo numbers [21]. In 2023, Tascı defined and examined Gaussian Leonardo numbers [26]. In 2023, Tan and his colleagues defined Leonardo p-numbers [25]. In 2024, Ozimamoglu discussed q Leonardo hybrid numbers [19]. Kuhapatanakul and Ruankong investigated genelizated p-Leonardo numbers [16]. Halici and Curuk obtained some important identities of these numbers using Pascal type triangles for Leonardo numbers [13].

For any natural number n and nonzero real numbers a,b we define the biperiodic Leonardo numbers $\mathcal{L}e_n$ as follows.

$$\mathcal{L}e_n=\begin{cases} b\,\mathcal{L}e_{n-1}+\mathcal{L}e_{n-2}+b\ ,\ n\ is\ even \\ a\mathcal{L}e_{n-1}+\mathcal{L}e_{n-2}+a\ ,\ n\ is\ odd\end{cases} \tag{13}$$

Here, $\mathcal{L}e_0=1\ ,\mathcal{L}e_1=2a-1$ are the initial values. Moreover, we can arrange this definition for numbers $n\geq 4$ as follows.

$$\mathcal{L}e_n=(ab+2)\mathcal{L}e_{n-2}-\mathcal{L}e_{n-4}+ab. \tag{14}$$

Some terms of the sequence are given below to be used throughout the study.

$$\{\mathcal{L}e_n\}_{n\geq 0} = \{1, 2a-1, 2ab+1, 2a^2b+4a-1, \cdots\}. \quad (15)$$

For $n \geq 2$ and different from each other real numbers a, b, a different definition for these numbers is given by Catarino and Spreafico in 2024 as follows [7].

$$GLe_n = \begin{cases} a\,GLe_{n-1} + GLe_{n-2} + a\ , n \text{ is even} \\ bGLe_{n-1} + GLe_{n-2} + b\ , n \text{ is odd} \end{cases}$$

where, $GLe_0 = 2a - 1\ , GLe_1 = 2ab - 1.$

In the table below, we have listed some biperiodic sequences named according to their initial values.

n	0	1	2	3	4	5	$\cdots$
q_n	0	1	a	$ab+1$	a^2b+2a	$a^2b^2+3ab+1$	$\cdots$
ℓ_n	2	a	$ab+2$	a^2b+3a	a^2b^2+4ab+	$a^3b^2+5a^2b$ +5a	$\cdots$
j_n	0	1	a	$ab+2$	a^2b+4a	$a^2b^2+6ab+4$	$\cdots$
c_n	2	a	$ab+4$	a^2b+6a	a^2b^2+8ab+	$a^3b^2 10a^2b+20$	$\cdots$
P_n	0	1	$2a$	$4ab+1$	$8a^2b+4a$	$16a^2b^2+12ab+$	$\cdots$
θ_n	2	$2a$	$4ab+$	$8a^2b+6a$	$16a^2b^2+16a$	$32a^3b^2+40a^2b$	$\cdots$
$\mathcal{L}e_n$	1	$2a-$	$12ab+$	$2a^2b+4a$	$2a^2b^2+6ab+$	$2a^3b^2+8a^2b+6$	$\cdots$

Table 1. Some special biperiodic numbers

The following some relationships between Leonardo, Fibonacci and Lucas numbers are

- $Le_n = 2F_{n+1} - 1.$
- $Le_n = F_n + L_{n-1}.$
- $Le_n = L_{n+2} - F_{n+2} - 1.$
- $Le_{n+1} = Le_n + 2F_n.$

For non zero real numbers a and b and for every natural number n, the biperiodic Fibonacci and Lucas numbers can be written, respectively

$$q_{n+2} = \begin{cases} aq_{n+1} + q_n, & n \equiv 0(mod2) \\ bq_{n+1} + q_n, & n \equiv 1(mod2) \end{cases}$$

and

$$\ell_{n+2} = \begin{cases} b\ell_{n+1} + \ell_n, & n \equiv 0(mod2) \\ a\ell_{n+1} + \ell_n, & n \equiv 1(mod2). \end{cases}$$

Where $q_0 = 0,\ q_1 = 1$ and $\ell_0 = 2,\ \ell_1 = a$. In [23], Fibonacci and Lucas $p-$numbers are defined as follows, respectively.

$$F_p(n) = F_p(n-1) + F_p(n-p-1),$$

and

$$L_p(n) = L_p(n-1) + L_p(n-p-1).$$

In here,

$$F_p(0) = 0 \text{ and } F_p(1) = F_p(2) = \cdots = F_p(p) = 1$$

and

$$L_p(0) = p + 1 \text{ and } L_p(1) = L_p(2) = \cdots = L_p(p) = 1.$$

In [24], Leonardo $p-$numbers, $Le_p(n)$ are defined as follows.

$$Le_p(n) = Le_p(n-1) + Le_p(n-p-1) + p, \quad n > p$$

$$Le_p(0) = Le_p(1) = Le_p(2) = \cdots = Le_p(p) = 1.$$

When $p = 1$, this sequence reduces to classical Leonardo numbers. In 2018, Yazlık and others defined and investigated the Fibonacci and Lucas

p numbers [27]. For $a, b \epsilon \mathbb{R}^+$ and $p \epsilon \mathbb{Z}^+$, biperiodic Fibonacci and Lucas p −sequences are defined as follows, respectively.

$$f_n = \begin{cases} af_{n-1} + f_{n-p-1}, n \equiv 0(mod\ 2) \\ bf_{n-1} + f_{n-p-1}, n \equiv 1(mod\ 2) \end{cases}$$

and

$$\ell_n = \begin{cases} b\ell_{n-1} + \ell_{n-p-1}, n \equiv 0(mod 2) \\ a\ell_{n-1} + \ell_{n-p-1}, n \equiv 1(mod 2) \end{cases}.$$

When $n \geq p + 1$, the initial values for f_n and ℓ_n are follows:

$$f_0 = 0, f_1 = 1, f_2 = a, \dots , f_p = a^{\lfloor \frac{p}{2} \rfloor} b^{\lfloor \frac{p-1}{2} \rfloor}$$

and

$$\ell_0 = p + 1, \ell_1 = a, \ell_2 = ab, \dots , \ell_p = a^{\lfloor \frac{p+1}{2} \rfloor} b^{\lfloor \frac{p}{2} \rfloor}.$$

Notice that these sequences defined above reduce to the classical Fibonacci and Lucas sequences, respectively, for $p = a = b = 1$.

$$f_n = f_{n-1} + f_{n-2},\ \ f_0 = 1, f_1 = 1,$$

$$\ell_n = \ell_{n-1} + \ell_{n-2},\ \ \ell_0 = 2, f_1 = 1.$$

In [13], in their study, the authors defined biperiodic Leonardo numbers. These numbers are given by the following recurrence relation, with $\mathcal{L}e_0 = 1, \mathcal{L}e_1 = 2a - 1$,

$$\mathcal{L}e_n = \begin{cases} b\mathcal{L}e_{n-1} + \mathcal{L}e_{n-2} + b, & n \equiv 0(mod\ 2) \\ a\mathcal{L}e_{n-1} + \mathcal{L}e_{n-2} + a, & n \equiv 1(mod\ 2) \end{cases}.$$

In this study, we will consider some different biperiodic Leonardo numbers, make definitions and examine the properties of the series.

Definition 1. For $a, b \in \mathbb{R}^{+}$ and $p \in \mathbb{Z}^{+},$ we define biperiyodik Leonardo p- sequence $\{\ell e_n\}_{n=0}^{\infty}$ with $\ell e_0 = 1$,$\ell e_1 = 2a - 1$, as follows.

$$\ell e_n = \begin{cases} b\ \ell e_{n-1} + \ell e_{n-p-1} + b, & n \equiv 0 (mod\ 2) \\ a\ \ell e_{n-1} + \ell e_{n-p-1} + a, & n \equiv 1 (mod\ 2) \end{cases}$$

$$\{\ell e_n\}_{n\geq 0} = \left\{1\ ,2a-1\ ,2ab+1\ , \dots , a^{\left\lfloor \frac{p}{2} \right\rfloor} b^{\left\lfloor \frac{p-1}{2} \right\rfloor}, \dots \right\}.$$

Diagrams can be given to more easily examine the relationships between the elements of the array. For the sequence$\{\ell e_n\}_{n\geq 0}$, we also give the following diagram.

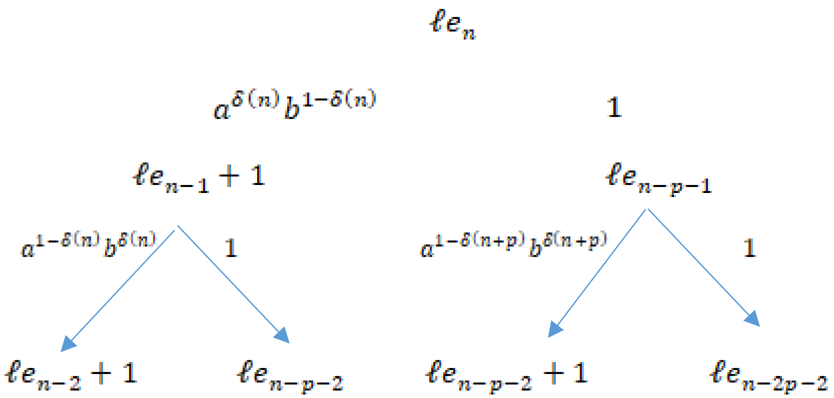


Figure 1. 3-diagram.

Theorem 1. For biperiyodik Leonardo p-sequence $\{\ell e_n\}_{n=0}^{\infty}$, we have

$$\ell e_n = \begin{cases} ab(\ell e_{n-2} + 2) + (a+b)\ell e_{n-p-2} + \ell e_{n-2p-2}, & p \equiv 0 (mod2) \\ ab(\ell e_{n-2} + 1) + 2\ell e_{n-p-1}, & p \equiv 1 (mod2) \end{cases}$$

Proof. Let's examine the definition of the above sequence according to whether p is odd or even:

$$\ell e_n = \begin{cases} b\,\ell e_{n-1} + \ell e_{n-p-1} + b, & n \equiv 0(mod\ 2) \\ a\,\ell e_{n-1} + \ell e_{n-p-1} + a, & n \equiv 1(mod\ 2) \end{cases}$$

Let p be odd. Then,

$$\ell e_n = a^{\delta(n)} b^{1-\delta(n)} \ell e_{n-1} + \ell e_{n-p-1} + a^{\delta(n)} b^{1-\delta(n)}$$

$$= ab\ell e_{n-2} + a^{\delta(n)} b^{1-\delta(n)} \ell e_{n-p-2} + ab + a^{\delta(n)} b^{1-\delta(n)} \ell e_{n-p-2} + \ell e_{n-2p-2} \\ + a^{\delta(n)} b^{1-\delta(n)} + a^{\delta(n)} b^{1-\delta(n)}$$

$$\ell e_n = ab\ell e_{n-2} + 2a^{\delta(n)} b^{1-\delta(n)} \ell e_{n-p-2} + \ell e_{n-2p-2} \\ + 2a^{\delta(n)} b^{1-\delta(n)} + ab$$

$$\ell e_n = ab\ell e_{n-2} + 2a^{\delta(n)} b^{1-\delta(n)} \left(\ell e_{n-p-2} + 1\right) + \ell e_{n-2p-2} \\ + ab$$

$$\ell e_n = ab\ell e_{n-2} + 2\ell e_{n-p-1} + ab$$

$$\ell e_n = ab(\ell e_{n-2}) + 2\ell e_{n-p-1}\,. \qquad (16)$$

Let p be even. Then,

$$\ell e_n = a^{\delta(n)} b^{1-\delta(n)} \ell e_{n-1} + \ell e_{n-p-1} + a^{\delta(n)} b^{1-\delta(n)}$$

$$= ab\ell e_{n-2} + a^{\delta(n)} b^{1-\delta(n)} \ell e_{n-p-2} + ab + a^{1-\delta(n)} b^{\delta(n)} \ell e_{n-p-2} + \ell e_{n-2p-2} \\ + a^{1-\delta(n)} b^{\delta(n)} + a^{\delta(n)} b^{1-\delta(n)}$$

$$= ab\ell e_{n-2} + \left(a^{\delta(n)} b^{1-\delta(n)} + a^{1-\delta(n)} b^{\delta(n)}\right)\ell e_{n-p-2} + \ell e_{n-2p-2} \\ + a^{1-\delta(n)} b^{\delta(n)} + a^{\delta(n)} b^{1-\delta(n)} + ab$$

$$\ell e_n = ab\ell e_{n-2} + (a+b)\ell e_{n-p-2} + \ell e_{n-2p-2} + 2ab$$

$$\ell e_n = ab(\ell e_{n-2} + 2) + (a+b)\ell e_{n-p-2} + \ell e_{n-2p-2}\,. \qquad (17)$$

From the equlities (16) ve (17) we get

$$\ell e_n \\ = \begin{cases} ab(\ell e_{n-2} + 2) + (a+b)\ell e_{n-p-2} + \ell e_{n-2p-2}, & p \equiv 0(mod2) \\ ab(\ell e_{n-2} + 1) + 2\ell e_{n-p-1}, & p \equiv 1(mod2). \end{cases}$$

Thus, the proof is completed.

We can define biperiodic p Leonardo polynomials as follows.

Definition 2. Biperiyodik p Leonardo polynomials are

$\ell e_p(x) = x^{2p+2} - abx^{2p} + 2ab - (a+b)x^p - 1, p$ is even

$\ell e_p(x) = x^{2p+2} - abx^{2p} - ab - 2x^{p+1}, p$ is odd .

If we take $x^2 = r$, then

$$\ell e_{p(r)} = \begin{cases} r^{p+1} - abr^p - (a+b)r^{\frac{p}{2}} - 2ab - 1, & p \equiv 0(mod2) \\ r^{p+1} - abr^p - 2r^{\frac{p+1}{2}} - ab, & p \equiv 1(mod2). \end{cases}$$

If p is odd, then

$$\ell e_p(x) = (x^{p+1} - 1)^2 - ab(x^{2p} + 1) - 1$$

and

$$\ell e_p'(x) = 2(x^{p+1} - 1)(p+1)x^p - 2pabx^{2p-1}$$

$$\ell e_p(x) = 0 \Leftrightarrow (x^{p+1} - 1)^2 - ab(x^{2p} + 1) - 1 = 0$$

$$ab = \frac{x^{p+1}(x^{p+1} - 2)}{x^{2p} + 1}$$

$$\ell e_p'(x) = 0 \Leftrightarrow 2(x^{p+1} - 1)(p+1)x^p - 2pabx^{2p-1} = 0$$

$$ab = \frac{(x^{p+1} - 1)(p+1)x^p}{px^{2p-1}}$$

$$ab = \frac{(p+1)x}{p} \cdot \frac{x^{p+1} - 1}{x^p}$$

$$x = \frac{p\sqrt{ab}}{p+1}.$$

In 2022, in their work, Ait-Amrane and Belbachir gave the definition of bi-periodic r-Fibonacci r-Lucas sequences [3].

$$U_n^{(r)} = \begin{cases} aU_{n-1}^{(r)} + cU_{n-r-1}^{(r)}, & n \equiv 0(mod2) \\ bU_{n-1}^{(r)} + dU_{n-r-1}^{(r)}, & n \equiv 1(mod2) \end{cases}.$$

Where $n \geq r+1$ and $U_0^{(r)} = 0, U_1^{(r)} = 1, U_2^{(r)} = a, \ldots, U_r^{(r)} = a^{\left\lfloor \frac{r}{2} \right\rfloor} b^{\left\lfloor \frac{r-1}{2} \right\rfloor}$.

Using this last definition, the definition of the biperiodic r- Leonardo series can be given.

Definition 3. We define Biperiyodik $r -$ Leonardo sequence $Le_n^{(r)}$ as follows.

$$Le_n^{(r)} = \begin{cases} bLe_{n-1}^{(r)} + dLe_{n-r-1}^{(r)} + b, & n \equiv 0(mod2) \\ aLe_{n-1}^{(r)} + cLe_{n-r-1}^{(r)} + a, & n \equiv 1(mod2) \end{cases}$$

with $Le_0^{(r)} = 1, Le_1^{(r)} = 2a - 1.$

Depending on the case of the number r , the following Theorem can be given for the sequence $Le_n^{(r)}$.

Theorem 2. For the sequence $Le_n^{(r)}$, we have

$$abLe_{n-2}^{(r)} + a^{\delta(n)} b^{1-\delta(n)} (c+d) Le_{n-r-2}^{(r)} \\ + c^{2\delta(n)} d^{2-2\delta(n)} Le_{n-2r-2}^{(r)} + a^{\delta(n)} b^{1-\delta(n)}, r\ odd$$

and

$$Le_n^{(r)} = abLe_{n-2}^{(r)} + (ad+bc)Le_{n-r-2}^{(r)} + cdLe_{n-2r-2}^{(r)} + \\ a^{\delta(n)} b^{1-\delta(n)}, \ \ r\ even$$

.

Proof.

$$Le_n^{(r)} = a^{\delta(n)} b^{1-\delta(n)} Le_{n-1}^{(r)} + c^{\delta(n)} d^{1-\delta(n)} Le_{n-r-1}^{(r)} + a^{\delta(n)} b^{1-\delta(n)}$$

$$Le_n^{(r)} = abLe_{n-2}^{(r)} + \left(a^{\delta(n)}b^{1-\delta(n)}c^{1-\delta(n)}d^{\delta(n)} + c^{\delta(n)}d^{1-\delta(n)}a^{1-\delta(n+r)}b^{\delta(n+r)}\right)Le_{n-r-2}^{(r)}$$

$$+c^{\delta(n)+1-\delta(n+r)}d^{1-\delta(n)+\delta(n+r)} + Le_{n-2r-2}^{(r)} + a^{\delta(n)}b^{1-\delta(n)}$$

From the equality $\delta(n+r) = \delta(n) + \delta(r) - 2\delta(n)\delta(r)$, in the case of r odd, $Le_n^{(r)}$ is equal to this: $Le_n^{(r)} = A + B$ where

$$A = abLe_{n-2}^{(r)} + \left(a^{\delta(n)}b^{1-\delta(n)}c^{1-\delta(n)}d^{\delta(n)} + c^{\delta(n)}d^{1-\delta(n)}a^{\delta(n)}b^{1-\delta(n)}\right)Le_{n-r-2}^{(r)}$$

$$B = c^{2\delta(n)}d^{2-2\delta(n)}Le_{n-2r-2}^{(r)} + a^{\delta(n)}b^{1-\delta(n)}.$$

If we take the necessary actions then

$$Le_n^{(r)} = abLe_{n-2}^{(r)} + a^{\delta(n)}b^{1-\delta(n)}(c+d)Le_{n-r-2}^{(r)}$$
$$+c^{2\delta(n)}d^{2-2\delta(n)}Le_{n-2r-2}^{(r)} + a^{\delta(n)}b^{1-\delta(n)}.$$

When r even, $Le_n^{(r)}$ is equal to this: $Le_n^{(r)} = C + D$ where C and D are respectively.

$$C = abLe_{n-2}^{(r)} + (a^{\delta(n)}b^{1-\delta(n)}c^{1-\delta(n)}d^{\delta(n)}$$

and

$$D = c^{\delta(n)}d^{1-\delta(n)}a^{\delta(n)}b^{1-\delta(n)})Le_{n-r-2}^{(r)} + cdLe_{n-2r-2}^{(r)} + a^{\delta(n)}b^{1-\delta(n)}.$$

Making some calculations, we get

$$Le_n^{(r)} = abLe_{n-2}^{(r)} + (ad+bc)Le_{n-r-2}^{(r)} + cdLe_{n-2r-2}^{(r)} + a^{\delta(n)}b^{1-\delta(n)}.$$

Thus, the proof is completed.

Theorem 3. The generating function for biperiodic r-Leonardo sequences is as follows.

$$G(x) = \frac{x + bx^2 + (-1)^{\delta(r)} dx^{r+2}}{1 - abx^2 - (b^{\delta(r+1)}c + a^{\delta(r+1)}d)x^{r+1+\delta(r+1)} - (-1)dcx^{2r+2}}.$$

Proof. Let's write the following equation using the generating function definition.

So, $G(x)$ is follows.

$$\frac{\sum_{k=0}^{2r+1} le_k^{(r)} x^k - abx^2 \sum_{k=0}^{2r-1} le_k^{(r)} x^k - (b^{\delta(r+1)}c + a^{\delta(r+1)}d)x^{r+1+d(r+1)} \sum_{k=0}^{r-\delta(r+1} le_k^{(r)} x^k}{1 - abx^2 - (b^{\delta(r+1)}c + a^{\delta(r+1)}d)x^{r+1+\delta(r+1)} - (-1)cdx^{2r+2}}.$$

In here, when r is odd we get

$$G(x) = \sum_{k=0} le_k^{(r)} x^k$$

$$abx^2 G(x) = -ab \sum_{k=0} le_k^{(r)} x^{k+2}$$

$$(c+d)x^{r+1} G(x) = dc \sum_{k=0} le_k^{(r)} x^{k+r+1}$$

$$(dc)x^{2r+2} G(x) = dc \sum_{k=0} le_k^{(r)} x^{k+2r+2}$$

If these statements are collected side by side, then

$$(1 - abx^2 - (cd)x^{r+1} + dcx^{2r++2})G(x) = E + F.$$

Where E and F are follows:

$$E = le_0^{(r)} + le_1^{(r)} x + \cdots + le_{2r+1}^{(r)} x^{2r+1} - able_0^{(r)} x^2 - able_1^{(r)} x^3 - \cdots - able_{2r-1}^{(r)} x^{2r+1}$$

and

$$F = -(c+d)le_1^{(r)} x^{r+1} - (c+d)le_1^{(r)} x^{r+2} \ldots - (c+d)le_r^{(r)} x^{2r+1}$$

respectively.

$$E+F=\sum_{k=0}^{2r+1} le_k^{(r)} x^k - abx^2 \sum_{K=0}^{2r-1} le_k^{(r)} x^k$$

$$-(c+d)x^{r+1} \sum_{k=0}^{r} le_k^{(r)} x^k$$

Thus, we get

$$G(x)=\frac{x+bx^2-dx^{r+2}}{1-abx^2-(c+d)x^{r+1}+cdx^{2r+2}}$$

When r is even number, then

$$G(x)=\frac{x+bx^2+dx^{r+2}}{1-abx^2-(bc+ad)x^{r+2}-dcx^{2r+2}}$$

Thus, the proof is completed.

In particular, if $r = 1$ it reduces to the biperiodic Leonardo generating function.

Conclusion. In this study, we examined the sequence called Leonardo sequence, which has been frequently studied recently. Then, we defined and examined the biperiodic nature of this We defined two new and different sequences by taking advantage of the properties of this new sequences and gave the important identities and generating functions provided by the elements of these.

REFERENCES

[1] Alp, Y., Kocer, E. G. **(2021).** Hybrid Leonardo numbers. *Chaos, Solitons & Fractals*, *150*, 111128.

[2] Alp, Y., Kocer, E. G. **(2021).** "Some properties of Leonardo numbers", *Konuralp Journal of Mathematics*, 9(1), 183-189.

[3] Aıt-amrane, N. R., Belbachir, H. **(2022).** Bi-periodic r -Fibonacci sequence and bi-periodic r-Lucas sequence of type s. *Hacettepe Journal of Mathematics and Statistics*, *51*(3), 680-699.

[4] Bilgici, G. **(2014).** Two generalizations of Lucas sequence. *Applied Mathematics and Computation*, *245*, 526-538.

[5] Catarino, P. M., Borges, A. **(2019).** On Leonardo numbers. *Acta Mathematica Universitatis Comenianae*, *89*(1), 75-86,

[6] Catarino, P. M. M. C., & Borges, A. **(2020).** A note on Incomplete Leonardo Numbers. *Integers: Electronic Journal of Combinatorial Number Theory*, *20*.

[7] Catarino, P. M. M. C., & Spreafico, E. **(2024).** A Note on Bi-Periodic Leonardo Sequence. *Armenian Journal of Mathematics*, *16*(5), 1-17.

[8] Coskun, A., Taskara, N. **(2016).** The matrix sequence in terms of bi-periodic Fibonacci numbers. *Communications Faculty of Sciences University of Ankara Series A1 Mathematics and Statistics*, *68*(2), 1939-1949.

[9] Dijkstra, E. W. **(1981)**. Archive: Fibonacci numbers and Leonardo numbers.(EWD 797).

[10] Edson, M., Yayenie, O. **(2009).** A new generalization of Fibonacci sequence & extended Binet's formula.

[11] Halici, S. **(2018)**. On bicomplex Fibonacci numbers and their generalization. In *Models and Theories in Social Systems* (pp. 509-524). Cham: Springer International Publishing.

[12] Halici, S., Curuk, S. **(2019)**. On dual bicomplex numbers and their some algebraic properties. *Journal of Science and Arts*, *19*(2), 387-398.

[13] Halici, S., Curuk, S**. (2024).** On the Leonardo Sequence via Pascal-Type Triangles. *Journal of Mathematics*, 2024, 2024.1: 9352986.,

[14] Karakus, S. O., Nurkan, S. K., & Turan, M. **(2022).** Hyper-dual Leonardo numbers. *Konuralp Journal of Mathematics*, *10*(2), 269-275.

[15] Karatas, A. **(2022).** On complex Leonardo numbers. *Notes on Number Theory and Discrete Mathematics*, *28*(3), 458-465.

[16] Kuhapatanakul, K., Ruankong, P. **(2024).** On generalized Leonardo p-numbers. *Journal of Integer Sequences*, *27*(2), 3.

[17] Kuruz, F., Dagdeviren, A., Catarino, P. **(2021).** On Leonardo Pisano Hybrinomials. *Mathematics*, *9*(22), 2923.

[18] Nurkan, S. K., & Güven, İ. A**. (2023).** Ordered Leonardo quadruple numbers. *Symmetry*, *15*(1), 149.

[19] Ozimamoglu, H. **(2024).** A new generalization of Leonardo hybrid numbers with q-integers. *Indian Journal of Pure and Applied Mathematics*, *55*(1), 325-334.

[20] Shannon, A. G. **(2019).** A note on generalized Leonardo numbers. *Notes on Number Theory and Discrete Mathematics*, *25*(3), 97-101.

[21] Shattuck, M. **(2022).** Combinatorial proofs of identities for the generalized Leonardo numbers. *Notes Number Theory Discrete Math*, *28,* 778-790,

[22] Soykan, Y. **(2021).** Generalized Leonardo numbers. *Journal of Progressive Research in Mathematics*, *18*(4), 58-84.

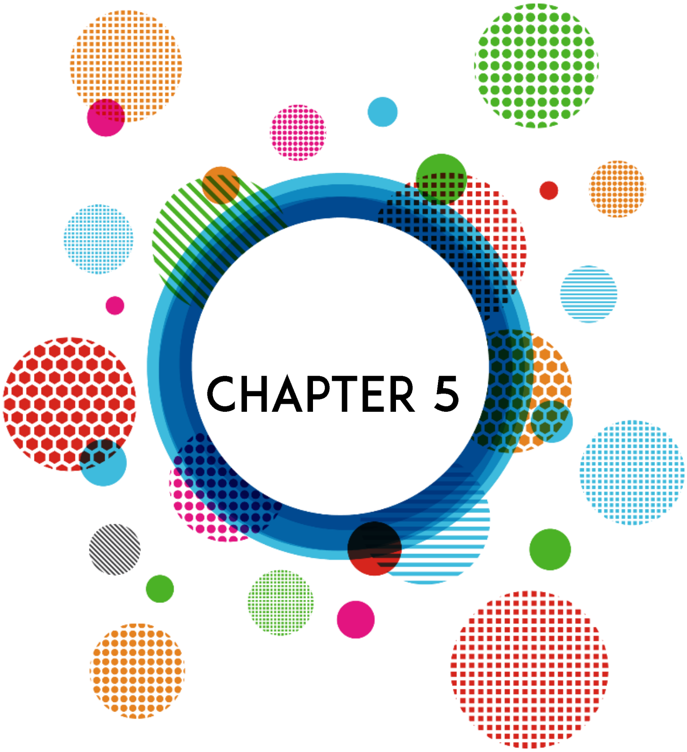
[23] Stakhov, A., Rozin, B. (2006). Theory of Binet formulas for Fibonacci and Lucas p-numbers. *Chaos, Solitons & Fractals*, *27*(5), 1162-1177.

[24] Tan, E., & Leung, H. H. **(2023).** On Leonardo p-numbers. *Integers: Electronic Journal of Combinatorial Number Theory*, *23*.

[25] Tan, E., Savin, D., & Yılmaz, S. (**2023).** A New Class of Leonardo Hybrid Numbers and Some Remarks on Leonardo Quaternions over Finite Fields. *Mathematics*, *11*(22), 4701.

[26] Tascı, D. **(2023).** On Gaussian Leonardo numbers. *Contrib. Math*, *7*, 34-40.

[27] Yazlik, Y., Köme, C., Madhusudanan, V. **(2018).** A new generalization of Fibonacci and Lucas p-numbers. *Journal of computational analysis and applications*, *25*(4), 657-669.



CHAPTER 5

Theoretical Investigation of Organobromine Compound Extracted Isolated From Algae in Gaseous and Solvent Environments: RMSD, NLO and NBO Analyses

Seçil Eren[1] *& Cem Cüneyt Ersanlı*[2]

---

[1] Sinop University, Institute of Graduate Studies, Department of Physics, Sinop/Turkey ORCID: 0009-0004-5109-290X

[2] Prof. Dr. Sinop University, Faculty of Arts and Science, Department of Physics, Sinop/Turkey, ORCID: 0000-0002-8113-5091

1. Introduction

The term algae is Latin and a plural of the term used for sea grasses. Algae are photoautotroph organisms with wide distributional range capable of inhabiting fresh water, salt and brackish water bodies and plants and animals, moist and illuminated caves, even the surface of snow. Algae can be unicellular or multicellular. Algae, as characterized by the presence of chlorophyll, are members of the group Thallophyta. Algae are divided into five broad categories according to the type of pigments found in them:

1. Blue-green algae (*Cyanophyta*): These are prokaryotic in cell structure and blue-green in color because of the blue pigments along with chlorophyll. They also possess some red pigment at times. They occur in fresh as well as sea Water.

2. Green algae (*Chlorophyta*): They are the most abundant group among the algae. Although they normally live in fresh water, they also live on moist rocks and tree trunks. They have eukaryotic cell structure and chloroplast and nucleus. They are greenish to yellowish green in color.

3. Diatoms (*Bacillariophyta*): These are relatively widespread in fresh water and marine environments and are usually golden yellow-brown colored. The cells are usually rectangular, triangular, round or oval in shape.

4. Red algae (*Rhodophyta*): They are usually found in saltwater and live in deeper water than other alga groups. They can be readily distinguished as being red-colored and branched.

5. Brown algae (*Ochrophyta*): They are widely distributed across cold as well as shallow waters. They grow by attaching to the base in the tidal zone and consist of a huge number of species (Akkayan, 1987).

Algae form the base of the food web as primary producers of aquatic ecosystems (Cirik & Cirik, 2011). The classification of algae is categorized into two major classes: Prokaryotic algae include only blue-green algae (*Cyanophyta*), while eukaryotic algae are explained under various classes like *Chlorophyta*, *Charophyta*, *Euglenozoa*, Bacillariophyta, *Cryptophyta*, *Haptophyta*, *Miozoa*, *Ochrophyta* and *Rhodophyta* (Guiry & Guiry, 2015). Apart from energy products such as biodiesel, biogas and bioethanol, foodstuffs, nutritional additives, raw materials for medicinals, animal feed ingredients, cosmetics and fertilizers come from algae. Apart from this, algae also possess remarkable potential especially in the discovery of new pharmaceuticals compounds by virtue of their high biological activity secondary metabolites (Gümüş, 2006; Cirik & Cirik, 2011).

The fact that they reduce the concentration of carbon dioxide in the environment and emit oxygen through photosynthesis has made algae an essential element for aquatic animals (Zeybek, et al., 2003). Due to that reason, blue-green algae growth in drinking and irrigation water, dams, rivers and recreation areas must be followed up with regular samples. There are several extensive scientific studies on the algal flora composition, distribution dynamics and interaction with environmental parameters of aquatic systems published in the literature (For example, Çelik & Ongun 2007; Tezel Ersanlı & Hasırcı, 2013; Tezel Ersanlı & Gönülol, 2014; Hasırcı Mustak & Tezel Ersanlı, 2015; Deniz & Tezel Ersanli, 2016a; Tezel Ersanlı & Hasırcı Mustak, 2017; Tezel Ersanlı & Öztürk, 2017; Yılmaz et al, 2018; Deniz & Tezel Ersanli, 2020a; Deniz & Tezel Ersanli, 2020b; Solak et al., 2020; Aswathy et al., 2021; Deniz & Tezel Ersanli, 2021a; Deniz & Tezel Ersanli, 2021b; Deniz & Tezel Ersanli, 2022). Nutritionally, algae are defined by the high content of fibre, minerals, proteins, minimal fat and easily metabolizable carbohydrates. For example, *Ulva* species are used in the form of dietary supplements due to their low caloric content, while in other countries they are used as antihelminthics in goitre and kidney diseases treatment. *Ulva lactuca*, which is widely used in South America, has goitre resistance-inducing activity as a result of its vitamin A content (Serrano et al., 1998). Algae also play important roles in bioremediation research in recent years. For example, *Spirogyra* sp. and *Rhizoclonium* sp. have been screened as bioadsorbents in the removal of synthetic dye contamination in water (Deniz & Tezel Ersanli, 2016b). Similarly, natural assemblages of macroalgae such as *Chaetomorpha* sp., *Polysiphonia* sp., *Ulva* sp. and *Cystoseira* sp. have also been investigated for their biosorptive potential (Sari & Tuzen, 2008; Li et al., 2015; Deniz & Tezel Ersanli, 2018a; Deniz & Tezel Ersanli, 2018b).

Laurencia (*Rhodophyta*) is a red algal genus that occurs on rocky surfaces of warm water intertidal regions (Masudai et al., 1996). There are 421 species described within this genus as per the databases of algae, but only 146 species are valid in the taxonomic context (Guiry & Guiry, 2015). *Laurencia* is a genus that possesses the capacity for biosynthesis of a wide variety of secondary metabolites that are marked by their unusual molecular structures (Suzuki et al., 2009). Such metabolites, especially rich in polyhalogenated terpenoid skeletons, are involved in the defense mechanism of the species (Kurata et al., 1998) and possess various biological activities such as antifeedant, anthelmintic, antimalarial, antifouling, antimicrobial and cytotoxic (Davyt et al., 2001; Paul et al., 2011). 8-Bromo-3,7,7-trimethyl-11-methylene-spiro[5.5]undec-1-en-3,9-diol, (**I**), is a new rigidol isomer, which has been isolated for the first time from Laurencia rigida species (Suescun et al., 2001).

Understanding the electronic character of the organic compounds is very beneficial for their chemical reactivity and potential applications. Especially in areas such as pharmaceutical chemistry, materials science and environmental chemistry, aspects such as rearrangability, electron donating/accepting ability and electrophilic/nucleophilic character of a compound directly affect its functionality (Parr & Pearson, 1983; Chattaraj et al., 2003). Root Mean Square Deviation (RMSD), root mean square difference, refers to a statistical measure used in scientific investigations to measure the deviation between two structures or data sets. It is widely used in areas such as computational chemistry, molecular modeling, bioinformatics and crystallography. Density functional theory (DFT) has widely been used in computation of electronic structure of molecules over the past few years. Following the DFT method, it is possible to obtain the energy levels of the HOMO and LUMO and determine global reactivity parameters such as ionisation energy (IE), electron affinity (EA), chemical hardness (η), chemical softness (S), chemical potential (μ), electronegativity (χ) and electrophilic index (ω) of a molecule (Parr et al., 1999). Nonlinear optical (NLO) materials are used to enable sophisticated optoelectronic functions such as laser technology, telecommunications and information processing (Chemla & Zyss, 1987). Organic molecules have been thoroughly studied for NLO applications due to the fact that they are light weight, processable and have high NLO response (Prasad & Williams, 1991). An understanding of molecular architecture and electronic properties of chemical bonds is one of the major goals of theoretical and computational chemistry. In this context, the NBO method is an effective analysis method that provides a natural chemical picture of the electron distribution and bond topology in molecular systems. In contrast with conventional molecular orbital theories, the NBO approach enables the interpretation of chemical bonds as it provides a more localized and Lewis-structured picture (Weinhold & Landis, 2005). NBO method is a post-processing technique that may be integrated into more advanced quantum chemistry calculations such as Hartree-Fock (HF), DFT and Møller-Plesset. With the aid of this method, bond donor (BD), anti-bond (BD*) as well as lone pair (LP) and Rydberg orbitals of the molecule may be identified and interatomic electron transitions, delocalisations and stabilisation energies may be estimated numerically (Reed et al., 1988).

Particularly, the second-order perturbation theory derived interaction energies [E(2)] explain electron transfer contributions towards bond stabilization and include valuable information in terms of molecular reactivity (Glendening et al., 2013). Structural features such as conjugation, hyperconjugation, lone pair interactions and resonance may be clarified with precision by virtue of NBO analyses. This provides major advantages in both basic research and applied fields such as drug design, materials science and molecular electronics (Weinhold, 2012).

In the context of this research, the molecular formula C15H23BrO2 (**I**) (Suescun et al., 2001) was calculated with the Gaussian 03 package (Frisch et al., 2004; Dennington et al, 2007) at the B3LYP/6-311G(d,p) level in the gas phase (ε=1) and in three solvents {chloroform (ε=4.8), methanol (ε=32.7) and dimethylsulfoxide [DMSO] (ε=46.7)} with different poly-ratios, and RMSD (root mean square difference of square root) values and global chemical parameters were derived. In addition, bromine (Br) bearing compound $C_{15}H_{23}BrO_2$ with π-conjugated system was also studied by DFT calculations in gas and solvent phases and NLO potential was evaluated. Finally, NBO study of the compound in the gas phase was conducted by the same method.

2. Material and Method

2.1. Theoretical Calculation Method

In order to determine the quantum chemical properties of the compound $C_{15}H_{23}BrO_2$ (Suescun et al., 2001) (Figure 1), B3LYP/6-311G(d,p) DFT was utilized with Gaussian software. B3LYP is a hybrid function derived from combining Becke’s three-parameter exchange function and Lee-Yang-Parr correlation function and has been used successfully widely in energy level and structural optimisation in organic compounds (Becke, 1993; Lee et al., 1988).

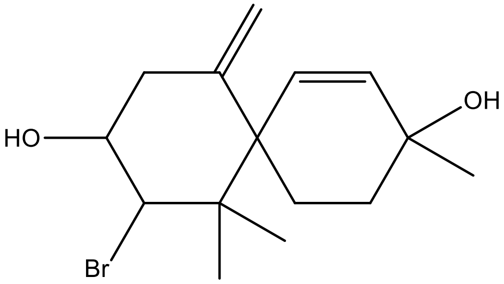


Figure 1. Chemical Diagram of (**I**) Molecule (Suescun et al., 2001).

2.2. Theoretical Approach

RMSD is the square root of the mean squared displacement of the positions of the corresponding atoms in two structures. In mathematical terms, RMSD is given by:

$$\mathrm{RMSD} = \sqrt{\frac{1}{\mathrm{N}}\sum_{\mathrm{i}=1}^{\mathrm{N}}\left(\mathrm{r}_{\mathrm{i}}^{\mathrm{model}} - \mathrm{r}_{\mathrm{i}}^{\mathrm{ref}}\right)^2} \qquad (1)$$

Where N is the number of atoms for comparison, $\mathrm{r}_{\mathrm{i}}^{\mathrm{model}}$ is the atom coordinates of the model structure and $\mathrm{r}_{\mathrm{i}}^{\mathrm{ref}}$ is the atom coordinates of the reference structure. RMSD can be explained as shown in Table 1.

Table 1. Concordance Level of Molecular Structures According to RMSD Values.

RMSD (Å)	Comment
< 0.5	Very good alignment
0.5–1.0	Good alignment
1.0–2.0	Acceptable, structural differences may exist
> 2.0	Structures differ significantly or alignment is poor

RMSD is a useful tool for comparing theoretical and experimental measurements and is particularly used in structural validations after geometry optimisation. RMSD is widely used in crystal and theoretical structure comparison, molecular docking and molecular dynamics simulations. In docking experiments, for example, if the RMSD value is below 2 Å, the binding site is likely to be considered successful.

2.3. Calculation of Global Chemical Parameters

After optimisation, HOMO and LUMO energy levels were employed to compute the global reactivity parameters using the equations outlined in Table 2 below (Parr & Pearson, 1983; Pearson, 1997).

Table 2. Quantum Chemical Global Reactivity Indicators and Related Equation Definitions.

Parameter	**Calculation Formula**
IE	$-E_{HOMO}$
EA	$-E_{LUMO}$
ΔE	$E_{LUMO} - E_{HOMO}$
χ	$(E_{HOMO} + E_{LUMO}) / 2$
μ	$-\chi$
η	$(E_{LUMO} - E_{HOMO}) / 2$
S	$1 / (2\eta)$
ω	$\mu^2 / (2\eta)$

With the help of these parameters, the reactivity of the compound, electron acceptor/donor activity and solvent environment effect were evaluated.

2.4. Energy Values (HF) and NLO Analysis

NLO parameters calculated to assess the applicability of molecules for use in optoelectronics supply valuable information regarding the polar nature and electron distribution of the molecule. In the current research work, solvent effects have been simulated for chloroform, methanol and DMSO solvents using Polarizable Continuum Model (PCM) according to data obtained by calculation at the B3LYP/6-311G(d,p) theoretical level according to Gaussian software for compound (**I**) and NLO calculations were performed for gas phase and solvent phases according to the help of data in the log file (Frisch et al., 2004). In addition, energy values for gas phase (ε=1) and solvent phases {chloroform (ε=4.8), methanol (ε=32.7) and dimethylsulfoxide [DMSO] (ε=46.7)} were retrieved from the log file. The calculated quantum chemical parameters are: dipole moment (μ), average polarisability ($\bar{\alpha}$) and total hyperpolarisability (β_{total}), average hyperpolarisability ($\langle\beta\rangle$).

Dipole Moment (μ)

The dipole moment is a measure of charge separation in the molecule and is composed of three components: μ_x, μ_y and μ_z. The total dipole moment (μ_{total}) can be obtained as:

$$\mu_{total} = \sqrt{\left(\mu_x^2 + \mu_y^2 + \mu_z^2\right)} \qquad 2$$

Mean (Isotropic) Polarisability ($\bar{\alpha}$)

Polarisability is a measure of the ease with which a molecule can be deformed in an electric field. Polarisability components along the principal axes are αxx, αyy and αzz. The mean polarisability is:

$$\bar{\alpha} = (\alpha_{xx} + \alpha_{yy} + \alpha_{zz})/3 \qquad 3$$

Total (vectorial) Hyperpolarisability

Total hyperpolarisability components: β_x, β_y and β_z. The total hyperpolarisability is:

$$\beta_{total} = \sqrt{(\beta_x^2 + \beta_y^2 + \beta_z^2)} \qquad 4$$

Here in terms of tensor components;

$$\begin{aligned} \beta_x &= \beta_{xxx} + \beta_{xyy} + \beta_{xzz} \\ \beta_y &= \beta_{yyy} + \beta_{yxx} + \beta_{yzz} \\ \beta_z &= \beta_{zzz} + \beta_{zxx} + \beta_{zyy} \end{aligned} \qquad 5$$

Mean (scalar) hyperpolarisability ($\langle\beta\rangle$)

$$\langle\beta\rangle = \frac{1}{5}\left[(\beta_{xxx} + \beta_{xyy} + \beta_{xzz}) + (\beta_{yyy} + \beta_{yxx} + \beta_{yzz}) + (\beta_{zzz} + \beta_{zxx} + \beta_{zyy})\right] \qquad 6$$

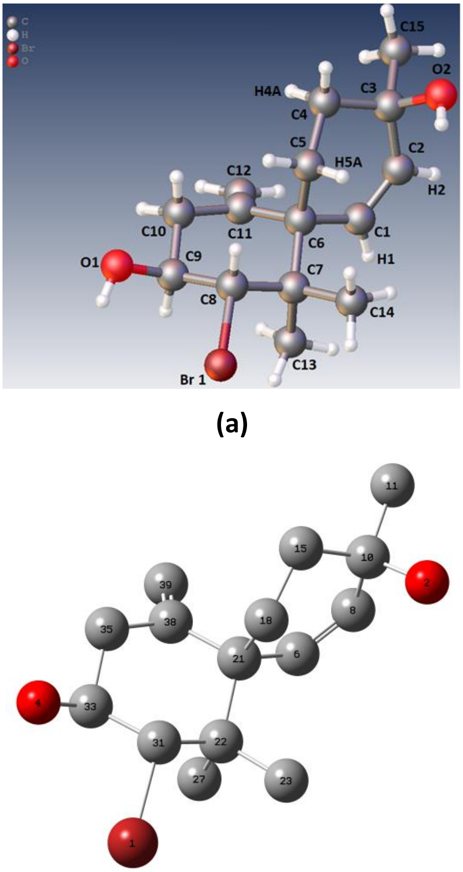
The above equation takes into account the symmetric contribution of all the Cartesian components.

2.5. NBO Analysis

To study the electronic structure of the compound, NBO analysis using the Gaussian 03 program at the B3LYP/6-311G(d,p) level provided important results in determining the bond characters and electron delocalisations in the molecule (Frisch et al., 2004; Glendening et al., 2013).

3. Findings and Discussion

Suescun et al. 2001 performed the crystallographic analysis of the molecule from the alga. Figure 2 depicts the Olex2-1.5 (Dolomanov et al., 2009) view of compound (I) (Suescun et al., 2001).



(a)

(b)

Figure 2. (a) The Olex (Dolomanov et al., 2009) Diagram of (I) Molecule (Suescun et al., 2001), **(b)** Optimised Structure View (Hydrogen Atoms are Omitted for Clarity) (Dennington et al., 2007).

3.1. RMSD

Figure 3 juxtaposes the RMSD values of the optimised geometries in three solvent environments (chloroform, methanol and DMSO) as well as the gas phase for compound (I) in relation to the reference structure. The RMSD value is the average squared deviation of atoms in the coordinate plane and plays an important role in the determination of the geometric stability of the molecular structure in relation to the environment. Calculations revealed that the compound had the lowest RMSD value (2.12 × 10-9 Å) in the gas phase. This indicates that the molecule is in a more ideal shape in the gaseous state where there are no solvent interactions and has the least deviation by way of geometry. When the effect of solvent environments was analyzed, RMSD values were higher in chloroform

(2.48 × 10-9 Å), methanol (2.57 × 10-9 Å) and DMSO (2.91 × 10-9 Å) solvents, respectively. This rise is directly proportional to the polarity of solvents and shows that especially high polarity solvents such as DMSO cause more effective conformational changes in the molecular structure. Hydrogen bonding and dipole-dipole interactions of the polar solvents with the functional groups such as hydroxyl groups affect the overall molecular shape and increase the deviations. These results indicate that the solvent effect has a significant impact on not only the energies but also on the molecular structures and such an effect must be taken into account in structural characterisation studies.

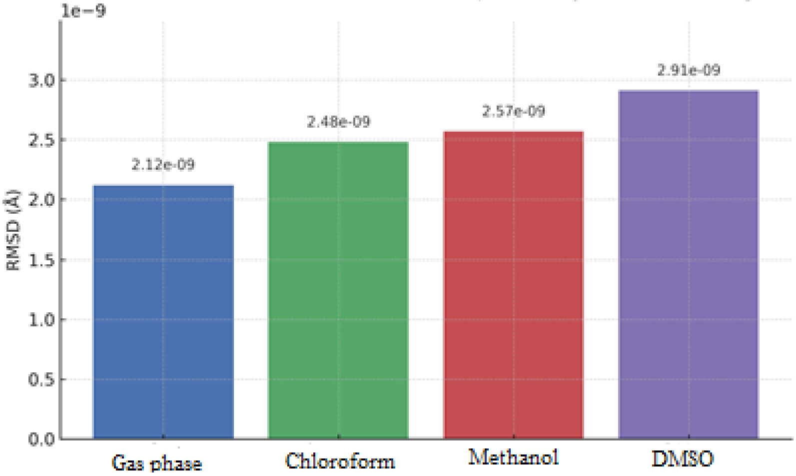


Figure 3. Variation of RMSD Values According to Gas Phase and Solvents.

3.2. Global Reactivity Parameters

Global reactivity parameters (Table 3) *IE*, *EA*, *ΔE*, χ from E_{HOMO} and E_{LUMO} energy values of compound (**I**) in gas phase and in three media of solvents [chloroform, methanol and DMSO] *IE*, *EA*, *ΔE*, χ, μ, η, *S* and ω were calculated from EHOMO and ELUMO energy values. These values provide important information on the electronic reactivity and behavior of the compound (Parr & Pearson, 1983). In the gas phase, the energy of E_{HOMO} was -7.1384 eV and E_{LUMO} energy -0.8441 eV. *ΔE* is thus maximum at 6.2943 eV, and this indicates that the compound is most stable and chemically less reactive when in the gas phase (Chattaraj et al., 2003). With the increase in dielectric constants of the solvent media, E_{HOMO} and E_{LUMO} energy levels move towards less negative values and the range of energy decreases. For instance, E_{HOMO} was -6.9487 eV and E_{LUMO} was -0.8253 eV in DMSO medium and ΔE value reached its lowest level with 6.1234 eV. This indicates that the molecule becomes more polarised and thus more reactive in the solvent system. The η is 3.1471 eV in the gaseous phase and the value of this falls in the solvents chloroform (3.0784 eV), methanol

(3.0626 eV) and DMSO (3.0617 eV), in order. That it falls indicates that the molecule softens and easily transfers electrons to the solvent effect. The *S* parameter also verifies this trend and the *S* value increases from 0.1589 to 0.1633 in solvents (Pearson, 1997). When the ω is obtained, the value of 2.5309 eV in the gas phase decreases marginally in solvents and goes down to 2.4674 eV in DMSO. This indicates that the electrophilic character of the compound decreases to a minor extent in solvent media, yet retains its electrophilicity as a whole. Consequently, high dielectric constant solvent conditions (notably DMSO and methanol) affect the electronic nature of the compound and increase the reactivity with lower energy range, increased softness and decreased electrophilicity to a certain extent. The findings suggest that the compound would be more active in polar solvents such as biological environmental conditions (Geerlings et al., 2003). These computations demonstrate once more how HOMO-LUMO data calculated from DFT computations is a useful tool for the assessment of global reactivity.

Table 3. Comparative Global Reactivity Parameters [B3LYP/6-311G(d,p)].

Parameter	**Gas phase (ε=1)**	**Chloroform (ε=4.8)**	**Methanol (ε=32.7)**	**DMSO (ε=46.7)**
E_{HOMO} (eV)	-7.1384	**–6.9841**	**–6.9506**	**–6.9487**
E_{LUMO} (eV)	-0.8441	**–0.8272**	**–0.8253**	**–0.8253**
IE (eV)	7.1384	**6.9841**	**6.9506**	**6.9487**
EA (eV)	0.8441	**0.8272**	**0.8253**	**0.8253**
ΔE (eV)	6.2943	6.1569	6.1253	6.1234
χ (eV)	3.9912	3.9057	3.8880	3.8870
μ (eV)	–3.9912	–3.9057	–3.8880	–3.8870
η (eV)	3.1471	3.0784	3.0626	3.0617
S (eV)$^{-1}$	0.1589	0.1624	0.1633	0.1633
ω (eV)	2.5309	2.4776	2.4678	2.4674

3.3. Hartree-Fock Energy Values and NLO Analysis

3.3.1. Hartree-Fock (HF) Energy Analysis

The HF total energy value is the ground-state electronic energy of a molecule and it has units of atomic units [a.u. or Hartree; 1 a.u. = 1 Hartree]. In the current study, the DFT computations at B3LYP/6-311G(d,p) were performed for compound (**I**) and Hartree-Fock energy values so obtained in the gas phase as well as in three of its precursors differing in polarity - chloroform, methanol and DMSO - were compared (Table 4). As is clear from these findings, the HF energy values obtained values are more negative with increased polarity of the solvent. Compared to the gas phase, even in low-polarity solvents such as chloroform, the changes in electron distribution stabilized the molecule. In high-polarity solvents such as methanol and DMSO, this reduction in energy is higher. Highest negative energy value was attained in DMSO (-3310.2091458 a.u.), indicating that the molecule was in the state of maximum stability in this solvent. This further suggests that solvent-molecule interactions are directly responsible for the overall energy balance within the system and electronic stability of the molecule increases with higher solvent polarity. Polar functional groups such as hydroxyl groups within the molecular structure are more in contact with polar solvents, decreasing the energy of the system and thus more stable structures are obtained. Therefore, especially in biological applications or solvent-sensitive biological systems, the dielectric nature of the medium plays an extremely crucial role from the perspective of molecu-lar stability (Cramer, 2013; Tomasi et al., 2005).

Table 4. Hartree-Fock Energy Values (a.u.).

Medium	Hartree-Fock Energy
Gas phase	-3310.2005116
Chloroform	-3310.2066095
Methanol	-3310.2090043
DMSO	-3310.2091458

3.3.2. Analysis of Dipole Moment (μ) Values

The dipole moment measures the asymmetry of electron distribution in a molecule quantitatively and represents the electrical polarity of the molecule. It is usually expressed in units of Debye, (D), and directly affects most of the physicochemical properties of the molecule such as chemical reactivity, solubility, biological interaction and intermolecular interactions (Cramer, 2013). DFT calculations at the level of B3LYP/6-311G(d,p) were performed for compound (**I**) and the dipole moment components of the molecule were investigated both in gas phase and in three solvents having different polarities (chloroform, methanol and DMSO) (Table 5). From the obtained data, it is evident that the total dipole moment value of the molecule changes with the change in the dielectric constant of the medium. The dipole moment, which is 1.6110420 D in the gaseous state, raised to 1.8722165 D in a moderately polar solvent such as chloroform, and 1.9711465 and 1.9776878 D in more polar solvents, methanol and DMSO, respectively. This increase indicates that the electric effects of polar solvents on the molecule become stronger and redistribute the electron density of the molecule in an even more asymmetric manner. Primarily polar functional groups such as hydroxyl (-OH) group increase the polarity of the molecule by the process of hydrogen bonding with solvent molecules (Tomasi et al., 2005). Increasing the dipole moment increases the solubility of the molecule in polar solvents such as water and increases interaction of the molecule with cell membranes in biological systems. The compound of interest in this regard exhibits features suitable for examination in biological applications.

Table 5. Dipole Moment Values (D).

Medium	**μ_x (a.u.)**	**μ_y (a.u.)**	**μ_z (a.u.)**	**Dipole Moment (D)**
Gas phase	-0.1893091	0.1409502	0.5882458	1.6110420
Chloroform	-0.2233163	0.1589564	0.6836773	1.8722165
Methanol	-0.2291522	0.1605677	0.7232650	1.9711465
DMSO	-0.2293740	0.1605308	0.7256203	1.9776878

Note: 1 atomic units (a.u.) = 2.541765 Debye, (D)

3.3.3. Polarisability

Polarizability (α) refers to the ability of a molecule to deform under an external electric field. The characteristic is very significant especially in intermolecular interactions and linear and nonlinear optical properties (Cramer, 2013). From Table 6, it is observed that with rising dielectric constant of the solvent, the components and average polarizability rise significantly. Even though the mean α value is close to 27.99 $Å^3$ when in the gas phase, it increases significantly in polar solvents to an estimate of 37.97 $Å^3$ when in DMSO. This suggests that polar solvents facilitate the electron distribution of the molecule to be more flexible and its polarizability to increase (Tomasi et al., 2005). In particular, hydrogen-bonding solvents (such as DMSO and methanol) increase the sensitivity of the molecule to external electric fields, hence increasing the factors of polarizability. Such an increase improves the functionality of the compound for linear and nonlinear optical applications. The higher the values of polarizability, the greater the corresponding high light-matter interaction and enhanced NLO response (Prasad & Williams, 1991). In addition, the increase in polarizability values is caused by the scattering of the molecular electronic cloud as a result of the solvent effect.

Table 6. Components and Average Values of Polarizability.

Medium	**α_{xx} (a.u.)**	**α_{yy} (a.u.)**	**α_{zz} (a.u.)**	**$\bar{\alpha}$ (Å^3)**
Gas phase (ε=1)	236.1053581	174.6213206	155.8030199	27.9865671
Chloroform (ε=4.8)	285.5292954	218.5325883	196.3937041	34.6025060
Methanol (ε=32.7)	305.1468523	240.4472216	218.9575788	37.7688516
DMSO (ε=46.7)	306.3146110	241.8506333	220.4560083	37.9698899

Note: 1 a.u. of polarizability = 0.1482×10^{-24} cm^3 or 1 a.u. = 0.1482 Å^3

3.3.4. Hyperpolarizability

Hyperpolarizability (***β***) is utilized to describe the nonlinear response of a molecule towards external electric fields and is a fundamental parameter reflecting the NLO properties of the molecule. Hyperpolarizable molecules are important in technologies such as electro-optic modulation, second harmonic generation, and frequency mixing (Prasad & Williams, 1991). Hyperpolarizability values derived from calculations performed by the Gaussian package of software at the B3LYP/6-311G(d,p) level are tabulated below in Table 7.

Table 7. Hyperpolarizability Components, Total and Average Hyperpolarizability Values **(**$\times 10^{-30}$ **esu).**

Medium	**β_x**	**β_y**	**β_z**	**β_{total}**	**$\langle\beta\rangle$**
Gas phase (ε=1)	0.65853	-0.07250	1.03283	1.22705	0.32377
Chloroform (ε=4.8)	1.80230	-0.42473	1.65391	2.48276	0.60630
Methanol (ε=32.7)	2.38254	-0.54211	1.91696	3.10566	0.75148
DMSO (ε=46.7)	2.41789	-0.54874	1.93230	3.14342	0.76029

Note: 1 a.u. of hiperpolarizabilite (β)=8.6393×10^{-33} electrostatic unit (esu)

As computed, both β_{total} and $\langle\beta\rangle$values of the molecule are significantly larger as the dielectric constant of the solvent medium is increased. While the total hyperpolarizability value in the gas phase is 1.22705×10^{-30} esu, it is 3.14342×10^{-30} esu in DMSO. This increase is attributed to the solvent polarity's ability to polarize the electron cloud of the molecule more readily (Tomasi et al., 2005). β_z is the most significant hyperpolarizability component.

It shows that the molecule is more responsive to electric fields along the *z*-axis direction and that this axis is dominant in nonlinear optical processes. This could be because the electronic structure and spatial symmetry of the molecule are allowing polarization in the *z*-direction (Frisch et al., 2004). The results show that the nonlinear optical activity of the molecule is enhanced in the solvent medium and that it is able to exhibit enhanced performance in NLO applications, especially in solvents with high dielectric constants.

3.3.5. NLO Analysis

Hyperpolarizability represents the second-order NLO responses of molecules and is usually connected with applications such as Second Harmonic Generation (SHG). In the case of compound (**I**), the total hyperpolarizability β_{total} was calculated to be 1.23×10^{-30} esu in the gas phase and 3.14×10^{-30} esu in DMSO. The significant increase obviously shows that the nonlinear optical responses are enhanced by polar solvents. For comparison purposes, the literature hyperpolarizability value for urea, a reference NLO molecule that is widely used, is approximately 0.3728×10^{-30} esu (Prasad & Williams, 1991). In this context, compound (**I**)’s βtotal value in DMSO is approximately 8.4 times larger than that of urea. This ratio indicates that compound (**I**) is a very good prospect for NLO applications.

3.4. NBO Analysis

Within the context of the quantum chemical investigation carried out on the compound under investigation (**I**), the geometric optimization was achieved at the B3LYP/6-311G(d,p) level using the DFT method in order to have an understanding of the electronic nature of the structure. The calculations were executed using the Gaussian 03 program package. Following the structure optimization, NBO analysis was achieved to provide a detailed investigation of the inherent bonding and electron distribution of the molecule. This analysis gave comprehensive details regarding the stability of the molecule, delocalization extent, and electronic structure by interpreting the covalent bond orbital occupancies, orbital energy levels, and second-order perturbation energies [E(2)]. According to the obtained NBO results tabulated in Table 8, bonds such as Br1–C8, O1–C9, O2–C3, C1–C2, C3–C15, C6–C7, and C10–C11 possess high occupancy values ranging from about 1.97 to 1.99. These values reveal that these bonds are extremely localized and possess classical covalent bond character. Examining the bond energy levels, it is apparent that especially the O–C and Br–C bonds possess lower (more negative) orbital energies. This indicates that these bonds exhibit high electron density and form highly stable structures. These polar covalent bonds within the molecule, particularly induced by the electronegative heteroatoms oxygen and bromine, affect the electron distribution as a whole, which in turn directly influences the reactivity and chemical properties of the molecule.

Table 8. Selected Covalent Bond Orbitals and Their Properties.

No	NBO (Donor)	Occupancy	Energy (a.u.)
1	BD(1) Br1–C8	1.97802	-0.58033
2	BD(1) O1–C9	1.98988	-0.83435
3	BD(1) O2–C3	1.98359	-0.80820
4	BD(1) C1–C2	1.97925	-0.74823
5	BD(1) C3–C15	1.96857	-0.60962
6	BD(1) C6–C7	1.92713	-0.56205
7	BD(1) C10–C11	1.96903	-0.62727

Second-order perturbation energy analysis [E(2)] reveals electron transfer-induced stabilization effects on bonds. It is clear from Table 9 that the C2–H2 bond $\sigma \rightarrow \sigma^*$ back-donation into the antibonding (BD*) orbital of C1–C6 results in tremendous intrinsic stabilization to the molecule with a gigantic energy of 7.09 kcal mol^{-1}. This value is a measure of the fact that the intramolecular charge distribution is very active and that the molecule possesses a conformationally rigid structure. Similarly, the $\pi \rightarrow \pi^*$ delocalization interaction from the C1–C2 π bond to the O2–C3 antibonding orbital is 6.93 kcal mol^{-1}, which shows efficient conjugation in the system. The C1–H1 $\sigma \rightarrow \sigma^*$ delocalization to the antibonding orbital of C2–C3 is 6.38 kcal mol^{-1}, exhibiting structural orientation allowing for the charge transfer within the carbon skeleton. In addition, the interaction $\pi \rightarrow \pi^*$ between the C3–C15 bond and the antibonding orbital of C4–C5 with 2.20 kcal mol^{-1} of energy, the conjugated structural properties are aiding the system.

Table 9. Selected Second-Order Perturbation Interactions.

Donor (i)	**Acceptor (j)**	**E(2) (kcal mol^{-}**	**Description**
BD(1) C1–H1	BD*(C2–C3)	6.38	σ → σ* delocalization
BD(2) C1–C2	BD*(O2–C3)	6.93	π → π* delocalization
BD(1) C2–H2	BD*(C1–C6)	7.09	σ → σ* back-donation
BD(1) C3–C15	BD*(C4–C5)	2.20	π → π* delocalization
BD(1) C4–H4A	BD*(C5–H5A)	2.88	σ → σ* bond effect

When all these outcomes are taken as a whole, it is observed that compound (**I**) possesses a delocalized electronic structure with high delocalization. Functional groups such as Br and OH in the molecule influence the electrostatic charge distribution and increase the reactivity profile of the molecule by donating electrons to antibonding orbitals. In particular, oxygen atom lone pair delocalizations enhance the molecule and bonding system's ability to engage in hydrogen bonding as well as expand the bonding framework by polar interactions. The NBO analysis performed, hence, demonstrates that compound (**I**) not only displays a stable framework but also displays a fertile profile when it comes to electron delocalizations. In this case, the compound stands out as a stable molecule to be looked at for potential NLO material application, both chemically and regarding its strengths of bonds as well as electronically.

4. Conclusions

In this work, the electronic and geometric properties of organobromine compound $C_{15}H_{23}BrO_2$ isolated from algae have been comprehensively investigated using DFT calculations at the B3LYP/6-311G(d,p) level in the gas phase along with three solvent media (chloroform, methanol, and DMSO). The geometry optimization results showed that the solvents' polarity significantly influences the molecular geometry as can be testified through the RMSD values calculated with reference to the gas phase. Among the solvents, the highest structural change (0.612 Å) was caused by methanol, followed by DMSO (0.468 Å) and chloroform (0.413 Å); these are also in the order of relative polarities of the solvents along with their hydrogen-bonding capacity. When compared to the gas phase, dipole moment values were higher significantly in all the solvent media with the highest in DMSO (5.2831 D), indicating greater polarization of the molecules by solvation effects. Similarly, the total first hyperpolarizability (β_{total}), an important parameter for nonlinear optical (NLO) activity, also attained the maximum in methanol (1.229×10^{-30} esu), reflecting the molecule's potentiality as an NLO material in polar solvents. The dipole moment and hyperpolarizability enhancements due to the solvent are found to be a result of enhanced electronic polarization and stabilization of charge-separated structures. NBO analysis of compound (**I**) reveals a stable electronic structure with highly localized covalent bonds and efficient electron delocalization. Highly occupied, negative orbital energy Br–C and O–C bonds show strong, polar covalent character. Successful intramolecular charge transfer and conjugation are evidenced by second-order perturbation interactions such as $\sigma \rightarrow \sigma^*$ and $\pi \rightarrow \pi^*$ transitions. These observations indicate the molecule's rigidity, increased stability, and the possibility of strong intermolecular interactions. Generally, the electronic characteristics of compound (**I**) indicate it to be a good candidate for NLO purposes based on its structure stability and high density of electron delocalization.

References

Akkayan, C. (1987). Microbiological problems in cellulose production. *Journal of Istanbul University Faculty of Forestry, B*(*37*), 141-159

Anastopoulos, I., & Kyzas, G. Z. (2015). Progress in batch biosorption of heavy metals onto algae. *Journal of Molecular Liquids, 209,* 77-86. https://doi.org/10.1016/j.molliq.2015.05.023

Aswathy Udayan, Pandey, A. K., Sharma, P., Sreekumar, N., & Kumar, S. (2021). Emerging industrial applications of microalgae: Challenges and future perspectives. *Systems Microbiology and Biomanufacturing, 1*(4), 411-431. https://doi.org/10.1007/s43393-021-00038-8

Becke, A. D. (1993). Density-functional thermochemistry. III. The role of exact exchange. *The Journal of Chemical Physics, 98*(7), 5648-5652. https://doi.org/10.1063/1.464913

Chattaraj, P. K., Maiti, B., & Sarkar, U. (2003). Philicity: A unified treatment of chemical reactivity and selectivity. *Journal of Physical Chemistry A, 107*(25), 4973-4975. https://doi.org/10.1021/jp027460z

Chemla, D. S., & Zyss, J. (1987). *Nonlinear optical properties of organic molecules and crystals*. Academic Press

Cirik, Ş., & Cirik, S. (2011). Aquatic plants I: Biology, ecology, and cultivation techniques of marine plants (Publication No. 58). Ege University Faculty of Fisheries Publications

Cramer, C. J. (2013). *Essentials of computational chemistry: Theories and models* (2nd ed.). John Wiley & Sons. https://doi.org/10.1002/9781118712278

Çelik, K., & Ongun, T. (2007). The influence of certain physical and chemical variables on the seasonal dynamics of phytoplankton assemblages of a source inlet and the outlet of the shallow hypertrophic Lake Manyas, Turkey. *Turkish Journal of Botany, 31*(6), 485-493

Davyt, D., Fernandez, R., Suescun, L., Mombru, A. W., Saldana, J., Dominguez, L., Coll, J., Fujii, M. T., & Manta, E. (2001). New sesquiterpene derivatives from the red alga *Laurencia scoparia*: Isolation, structure determination, and anthelmintic activity. *Journal of Natural Products, 64,* 1552-1555

Deniz, F., & Tezel Ersanlı, E. (2016a). Simultaneous bioremoval of two unsafe dyes from aqueous solution using a novel green composite biosorbent. *Microchemical Journal, 128,* 312-319

Deniz, F., & Tezel Ersanlı, E. (2016b). Removal of colorant from simulated wastewater by phyco-composite material: Equilibrium, kinetic and mechanism studies in a lab-scale application. *Journal of Molecular Liquids, 220*, 120-128

Deniz, F., & Tezel Ersanlı, E. (2018a). An ecofriendly approach for bioremediation of contaminated water environment: Potential contribution of a coastal seaweed community to environmental improvement. *International Journal of Phytoremediation*, *20*(3), 256-263

Deniz, F., & Tezel Ersanlı, E. (2018b). A natural macroalgae consortium for biosorption of copper from aqueous solution: Optimization, modeling and design studies. *International Journal of Phytoremediation*, *20*(4), 362-368

Deniz, F., & Tezel Ersanlı, E. (2020a). An effectual biosorbent substance for removal of manganese ions from aquatic environment: A promising environmental remediation study with activated coastal waste of *Zostera marina* plant. *BioMed Research International*, *2020*, 7806154. https://doi.org/10.1155/2020/7806154

Deniz, F., & Tezel Ersanlı, E. (2020b). A low-cost and eco-friendly biosorbent material for effective synthetic dye removal from aquatic environment: Characterization, optimization, kinetic, isotherm and thermodynamic studies. *International Journal of Phytoremediation*, *22*(4), 353-362. https://doi.org/10.1080/15226514.2019.1663485

Deniz, F., & Tezel Ersanli, E. (2021a). A renewable biosorbent material for green decontamination of heavy metal pollution from aquatic medium: A case study on manganese removal. *International Journal of Phytoremediation, 23*(3), 231-237. https://doi.org/10.1080/15226514.2020.1807905

Deniz, F., & Tezel Ersanli, E. (2021b). Purification of malachite green as a model biocidal agent from aqueous system by using a natural widespread coastal biowaste (*Zostera marina*). *International Journal of Phytoremediation, 23*(7), 772-779. https://doi.org/10.1080/15226514.2020.1857684

Deniz, F., & Tezel Ersanlı, E. (2022). A novel biowaste-based biosorbent material for effective purification of methylene blue from water environment. *International Journal of Phytoremediation*, *24*(12), 1243-1250. https://doi.org/10.1080/15226514.2021.2025039

Dennington, R., Keith, T., & Millam, J. (2007). *GaussView* (Version 4.1.2). Semichem Inc.

Dolomanov, O.V., Bourhis, L.J., Gildea, R.J., Howard, J.A.K. and Puschmann, H. (2009) OLEX2: A Complete Structure Solution, Refinement and Analysis Program. *Journal of Applied Crystallography*, 42, 339-341. http://dx.doi.org/10.1107/S0021889808042726

Frisch, M. J., Trucks, G. W., Schlegel, H. B., Scuseria, G. E., Robb, M. A., Cheeseman, J. R., Montgomery, J. A., Jr., Vreven, T., Kudin, K. N., Burant, J. C., Millam, J. M., Iyengar, S. S., Tomasi, J., Barone, V., Mennucci, B., Cossi, M., Scalmani, G., Rega, N., Petersson, G. A., Nakatsuji, H., Hada, M., Ehara, M., Toyota, K., Fukuda, R., Hasegawa, J., Ishida, M., Nakajima, T., Honda, Y., Kitao, O., Nakai, H., Klene, M., Li, X., Knox, J. E., Hratchian, H. P., Cross, J. B., Bakken, V., Adamo, C., Jaramillo, J., Gomperts, R., Stratmann, R. E., Yazyev, O., Austin, A. J., Cammi, R., Pomelli, C., Ochterski, J. W., Ayala, P. Y., Morokuma, K., Voth, G. A., Salvador, P., Dannenberg, J. J., Zakrzewski, V. G., Dapprich, S., Daniels, A. D., Strain, M. C., Farkas, O., Malick, D. K., Rabuck, A. D., Raghavachari, K., Foresman, J. B., Ortiz, J. V., Cui, Q., Baboul, A. G., Clifford, S., Cioslowski, J., Stefanov, B. B., Liu, G., Liashenko, A., Piskorz, P., Komaromi, I., Martin, R. L., Fox, D. J., Keith, T., Al-Laham, M. A., Peng, C. Y., Nanayakkara, A., Challacombe, M., Gill, P. M. W., Johnson, B., Chen, W., Wong, M. W., Gonzalez, C., & Pople, J. A. (2004). *Gaussian 03, Revision C.02*. Gaussian, Inc.

Geerlings, P., De Proft, F., & Langenaeker, W. (2003). Conceptual density functional theory. *Chemical Reviews, 103*(5), 1793-1874. https://doi.org/10.1021/cr990029p

Glendening, E. D., Landis, C. R., & Weinhold, F. (2013). Natural bond orbital methods. *Wiley Interdisciplinary Reviews: Computational Molecular Science, 2*(1), 1-42. https://doi.org/10.1002/wcms.51

Guiry, M. D., & Guiry, G. M. (2015). *AlgaeBase: World-wide electronic publication*. National University of Ireland, Galway. http://www.algaebase.org

Gümüş, G. (2006). *Investigation of the chemical composition of sea lettuce* (Master's thesis). Ege University Institute of Science.

Hasırcı Mustak, S., & Tezel Ersanlı, E. (2015). Spatial and temporal characterization of the physicochemical parameters and phytoplankton assemblages in Dodurga Reservoir (Sinop, Turkey). *Turkish Journal of Botany, 39*(3), 547-554. https://doi.org/10.3906/bot-1407-32

Kurata, K., Taniguchi, K., Agatsuma, Y., & Suzuki, M. (1998). Diterpenoid feeding-deterrents from *Laurencia saitoi*. *Phytochemistry, 47,* 363-369

Lee, C. T., Yang, W. T., & Parr, R. G. (1988). Development of the Colle-Salvetti correlation-energy formula into a functional of the electron density. *Physical Review B, 37*, 785-789

Li, Y. X., Wang, Y., & Zhao, F. J. (2015). Kinetic and equilibrium studies of chromium (VI) biosorption by spent macroalgae Polysiphonia urceolata and Chondrus *ocellatus. Biotechnology & Biotechnological Equipment, 29(3), 498-505. https://doi.org/10.1080/13102818.2015.1011374*

Masuda, M., Abe, T., Suzuki, T., & Suzuki, M. (1996). Morphological and chemotaxonomic studies on *Laurencia composita* and *L. okamurae* (Ceramiales, Rhodophyta). *Phycologia, 35,* 550-562

Parr, R. G., & Pearson, R. G. (1983). Absolute hardness: Companion parameter to absolute electronegativity. *Journal of the American Chemical Society, 105*(26)*,* 7512-7516. https://doi.org/10.1021/ja00364a005

Parr, R. G., Szentpály, L. V., & Liu, S. (1999). Electrophilicity index. *Journal of the American Chemical Society, 121*(9)*,* 1922-1924. https://doi.org/10.1021/ja983494x

Paul, V. J., Ritson-Williams, R., & Sharp, K. (2011). Marine chemical ecology in benthic environments. *Natural Product Reports, 28,* 345-387

Pearson, R. G. (1997). *Chemical hardness: Applications from molecules to solids*. Wiley-VCH.

Prasad, P. N., & Williams, D. J. (1991). *Introduction to nonlinear optical effects in molecules and polymers*. Wiley-Interscience.

Reed, A. E., Curtiss, L. A., & Weinhold, F. (1988). Intermolecular interactions from a natural bond orbital, donor–acceptor viewpoint. *Chemical Reviews, 88*(6), 899-926. https://doi.org/10.1021/cr00088a005

Sari, A., & Tuzen, M. (2008). Biosorption of Pb(II) and Cd(II) from aqueous solution using green alga (*Ulva lactuca*) biomass. *Journal of Hazardous Materials, 152*(1)*,* 302-308. https://doi.org/10.1016/j.jhazmat.2007.06.097

Serrano, A., Palacios, C., Roy, G., et al. (1998). Derivatives of gallic acid induce apoptosis in tumoral cell lines and inhibit lymphocyte proliferation. *Archives of Biochemistry and Biophysics, 350,* 49-54

Solak, C. N., Peszek, Ł., Yilmaz, E., Ergül, H. A., Kayal, M., Ekmekçi, F., Várbíró, G., Yüce, A. M., Canli, O., Binici, M. S., & Ács, É. (2020). Use of diatoms in monitoring the Sakarya River Basin, Turkey. *Water, 12*(3)*,* 703. https://doi.org/10.3390/w12030703

Suescun, L., Mombru, A. W., Mariezcurrena, R. Â., Davyt, D., Fernandez, R., & Manta, E. (2001). Two natural products from the algae *Laurencia scoparia*. *Acta Crystallographica Section C: Structural Chemistry, 57,* 286-288

Suzuki, M., Takahashi, Y., Nakano, S., Abe, T., Masuda, M., Ohnishi, T., Noya, Y., & Seki, K.-I. (2009). An experimental approach to study the biosynthesis of brominated metabolites by the red algal genus *Laurencia*. *Phytochemistry, 70,* 1410-1415

Tezel Ersanlı, E., & Gönülol, A. (2014). Phytoplankton dynamics and some physicochemical variables in Cakmak Reservoir, Samsun, Turkey. *MANAS Journal of Agriculture and Life Sciences*, *4*(1), 17-25

Tezel Ersanlı, E., & Hasırcı, S. (2013). The relationship between environmental variables and the vertical and horizontal assemblages of phytoplankton in Erfelek Reservoir in Sinop, Turkey. *Turkish Journal of Botany, 37*(4), 715-726. https://doi.org/10.3906/bot-1207-21

Tezel Ersanlı, E., & Hasırcı Mustak, S. (2017). Distribution dynamics of vegetative cells and cyst of *Ceratium hirundinella* in two reservoirs, Turkey. *Süleyman Demirel University Journal of Natural and Applied Sciences*, *21*(1), 247-253

Tezel Ersanlı, E., & Öztürk, R. (2017). Ecological and statistical evaluation of algal flora and water quality of Karasu Stream. *KSU Journal of Natural Sciences, 20*(3), 193-200

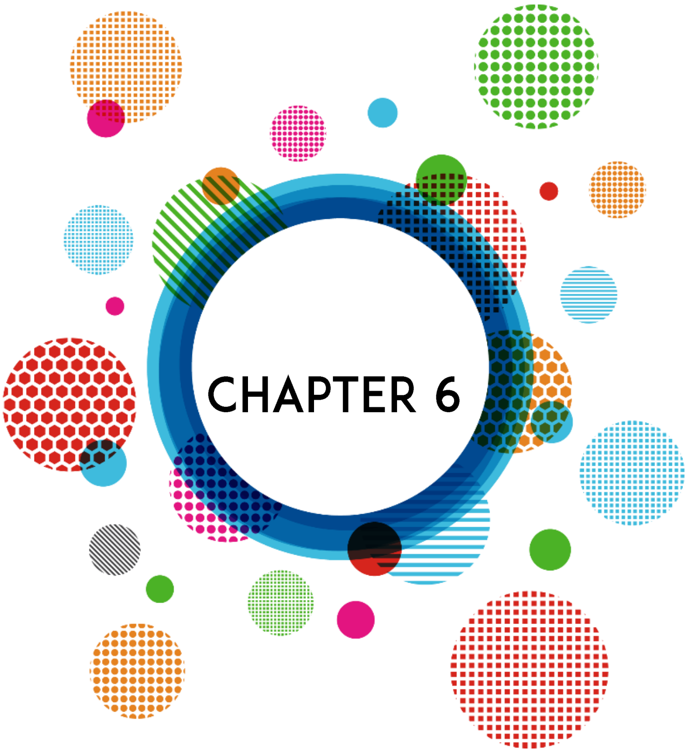
Tomasi, J., Mennucci, B., & Cammi, R. (2005). Quantum mechanical continuum solvation models. *Chemical Reviews, 105*(8), 2999-3093. https://doi.org/10.1021/cr9904009

Weinhold, F. (2012). *Discovering chemistry with natural bond orbitals*. Wiley.

Weinhold, F., & Landis, C. R. (2005). *Valency and bonding: A natural bond orbital donor-acceptor perspective*. Cambridge University Press.

Yılmaz, N., Yardımcı, C. H., Elhag, M., & Dumitrache, C. A. (2018). Phytoplankton composition and water quality of Kamil Abduş Lagoon (Tuzla Lake), Istanbul-Turkey. *Water, 10*(5), 603. https://doi.org/10.3390/w10050603

Zeybek, N., Zeybek, U., & Saygıner, B. (2003). *Pharmaceutical botany*. Meta Publishing House.



CHAPTER 6

Green AI: Sustainability-Focused Artificial Intelligence Approaches and Future Strategies

Özge Taş[1] & İsmail Emre Deniz[2]

---

[1] Öğr.Gör., Kapadokya Üniversitesi, ORCID: 0000-0001-7220-5054

[2] Bursa Uludağ Üniversitesi, ORCID:0000-0003-4883-9959

1.INTRODUCTION

Green artificial intelligence (AI), in conjunction with sustainability, is an emerging interdisciplinary field. Its primary focus is the enhancement of the environmental sustainability of AI technologies, in addition to the leveraging of AI to address ecological challenges. Since its inception around 2019, Green AI has garnered attention due to the escalating concerns about the energy consumption and carbon footprint associated with advanced AI systems, particularly large language models (LLMs). This movement advocates for responsible technological development that aligns with global sustainability goals and addresses the pressing ecological impacts of AI advancements.Green AI encompasses two primary variants: The concept of "Green-in-AI" aims to minimise the environmental impact of AI technologies themselves by optimising algorithms and energy use. In contrast, "Green-by-AI" employs AI to address environmental issues, such as enhancing agricultural practices and biodiversity monitoring. As organisations increasingly rely on AI for various applications, the potential for significant reductions in greenhouse gas emissions through efficient energy management and resource allocation has become a focal point of research and application (Yang J., E.i. 2019; Brevini, B. 2020). Notwithstanding the promise of Green AI, notable controversies persist regarding its dual role as both a tool for sustainability and a contributor to environmental degradation. To illustrate, the energy-intensive processes necessary to train voluminous AI models can engender considerable carbon emissions, thus giving rise to questions surrounding the overall ecological merits of such technologies. Projections indicate that data centres, which are pivotal for AI operations, may consume up to 21% of global energy demand by 2030. This necessitates an urgent re-evaluation of energy practices within the tech sector. As the field evolves, it faces challenges such as algorithmic bias, regulatory inadequacies, and the need for enhanced energy efficiency. The term "stakeholders" is employed to denote the individuals or groups with a vested interest in the subject under discussion. Ultimately, the future of Green AI will depend on balancing technological innovation with sustainable practices to foster a greener and more equitable world.

2. Literature

Green AI has emerged as a significant field within artificial intelligence (AI) since around 2019, focusing on the sustainability of AI technologies, particularly regarding their energy efficiency and environmental impact. This movement promotes responsible technological development aimed at addressing the ecological challenges posed by rapid advancements in AI capabilities.

Table 1. A look at the history of green AI technologies

Author	**Objectives**	**Result**
(Khakurel et al., 2018)	Explore AI's long-term impacts on sustainability dimensions. Analyze positive and negative influences of AI on sustainable development.	AI has significant impacts on all five sustainability dimensions.Value, collaboration, sharing responsibilities, and ethics are crucial for sustainable development of AI.
(Yigitcanlar & Cugurullo, 2020)	Explore sustainability of AI in smart cities.Inform policymakers on sustainable AI adoption	Explores sustainability of AI in smart cities.Provides insights into emerging urban artificial intelligences
(Liao & Wang, 2020)	Map intersections of sustainability and AI research. Expand community of practice for AI in sustainable development.	Central body of work on green and sustainable science and technology Interactions are necessary, challenging, and promising
(Mercier-Laurent, 2021)	Explore AI's role in sustainable development challenges. Innovate approaches to achieve United Nations Sustainable Development Goals.	AI can innovate the way of facing the Planet Crisis AI can help achieve some of the United Nations Sustainable Development Goals
(Nicodeme, 2021)	Overview of AI's potential for sustainability in Smart Cities. Highlight AI's energy consumption drawbacks and propose greener methodologies.	AI has potential for sustainability in Smart cities. AI's energy consumption has negative ecological impact.

(Walshe et al., 2021)	Discuss AI's role in achieving Sustainable Development Goals. Address sustainability issues while balancing negative impacts of AI.	AI can be an enabler for achieving sustainability goals A balanced approach is needed to avoid negative impacts
(Yigitcanlar et al., 2021)	Highlight shortfalls in mainstream AI conceptualization and practice. Advocate for a consolidated green AI approach for smart cities.	Highlighting the shortfalls in mainstream AI system conceptualization and practice Advocating the need for a consolidated AI approach (green AI) to support smart city transformation
(Bracarense et al., 2022)	Analyze academic research on AI and sustainability trends. Propose a robust agenda for future research.	Research focuses on energy efficiency, smart grid, renewable energy. Identified eight main shortcomings in AI for sustainability research.
(Utilizing Artificial Intelligence for Environmental Sustainability, 2022)	Examine AI's role in achieving environmental sustainability. Assess AI's impact on sustainable development goals.	AI can be used to achieve optimal outcomes in various industries. AI intervention is essential in attaining the United Nations Sustainable Development Goals.
(Taghikhah et al., 2022)	AI's potential in overcoming socioenvironmental challenges Data-driven interventions and leadership strategies for sustainability	AI can support interventions for promoting proenvironmental behavior AI can aid in efficient management of wildfires and renewable energy production
(Samoilenko, 2023)	Importance and applications of AI technologies in sustainability Contribution of AI technologies to sustainability goals	Artificial intelligence can be used to achieve sustainability goals. Ethical and legal regulations should be increased.

(Akter, 2024)	Examine AI applications for sustainability across various sectors. Discuss trends, challenges, and future research directions.	AI mitigates environmental impacts and promotes sustainability. Highlights key applications, trends, and future research directions.
(Gambhir & Bhatt, 2022)	Evaluate AI impact on Sustainable Development Goals. Study the balance for global sustainability between AI and SD.	AI's impact on Sustainable Development Goals is being studied. AI and SD are crucial for global sustainability.
(Li, n.d.)	Analyze artificial intelligence's influence on corporate sustainability strategies. Evaluate ethical implications of AI in corporate management.	Artificial intelligence influences corporate sustainability strategies positively. Ethical use of AI is crucial for corporations.
(Swiatek, 2024)	Enhance businesses' sustainability efforts through bounded AI. Address unresolved issues surrounding AI's environmental and ethical impacts.	Businesses must green AI for sustainability and ethics. NearMap case study illustrates successful bounded AI implementation.
(Raman et al., 2024)	Identify thematic clusters in Green and Sustainable AI literature. Uncover emerging topics in AI research related to sustainability and ethics.	Identified three major thematic clusters in AI research. Uncovered five emerging topics related to ethical and sustainable AI.
(Yigitcanlar et al., 2021)	Highlight shortfalls in mainstream AI conceptualization and practice. Advocate for a consolidated green AI approach for smart cities.	Highlighting the shortfalls in mainstream AI system conceptualization and practice Advocating the need for a consolidated AI approach (green AI) to support smart city transformation

(Akter, 2024)	Examine AI applications for environmental sustainability. Discuss trends, challenges, and future research directions.	AI optimizes energy consumption and resource management. AI enhances conservation efforts and predicts environmental risks.
(Bracarense et al., 2022)	Analyze academic research on AI and sustainability trends. Propose a robust agenda for future research.	Research focuses on energy efficiency, smart grid, renewable energy. Identified eight main shortcomings in AI for sustainability research.
(Lohani, 2024)	Examine AI's role in enhancing environmental sustainability efforts. Identify challenges and opportunities for AI applications in conservation.	AI enhances sustainability efforts in resource management and climate change. AI applications include pollution prevention, climate modeling, and renewable energy optimization.

3. Variants of Green AI

Green AI can be divided into two main variants:

Green-in-AI

This variant emphasises the implementation of sustainability strategies within the AI domain itself. A salient issue in this domain pertains to the energy consumption of large language models (LLMs), such as OpenAI's ChatGPT and Google's Gemini. These models have demonstrated superior data processing capabilities in comparison to human brains, yet they require significant energy resources. It is imperative to acknowledge the significance of comprehending the energy dynamics of AI systems in order to enhance their sustainability and mitigate their ecological impact (Masanet, E. E. I., 2020).

Green-by-AI

The second variant places emphasis on the utilisation of AI technologies for the purpose of addressing specific environmental challenges, including the enhancement of agricultural practices and the promotion of biodiversity. Recent technological developments, such as artificial intelligence (AI) and the Internet of Things (IoT), have witnessed a surge in their application in the domains of ecological research and environmental management. These technologies have been instrumental in enhancing the efficiency of data collection and analysis, thereby contributing to a more comprehensive and informed understanding of environmental issues. For instance, the utilisation of motion-sensing cameras in the collection of extensive biodiversity data can be complemented by artificial intelligence (AI) for the purpose of informing conservation strategies and enhancing ecosystem management (Parker D. S. 2009; Bolon-Canedo et. al. 2024). This approach has the potential to not only deepen our comprehension of intricate ecological interactions but also to facilitate effective decision-making in uncertain conditions.(Adnan M, e.i 2024),(Zewe A. 2025)

Challenges and Innovations

As the field of Green AI continues to evolve, it is confronted with the significant challenge of analysing vast quantities of data in order to achieve effective understanding of ecosystems. It is evident that traditional methodologies are frequently inadequate in addressing the intricacies inherent in such contexts. Advanced AI technologies, therefore, emerge as a pivotal element in navigating this complexity. Consequently, innovations in AI, such as machine learning and cognitive AI, are increasingly recognised for their potential to support sustainable development initiatives (Pancholi K. And Shukla P. 2025),(Dinçer et.al. 2022).

Current Status of AI Technologies

The field of artificial intelligence (AI) is undergoing rapid development, with considerable ramifications for diverse sectors, particularly in regard to environmental, social, and governance (ESG) issues. Current artificial intelligence (AI) technologies have the potential to reduce greenhouse gas emissions by optimising energy consumption patterns through advanced analytics. It is suggested that the utilisation of artificial intelligence may facilitate enhanced efficiency in energy management, thereby contributing to the mitigation of climate change. (Bolon-Canedo e.i 2024).

Energy Efficiency Improvements

The implementation of AI technologies has been increasingly adopted to enhance energy efficiency across a variety of industrial sectors. For instance, research indicates that the application of AI can lead to energy efficiency improvements ranging from 10.2% to 40% in specific settings through techniques such as Model Predictive Control (MPC). These advancements underscore the ability of AI not only to optimise energy usage, but also to mitigate operational costs.

Impact on Healthcare and Accessibility

Within the healthcare sector, AI technology is playing a crucial role in increasing access to medical services for vulnerable populations. This application is of particular significance in enhancing productivity by facilitating greater access to essential health products and services for financially underprivileged communities (Bolon-Canedo, et.al 2024). When harnessed effectively, the benefits of AI in healthcare can drive significant advancements in public health and service delivery.

Data Centers and Energy Demand

As artificial intelligence (AI) technology becomes increasingly prevalent, there is a concomitant increase in demand for computational power. This has given rise to concerns regarding energy consumption and sustainability. Current projections indicate that data centres, which underpin AI operations, could account for up to 21% of overall global energy demand by 2030. The computational requirements for training and maintaining AI systems are increasing rapidly, with estimates indicating an annual growth rate of energy consumption between 26% and 36% (Zewe A., 2025). This surge necessitates a reevaluation of sustainability practices within the technology sector.

Carbon Footprint and Environmental Concerns

While there is considerable potential for artificial intelligence (AI) to contribute to the resolution of environmental issues, it is important to acknowledge the challenges that this technology poses. The training of popular AI models has been shown to generate substantial carbon emissions, with estimates indicating that such processes can result in approximately 626,000 pounds of CO2 being emitted — the equivalent of the emissions from 300 round trips between New York and San Francisco. As artificial intelligence (AI) technologies continue to advance, it is imperative for stakeholders to develop strategies that mitigate their environmental impact while maximising their potential benefits in sustainability initiatives.

Strategies for Green AI

Green AI is a term used to describe a range of strategies that are intended to facilitate the development of artificial intelligence technologies that are environmentally sustainable. The focus of these strategies is on optimising algorithms, hardware, and operational processes with a view to reducing energy consumption and minimising the carbon footprint of AI systems (Belenguer L., 2022).

Optimization of Algorithms and Models

A fundamental approach in Green AI is the optimisation of algorithms. This approach entails the conceptualisation of models that necessitate a reduced number of data points for training, thereby leading to a decrease in energy consumption during the training process. Furthermore, researchers are developing resource-aware algorithms that intelligently manage computational resources, thereby minimising waste and enhancing efficiency (Belenguer, L., 2022).

Energy-Efficient Hardware

It is imperative to acknowledge the significance of eco-friendly hardware designs as a pivotal strategy in this context. As posited by Belenguer (2022), the development of energy-efficient computational hardware has the potential to markedly reduce the power requirements of AI systems. Organisations are encouraged to consider upgrading or retrofitting existing hardware rather than replacing it entirely, which can extend its lifespan and reduce electronic waste (Nishant R e.i 2020), (Alzoubi Y. et.al 2024).

Sustainable Data Center Operations

The enhancement of data centre operations is also of paramount importance for the realisation of Green AI. In the contemporary business environment, organisations are engaged in the exploration of methodologies designed to enhance the energy efficiency of their data centres. This exploration encompasses the implementation of advanced cooling techniques and the optimisation of server utilisation (Belenguer, L., 2022). This objective is consistent with the overarching goals of promoting energy efficiency and establishing a sustainable operational framework for AI applications.

Practices for Extending Hardware Lifespan

In order to enhance sustainability, organisations have the capacity to adopt practices that extend the lifespan of hardware. Maintenance, software updates and hardware inspections are all vital components in ensuring that equipment operates efficiently over time (Nishant R et. al. 2020; Alzoubi Y. et. al. 2024). Moreover, the promotion of behaviours that enhance energy efficiency among employees has the potential to contribute to a more sustainable operational environment (Galaz V. et al., 2021).

Integration of Ethical Frameworks

The integration of ethical frameworks within the development of artificial intelligence (AI) technologies is imperative to ensure that such technologies are aligned with the objectives of sustainability. As emphasised by numerous international initiatives, the incorporation of ethical considerations into the process of formulating AI policies can facilitate the utilisation of AI for the purpose of addressing intricate environmental and developmental challenges. This approach also serves to address human rights practices (Zewe A., 2025).

Future Directions

The future of green artificial intelligence (AI) is at a critical juncture, where there is a need for technological advancement to be aligned with sustainability goals. As research continues, several key areas for development have emerged that have the potential to enhance the environmental sustainability of AI systems.

Sustainable Energy Integration

A significant direction in this field is the integration of renewable energy sources into the infrastructure of artificial intelligence. Coglianese (2024) emphasises that the advancement of AI technologies for the utilisation of sustainable energy will complement the broader transition of the economy towards renewable sources, such as wind and solar power. The primary objective of the present research endeavour is to enhance the energy efficiency of manufacturing, production and transportation sectors, with a view to minimising the carbon footprint of AI operations. The transition to cleaner energy sources is imperative in order to mitigate the negative environmental impacts of AI and thereby support global sustainability objectives.

Enhanced Data Analytics for Sustainability

The capacity of AI to process vast amounts of environmental data represents a promising avenue for future developments. It is evident that companies such as Microsoft are already leveraging artificial intelligence (AI) to analyse environmental data, thereby providing insights that can drive more effective sustainability strategies. This capability facilitates the identification of patterns and the prediction of outcomes, thereby rendering sustainability efforts not merely data-driven, but also insight-driven. As artificial intelligence (AI) technologies advance, their role in facilitating real-time environmental monitoring and management will become increasingly critical. This will enable timely interventions and policy adjustments.

Policy and Regulation Considerations

In the context of accelerating advancements in artificial intelligence (AI), it is imperative to prioritise the balance between rapid technological progress and the safeguarding of public safety and the upholding of ethical standards. It is incumbent upon policymakers to confront the challenge of overseeing such innovations whilst concomitantly addressing the risks associated with them, including, but not limited to, privacy, bias, and manipulation (Sundberg N., 2024). In order to ensure the sustainable development and deployment of AI technologies, future research must concentrate on the establishment of frameworks that govern such technologies. It is vital that these frameworks ensure the alignment of AI technologies with environmental goals, without compromising ethical considerations.

Circular Economy Approaches

The adoption of circular economy principles is imperative for the sustainable development of AI. The concept of environmental sustainability is predicated on the consumption of natural resources at a rate that is sustainable in the long term. Artificial intelligence (AI) has the potential to contribute to this objective by optimising the use of resources and minimising waste (QECD, 2022). Future efforts should therefore aim to develop AI systems that are not only efficient but also capable of supporting circular economy initiatives, thus promoting long-term sustainability.

Addressing Challenges

Finally, it is imperative to address the challenges associated with electronic waste and the carbon emissions resulting from AI's energy consumption (Verdecchia, R. et.al., 2023). It is evident that strategies which encompass the development of enhanced energy-efficient artificial intelligence systems, in conjunction with the utilisation of renewable energy sources, have the potential to markedly mitigate the environmental impact of artificial intelligence technologies. Furthermore, it is imperative to emphasise the necessity of nurturing innovation in sustainable practices within the AI sector, as this will play a pivotal role in addressing the adverse environmental implications associated with technological advancements.

Case Studies

Overview of AI in Sustainability

Recent studies illustrate the transformative role of artificial intelligence (AI) in enhancing sustainability across various industries. In the contemporary business landscape, there is an increasing trend of enterprises leveraging artificial intelligence (AI) to enhance operational efficiency, with a notable emphasis on reducing their carbon footprint. This strategic direction is underpinned by both ethical considerations and the mounting regulatory pressures and consumer expectations related to environmental sustainability.

Implementing Sustainable Supply Chains

The utilisation of AI technologies has been identified as a pivotal factor in the development of sustainable supply chains, as evidenced by numerous case studies. In the contemporary business landscape, artificial intelligence (AI) is being utilised by companies to enhance resource allocation, reduce waste, and optimise logistics processes. The integration of big data analytics and machine learning within business operations has been demonstrated to facilitate more accurate demand forecasting, thereby reducing excess inventory and optimising transportation routes. Consequently, these advancements have been shown to result in a reduction of emissions and cost savings, thereby providing a compelling case for the coexistence of sustainability and profitability.

Energy-Efficient AI Technologies

The focus of research in Green AI is the creation of AI solutions that are environmentally sustainable. The objective of this focus is to reduce energy consumption and minimise carbon footprints. The exploration of techniques, including but not limited to energy-efficient model training and resource-aware algorithms, is underway. For instance, companies are investing in eco-friendly hardware designs that not only enhance computational efficiency but also align with sustainability goals. It is imperative to acknowledge the pivotal role that such innovations play in mitigating the environmental impacts of AI applications and promoting energy efficiency (Tabbakh A. Et al. 2024).

Coherent ESG Reporting

Another critical area in which AI contributes to sustainability is through enhanced Environmental, Social, and Governance (ESG) reporting. In the corporate context, there has been an increasing adoption of AI-driven analytics with the aim of providing coherent and comprehensive ESG data, thereby facilitating enhanced transparency and accountability. This reporting is becoming increasingly significant as stakeholders and consumers demand greater insight into a company's sustainability practices, thereby influencing their purchasing decisions.

Challenges and Considerations

Notwithstanding the considerable potential of AI in promoting sustainability, there are still several challenges to be addressed. The extant literature and research methodologies in this field are limited in scope, and as a consequence, may overlook relevant insights with regard to Green AI. It is imperative to acknowledge the potential impact of two key factors on the comprehensiveness of findings: the scope of the database and the subjective nature of theme interpretation. These elements necessitate further critical review and validation by experts in the field to ensure the robustness of the research outcomes. Notwithstanding the challenges previously mentioned, the continuous progression of AI technologies provides a number of potential avenues for achieving enhanced sustainability across a variety of sectors.

Challenges and Barriers

Conclusion

The integration of artificial intelligence (AI) within sustainability efforts, frequently termed 'Green AI', is confronted by numerous challenges and barriers that hinder its prospective influence across diverse sectors. A significant concern is that of algorithmic bias, which has the potential to result in unequal access and benefits, thus serving to exacerbate existing inequalities rather than alleviate them. Furthermore, there is an increasing level of public scrutiny with regard to the fairness and transparency of AI-powered solutions, particularly in sensitive areas such as human resources and healthcare (Varsha P.S., 2023). Another potential impediment pertains to the possibility of cascading failures and external disruptions that may emerge from reliance on complex AI systems. The aforementioned systemic risks serve to emphasise the trade-offs between efficiency and resilience. It is suggested that, whilst AI has the capacity to optimise specific processes, it may concomitantly engender vulnerabilities that could be exploited during crises (Tabbakh, A. et al., 2024). Moreover, the prevailing governance frameworks frequently prove to be deficient in their capacity to address the sustainability risks that are concomitant with AI. This necessity has given rise to a requirement for enhanced regulatory oversight and the establishment of ethical guidelines. Furthermore, the environmental implications of implementing AI technologies, including the substantial energy consumption necessitated for training voluminous models, present considerable obstacles to the realisation of genuine sustainability. This issue highlights the necessity for the development of algorithms that are more energy-efficient, and the promotion of practices that minimise ecological footprints. In order to address the aforementioned challenges, it is imperative to adopt optimal practices and guidelines, whilst also fostering enhanced collaboration between government entities, industry, and research institutions. This collaborative effort is crucial for the effective implementation of Green AI initiatives.

REFERENCES

J. Yang, W. Xiao, C. Jiang, M. S. Hossain, G. Muhammad and S. U. Amin, "AI-Powered Green Cloud and Data Center," in IEEE Access, vol. 7, pp. 4195-4203, 2019, doi: 10.1109/ACCESS.2018.2888976.

keywords: {Cloud computing;Data centers;Engines;Energy consumption;Processor scheduling;Green products;Optimization;Green cloud and data center;energy optimizing;deep learning;particle swarm optimization},

Black boxes, not green: Mythologizing artificial intelligence and omitting the environment. *Big Data & Society*, *7*(2), 2053951720935141.

Khakurel, J., Penzenstadler, B., Porras, J., Knutas, A., & Zhang, W. (2018). The Rise of Artificial Intelligence under the Lens of Sustainability. 6(4), 100. https://doi.org/10.3390/TECHNOLOGIES6040100.

Yigitcanlar, T., & Cugurullo, F. (2020). The Sustainability of Artificial Intelligence: An Urbanistic Viewpoint from the Lens of Smart and Sustainable Cities. Sustainability, 12(20), 8548. https://doi.org/10.3390/SU12208548

Liao, H.-T., & Wang, Z. (2020). Sustainability and Artificial Intelligence: Necessary, Challenging, and Promising Intersections. https://doi.org/10.1109/MSIEID52046.2020.00076

Mercier-Laurent, E. (2021). Can Artificial Intelligence Effectively Support Sustainable Development (pp. 144–159). Springer, Cham. https://doi.org/10.1007/978-3-030-80847-1_10

Nicodeme, C. (2021). AI Legitimacy for Sustainability. IEEE Conference on Technologies for Sustainability, 1–5. https://doi.org/10.1109/SUSTECH51236.2021.9467431

Walshe, R., Koene, A., Baumann, S., Panella, M., Maglaras, L. A., & Medeiros, F. (2021). Artificial Intelligence as Enabler for Sustainable Development. IEEE International Conference on Engineering and Technology, 1–7. https://doi.org/10.1109/ICE/ITMC52061.2021.9570215

Yigitcanlar, T., Mehmood, R., & Corchado, J. M. (2021). Green Artificial Intelligence: Towards an Efficient, Sustainable and Equitable Technology for Smart Cities and Futures. Sustainability, 13(16), 8952. https://doi.org/10.3390/SU13168952

Bracarense, N., Bawack, R. E., Wamba, S. F., & Carillo, K. D. A. (2022). Artificial Intelligence and Sustainability: A Bibliometric Analysis and Future Research Directions. Pacific Asia Journal of the Association for Information Systems. https://doi.org/10.17705/1pais.14209

Utilizing artificial intelligence for environmental sustainability (pp. 259–279). (2022). Elsevier eBooks. https://doi.org/10.1016/b978-0-323-90396-7.00010-9

Taghikhah, F., Erfani, E., Bakhshayeshi, I., Tayari, S., Karatopouzis, A., & Hanna, B. (2022). Artificial intelligence and sustainability (pp. 93–108). https://doi.org/10.1016/b978-0-323-90508-4.00006-x

Samoilenko, S. (2023). Artificial Intelligence and Sustainability. 1, 26–33. https://doi.org/10.59287/iccar.734

Akter, S. (2024). AI for Sustainability: Leveraging Technology to Address Global Environmental. https://doi.org/10.60087/jaigs.v3i1.64

Gambhir, V., & Bhatt, D. (2022). study on achieving sustainability through artificial intelligence. International Journal of Health Sciences (IJHS). https://doi.org/10.53730/ijhs.v6ns2.8144

Li, R. (n.d.). Research on Artificial Intelligence Influence towards Corporate Sustainability Strategies in Management. https://doi.org/10.4108/eai.1-9-2023.2338700

Swiatek, L. (2024). Strengthening the Sustainability of Artificial Intelligence: Fostering Green Intelligence for a More Ethical Future (pp. 83–103). https://doi.org/10.1007/978-3-031-49979-1_5

Raman, R., Pattnaik, D., Lathabai, H. H., Govindan, K., & Nedungadi, P. (2024). Green and sustainable AI research: an integrated thematic and topic modeling analysis. 11, 1–28. https://doi.org/10.1186/s40537-024-00920-x

Yigitcanlar, T., Mehmood, R., & Corchado, J. M. (2021). Green Artificial Intelligence: Towards an Efficient, Sustainable and Equitable Technology for Smart Cities and Futures. Sustainability, 13(16), 8952. https://doi.org/10.3390/SU13168952

Akter, S. (2024). Harnessing Technology for Environmental Sustainability: Utilizing AI to Tackle Global Ecological Challenges. Deleted Journal, 2(1), 49–57. https://doi.org/10.60087/jaigs.v2i1.p57

Bracarense, N., Bawack, R. E., Wamba, S. F., & Carillo, K. D. A. (2022). Artificial Intelligence and Sustainability: A Bibliometric Analysis and Future Research Directions. Pacific Asia Journal of the Association for Information Systems. https://doi.org/10.17705/1pais.14209

Lohani, N. (2024). AI-based Environmental Sustainability: Transforming Conservation Efforts. International Journal For Multidisciplinary Research. https://doi.org/10.36948/ijfmr.2024.v06i02.16997

Masanet, E., Shehabi, A., Lei, N., Smith, S., & Koomey, J. (2020). Recalibrating global data center energy-use estimates. *Science*, *367*(6481), 984-986.

Parker, D. S. (2009). Very low energy homes in the United States: Perspectives on performance from measured data. *Energy and buildings, 41*(5), 512-520.

Bolón-Canedo, V., Morán-Fernández, L., Cancela, B., & Alonso-Betanzos, A. (2024). A review of green artificial intelligence: Towards a more sustainable future. *Neurocomputing*, 128096.

Adnan, M., Xiao, B., Ali, M. U., Bibi, S., Yu, H., Xiao, P., ... & An, X. (2024). Human inventions and its environmental challenges, especially artificial intelligence: New challenges require new thinking. *Environmental Challenges*, 100976.

Zewe A. (2025) https://news.mit.edu/2025/explained-generative-ai-environmental-impact-0117. January 17, 2025

Pancholi, K., & Shukla, P. (2025). Harnessing AI for Sustainability: Innovations, Policies, and Investment Paradigms. In *Diversity, AI, and Sustainability for Financial Growth* (pp. 97-124). IGI Global Scientific Publishing.

Dinçer, İ., Arcaklıoğlu, P. D. E., & Ezan, M. A. ENERJİDE YAPAY ZEKÂNIN ROLÜ RAPORU.

Bolón-Canedo, V., Morán-Fernández, L., Cancela, B., & Alonso-Betanzos, A. (2024). A review of green artificial intelligence: Towards a more sustainable future. *Neurocomputing*, 128096.

Belenguer, L. (2022). AI bias: exploring discriminatory algorithmic decision-making models and the application of possible machine-centric solutions adapted from the pharmaceutical industry. *AI and Ethics*, *2*(4), 771-787.

Nishant, R., Kennedy, M., & Corbett, J. (2020). Artificial intelligence for sustainability: Challenges, opportunities, and a research agenda. *International journal of information management*, *53,* 102104.

Alzoubi, Y. I., & Mishra, A. (2024). Green artificial intelligence initiatives: Potentials and challenges. *Journal of Cleaner Production*, 143090.

Galaz, V., Centeno, M. A., Callahan, P. W., Causevic, A., Patterson, T., Brass, I., ... & Levy, K. (2021). Artificial intelligence, systemic risks, and sustainability. *Technology in society*, *67,* 101741.

Sundberg, N. (2024). Tackling AI's climate change problem. *MIT Sloan management review*, *65*(2), 38-41.

https://appinventiv.com/blog/green-ai-applications/

OECD (2022), "Yapay zeka hesaplama ve uygulamalarının çevresel etkilerinin ölçülmesi: Yapay zeka ayak izi", *OECD Dijital Ekonomi Makaleleri* , No. 341, OECD Yayıncılık, Paris, https://doi.org/10.1787/7babf571-en .

Verdecchia, R., Sallou, J., & Cruz, L. (2023). A systematic review of Green AI. *Wiley Interdisciplinary Reviews: Data Mining and Knowledge Discovery*, *13*(4), e1507.

https://www.ibm.com/think/insights/future-ai-energy-efficiency

https://ruralhandmade.com/blog/case-studies-of-how-ai-is-being-used-to-improve-sustainable

https://www.e-spincorp.com/green-ai-sustainability-artificial-intelligence-greener-future/ grafikleri çizdir buna göre

Tabbakh, A., Al Amin, L., Islam, M. *et al.* Towards sustainable AI: a comprehensive framework for Green AI. *Discov Sustain* 5, 408 (2024). https://doi.org/10.1007/s43621-024-00641-4

https://www.ey.com/en_nl/insights/climate-change-sustainability-services/ai-and-sustainability-opportunities-challenges-and-impact

Varsha, P. S. (2023). How can we manage biases in artificial intelligence systems–A systematic literature review. *International Journal of Information Management Data Insights*, *3*(1), 100165.