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Progress in heterogeneous catalysis for renewable energy and petrochemical production from biomass

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ABSTRACT

Historically, catalytic advances often occurred during events such as wars or embargoes. However, research efforts are focused on better understanding catalytic processes, minimising feedstock and process costs, developing new catalytic materials, and addressing environmental concerns. This study provides an overview of the global energy system, which forms the basis for the need for alternative energy sources as a panacea for reducing greenhouse gas emissions and providing clean and affordable energy sources through heterogeneous catalysis. It also discusses the development of numerous heterogeneous catalytic materials and processes, focusing on the catalytic conversion of biomass and its derivatives, particularly into fuel blendstocks and petrochemicals. In this context, the analysis of the techno-economic and environmental impact of the different biomass conversion technologies was emphasised. Despite the numerous catalysts and technologies developed and documented over the last century, catalytic processes still have some drawbacks. This study further examined the challenges and offered technological opportunities for developing catalytic materials and processes. It also provided a framework for advancing clean and affordable energy in the renewable energy sector using catalytic materials.

1. Introduction

The world's population and economic growth surge have led to a rapid rise in global energy demand [1]. According to the International Energy Agency, IEA [2], global energy consumption reached 439 EJ in 2021 and is expected to rise by 23 % to 543 EJ by 2050. Fossil fuels dominate our energy mix with a share of over 80 %, with natural gas, oil, and coal accounting for a significant proportion [3]. Currently, fossil fuels play a central role in the energy sector, especially in chemical production, where 90 % of fossil carbon sources in some regions, including Europe and Africa, are used for chemical synthesis [4]. There are concerns that oil and gas reserves could be depleted within the next five decades, whereas coal is expected to last centuries [1]. In addition to concerns about the finite nature of supply, using fossil fuels also raises concerns about CO_2 emissions [5]. According to forecasts by the International Energy Agency, the carbon footprint will remain at 33 Gt in the 2040s [1]. Consequently, the persistent rise in CO_2 emissions, largely due to human activities, including the combustion of fossil fuels (coal, oil and natural gas) [6] (Fig. 1a) in various sectors, including transport, electricity generation, industrial processes and other sectors (Fig. 1b), poses a significant threat to the environment and human health. The widespread availability and high dependence on fossil fuels combined with an increase in CO_2 emissions is driven by factors such as gross domestic product (GDP) per capita based on purchasing power parity (PPP), population growth and energy intensity (Fig. 1c). As the world's population continues to grow, the search for sustainable energy resources will become a key challenge of the 21st century.

Heterogeneous catalysis remains a focal point of numerous industrial operations, profoundly influencing the global economy. It commands a significant market share, representing approximately 80 % of catalytic processes, with annual sales rising to $1.5 trillion and impacting roughly 35 % of the world's GDP [7]. Heterogeneous catalysis plays a crucial role in the conversion of biomass into renewable energy and petrochemical products and represents a sustainable alternative to fossil fuels [8]. In renewable energy applications, heterogeneous catalysts are used to convert biomass into biofuels through processes such as catalytic fast

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pyrolysis [9–11], hydrothermal liquefaction [12–14], and hydrodeoxygenation [15,16]. These processes convert organic materials into bio-oils that can be refined into fuels like gasoline and diesel. Catalysts also help produce hydrogen from biomass through steam reforming and facilitate biogas conversion into synthesis gas for further processing into fuels. For petrochemical production, heterogeneous catalysts are essential for converting biomass-derived molecules into valuable chemicals [9,17]. Sugars from biomass can be catalytically converted into platform chemicals, while lignin is broken down into aromatic compounds, creating bio-based alternatives to petroleum-derived chemicals [18]. Catalysts are also used in refining bio-oils and upgrading biomass-derived intermediates into products that can replace conventional petrochemicals, including olefins and aromatics used in the manufacture of plastics and other materials [19]. Through these catalytic processes, biomass can be effectively converted into renewable fuels and chemicals, reducing dependence on fossil fuels, lowering emissions, and promoting sustainability in energy production and the petrochemical industry.

Similarly, waste energy can be recovered through catalytic energy recovery or converted into usable forms, promoting greater energy efficiency and sustainability. This approach is particularly important in renewable energy systems, where catalysts help to convert excess energy or by-products into valuable resources such as chemicals, fuels, or electricity. A key area is waste heat utilisation, where catalysts are used in thermochemical cycles to convert waste heat from industrial processes into chemical energy or fuels [20]. For example, solid oxide fuel cells (SOFC) and thermochemical cycle systems use catalysts to convert heat into hydrogen or electricity, thus regenerating energy from thermal waste [20–22]. Another important application is chemical energy storage, where catalysts enable the conversion of surplus renewable energy (e.g. solar or wind energy) into chemical forms that can be stored. Technologies such as power-to-gas rely on catalytic processes to convert excess electricity into hydrogen or methane, enabling long-term energy storage and later utilisation [23]. Catalysts also play a crucial role in the conversion of biomass, where organic materials are converted into biofuels or other energy-rich substances. This process regenerates energy from renewable sources, which aligns with the principles of the circular economy and represents a sustainable alternative to fossil fuels. In essence, catalytic energy recovery offers an important means of improving energy efficiency, reducing waste and supporting the global transition to cleaner, renewable energy systems.

Several studies have reviewed advances in heterogeneous catalysis. Chen, et al. [25] explored computational methods, focusing on microkinetic modeling and kinetic Monte Carlo simulations, while Mou, et al. [26] discussed machine learning applications in catalyst discovery and reaction pathway analysis. Vogt and Weckhuysen [27] examined key concepts such as turnover frequency and structure sensitivity, comparing catalytic principles from enzymatic and homogeneous catalysis. Other reviews focused on biodiesel production using heterogeneous catalysts [28–30], microwave-assisted catalysis [31], metal-organic frameworks [32], and ammonia synthesis [33]. Recent reviews by Li, et al. [34] and Zhang, et al. [35] examined liquid biofuel synthesis from lignocellulose and CO_2 conversion into carboxylic acids, respectively. While these studies cover various aspects of heterogeneous catalysis, the cost and environmental implications of these processes have often been overlooked and insufficiently addressed. This review aims to fill that gap by providing a comprehensive overview of heterogeneous catalysts employed in biomass conversion to fuels and petrochemicals, with special attention to their techno-economic and environmental impacts. The study also highlights current perspectives, challenges and prospects for improved heterogeneous catalysis.

1.1. Bibliometric analysis of research trends in heterogeneous catalysis

To understand the evolving research trends in heterogeneous catalysis, a bibliometric analysis was conducted using the Web of Science database, focusing on publications related to heterogeneous catalysis for renewable energy and petrochemical production from biomass. This approach provided a comprehensive overview of the field's development, highlighting key growth areas and emerging research priorities. To ensure the precision and relevance of the data, keywords such as "heterogeneous catalysis," "heterogeneous catalyst," "biomass valorisation," "biomass conversion," "renewable energy," "fuel," and "petrochemical" were used. The search was restricted to the period from 2000 to 2025 and included only articles and review articles published in English. Research areas of interest included chemistry, engineering, material science, environmental science, and energy and fuels. Special attention was given to studies contributing to Sustainable Development Goals (SDGs) 7 (Affordable and Clean Energy), 12 (Responsible Consumption and Production), and 13 (Climate Action). After applying these criteria, 1206 research documents were retrieved, with China leading in research output (407 publications), followed by India (106), the USA (103), Germany (95), and Spain (80), indicating China's dominant role in advancing this research field over the past two decades. To assess the research trends in heterogeneous catalysis within the academic community, the co-occurrence counting method was employed

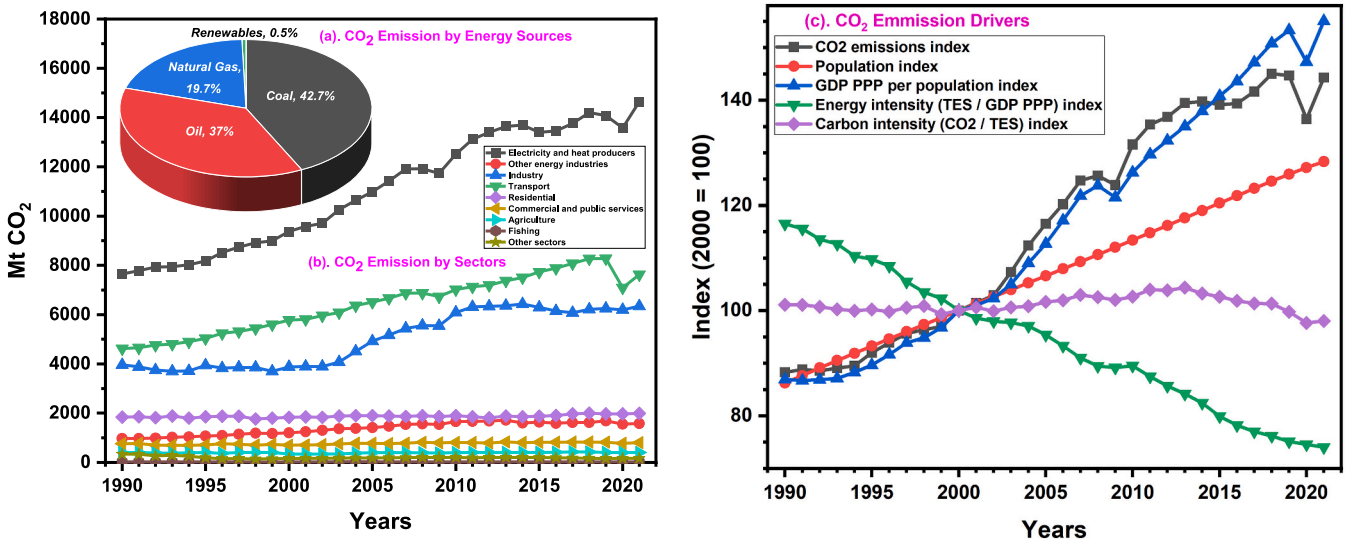

Fig. 1. CO_2 Emissions by (a) sectors and (b) energy sources from 1990 to 2021 [24]. (c) CO_2 emission drivers showing trends from 1990 to 2021 [24].

using VOSviewer (*v1.6.20*). A minimum threshold of 15 keyword occurrences was applied, yielding 147 qualifying keywords. The resulting visualization map generated by VOSviewer highlights the prominence and interrelationships of key terms, offering insight into the major research themes and areas of focus within the dataset (Fig. 2a).

The quantitative trend in publications shows steady growth from 2000 to 2025, increasing from 6 publications in 2000 to 86 in 2020, with notable peaks during 2017 and 2020. A slight dip was observed in 2019, where publication output dropped to 59, possibly due to shifts in funding priorities, emerging focus on other renewable technologies, and global economic uncertainties prior to the pandemic (Fig. 2b). After 2019, research activity rebounded strongly, reflecting renewed international commitment to sustainable energy transitions. As of April 2025, 23 publications have been recorded; extrapolating based on the average monthly publication rate suggests that approximately 65–75 papers could be published by the end of the year. The bibliometric analysis highlights the growing interest in heterogeneous catalysis for energy production, particularly in renewable and sustainable technologies, but underscores the need for continued exploration in this field. The field of heterogeneous catalysis for biomass valorisation remains vibrant and integral to achieving global sustainability and clean energy goals.

1.2. Energy sources – overview of fossil fuel and renewable energy sources

Energy is now an essential part of people's way of life worldwide and a vital factor for the development of any country. It also has a significant impact on the ecosystem. When it comes to meeting the global energy needs, fossil fuels and renewable energy sources are of great importance. Fossil fuels, including oil, coal and natural gas, are responsible for 80 % of the world's energy consumption. However, the combustion of fossil fuels leads to an increase in greenhouse gas (GHG) emissions and contributes to climate change [36]. On the other hand, renewable energy sources such as solar, wind, and wave energy offer alternatives to fossil fuels that are less harmful to the environment. Not only are these sources

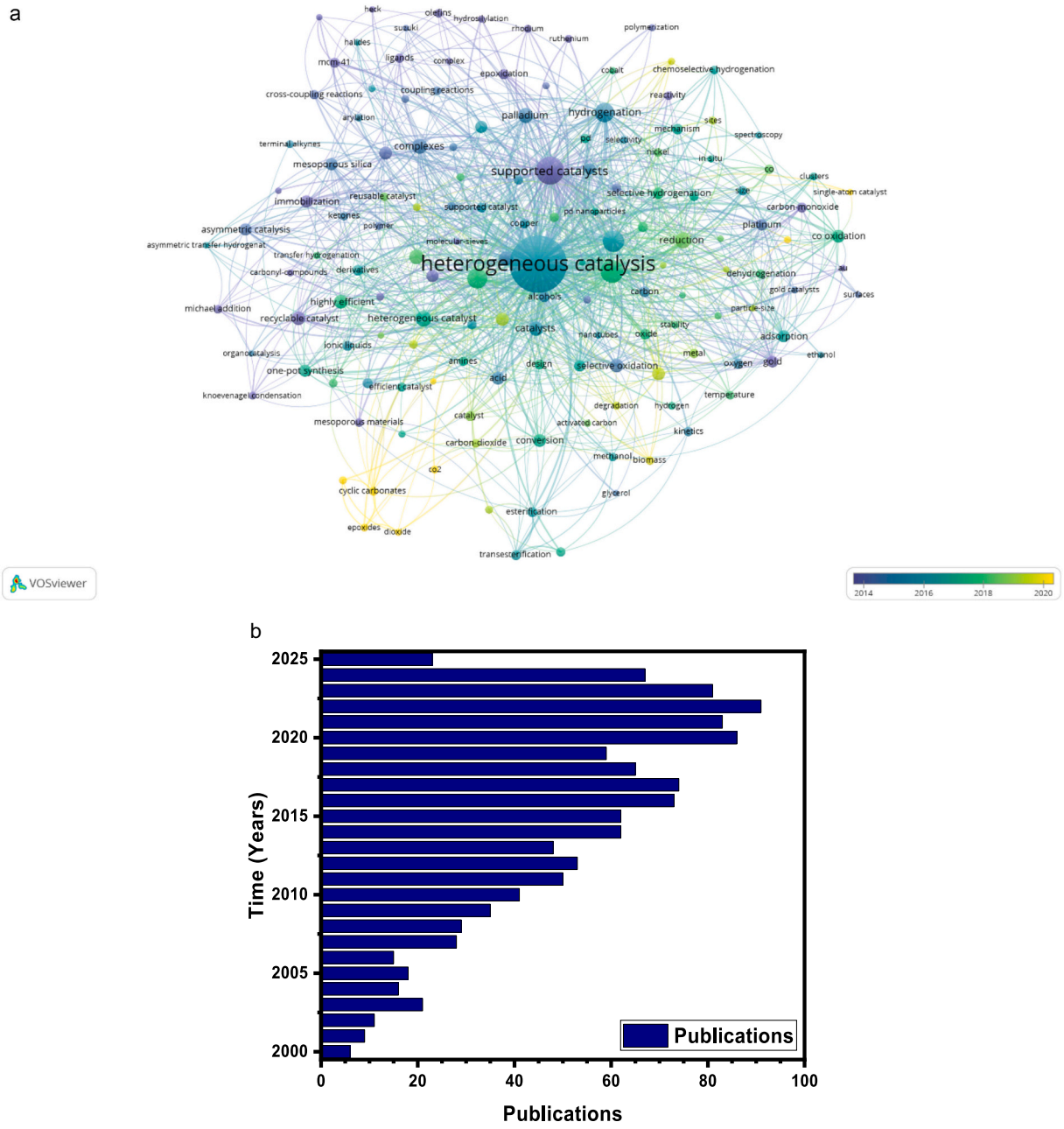

Fig. 2. a. Overlay visual of keyword distribution across average publication year. b. Research/publication trends on heterogeneous catalysis from 2000 to 2025.

inherently renewable, but they also do not run out over time [37]. Although renewable energy sources have advantages, including the ability to reduce environmental impact and the fact that they are sustainable, they also have disadvantages, including high initial prices and dependence on certain weather conditions. Therefore, it is important to mix renewable and non-renewable energy sources to meet the demands of the global energy market. Combining combined heat and power (CHP) with renewable energy sources is one method used to improve the efficiency of renewable energy technologies [37].

1.2.1. The place of fossil fuel in the present decade

Fossil fuels continue to play a critical role in the global energy mix, with oil, natural gas, and coal being the primary sources of energy consumption, accounting for 80 % of global energy. Despite a declining share, fossil fuels are expected to dominate energy consumption until 2050 due to their energy intensity, reliability, and lack of easily substitutable alternatives. The target for carbon neutrality by 2035 has motivated a decision on the phasing out of fossil fuels. Michaux, et al. [38] reported the phasing out of fossil fuels in Finland. Oil is particularly important as it supplies a significant proportion of the world's energy and serves as the predominant transportation fuel. An oil shortage could lead to bottlenecks in the supply of all other fossil fuels. Although alternative energy sources such as renewables have the growth potential, they are likely to continue to dominate, given the increasing global demand for energy and the advantages of fossil fuels in terms of energy density and transportability [39,40]. Fossil fuel extraction and combustion contribute to global CO_2 emissions, with major producers responsible for a substantial portion of industrial emissions. Moreover, the exploration and exploitation of fossil fuels lead to water resources being polluted, affecting aquatic ecosystems [41]. Additionally, the toxic chemicals in crude oil, such as benzene, pose health risks to humans and marine life when oil spills occur [42]. According to the International Energy Agency, IEA [2], oil and gas operations account for 15 % of global energy-related greenhouse gas (GHG) emissions. The place of fossil fuels in the present decade is undergoing significant scrutiny and transition. While fossil fuels have long been the dominant source of energy globally, concerns over climate change, air pollution, and energy security are driving a shift towards cleaner and more sustainable alternatives.

Despite efforts to phase out fossil fuels for carbon neutrality by 2035, they continue to be critical, especially crude oil, which is vital for the production of transportation. However, the environmental impact of fossil fuel extraction and use is significant, contributing heavily to CO_2 emissions and pollution. As concerns over climate change and energy security grow, there is increasing momentum to transition towards cleaner, more sustainable energy alternatives.

1.2.2. Renewable energy sources

Renewable energy sources dominate the discussion in today's environmental crisis due to pollution, climate change, and ecosystem disruption. Renewable energy sources are forms of energy derived from natural processes that are replenished on a human timescale. These sources are abundant, environmentally friendly, and offer significant potential to meet global energy needs while minimising GHG emissions and mitigating climate change [43]. However, many challenges are associated with the commercial deployment of some of the renewable energy technologies, which necessitate further research to improve their performance. Table 1 shows various renewable energy sources, the associated technological challenges, and current research directions. Renewable energy sources offer diverse options for meeting energy demand while reducing environmental impacts and advancing sustainable development goals. Continued technological innovation, policy support, and investment are essential to accelerate the transition to a renewable energy future. Hao, et al. [44] reported a 5.4 % efficiency improvement in clean energy using digitalization. The most discussed renewable energy sources are wind, direct, solar, hydropower, geothermal, ocean,

Table 1
Technological research directions to renewable energy sources.

Renewable energy sources	Advances in process and technologies	Ref.
Solar Energy	• Materials, catalysis, and thermal storage advances boost solar energy and photovoltaic performance. • Aggregation-induced emission (AIE) materials aid luminescent solar concentrators and solar steam generation. • Cobalt-based nitrides are effective photo (electro)catalysis catalysts. • Innovations increase global solar capacity 20-fold, enhancing efficiency and power output. • Improved storage methods (flywheels, superconducting magnets, phase change materials) boost efficiency and cut costs.	[47,48]
Wind Energy	• Progress in wind farm systems and control for sustainable energy. • Improved modeling, optimization, and monitoring enhance turbine efficiency. • Focus on fault detection with vibration analysis, thermography, and machine learning. • Grid integration challenges due to voltage stability and power quality issues • Wind energy is one of the fastest-growing renewable energy sources globally.	[49,50]
Hydroelectric Power	• Hydroelectric power harnesses energy from flowing water via dams or river currents. • Turbines convert water's kinetic energy into electricity. • Large-scale hydroelectric projects are a mature, reliable renewable energy source.	
Geothermal Energy	• Geothermal energy is derived from heat beneath the Earth's surface. • It can be used for electricity generation via geothermal power plants and for heating/cooling buildings via geothermal heat pumps. • Abundant and reliable, especially in regions with high geothermal activity. • Progress includes numerical modeling for optimal design • Advances in cooling systems and geothermal heat exchangers (vertical wells, piles, deep wells).	[51]
Tidal and Wave Energy	• Tidal and wave energy harnesses ocean tides and waves using tidal barrages, turbines, wave buoys, and oscillating water columns. • These technologies capture kinetic energy to generate renewable power. • Marine energy offers a consistent and predictable renewable energy source	[52]
Hydrogen Energy	• Hydrogen, produced via electrolysis with renewable electricity, is a versatile energy carrier for storing and transporting renewable energy. • It finds applications in transportation, heating, and industry, offering flexibility and zero-emission potential when sourced sustainably. • Advances include high-performance storage materials like magnesium and titanium-based metal hydrides. • Ongoing research focuses on electrolysis, storage techniques, fuel cells, and hydrogen use for clean energy development. • Future prospects include environmentally friendly hydrogen production methods and optimizing economic and energy efficiency supply chains.	[53–55]
Biomass Energy	• Biomass energy comes from organic materials like wood, agricultural residues, and organic waste. • Materials can be burned for heat or converted into biofuels (ethanol, biodiesel) for transport and electricity. • Biomass energy reduces fossil fuel reliance and helps manage organic waste.	

hydrogen, and bioenergy. Fig. 3a presents the global Total Energy Supply (TES) from different energy sources, highlighting the trends from 1990 to 2021. This data visualization provides insights into the changing energy landscape over the past three decades, showcasing the contributions of fossil fuels, renewables, and other energy sources to the global energy mix. The global Total Energy Production (TEP), focusing on the global share of biofuel production and its consumption from various sources, is shown in Fig. 3b & c. Fig. 3d & e shows the Total Final Consumption (TFC) of the various energy sources in the different sectors.

While the global energy landscape is often described through overarching trends, a more quantified understanding of the role of biomass is

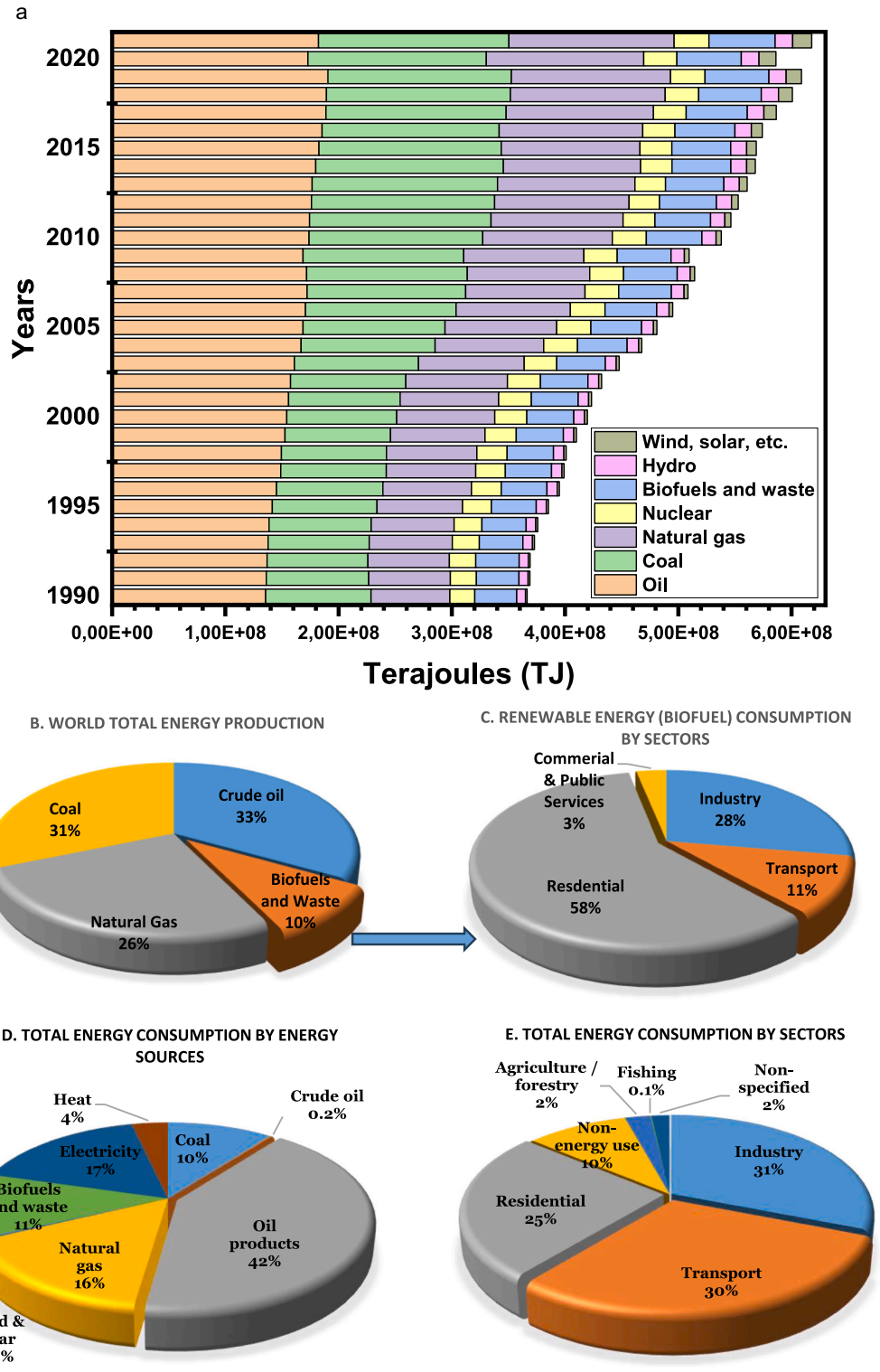

Fig. 3. a. Global Total Energy Supply (TES) from various energy sources (1990–2021) [24]. b. Global Total Energy Production (TEP), (c) Renewable energy (biofuel) consumption. (3d & e). Total Final Consumption (TFC) by (d) energy sources (e) sectors from 1990 to 2022 [24].

crucial for evaluating its strategic potential in future energy systems. According to the International Energy Agency (IEA), biomass currently contributes approximately 13 % of global final energy consumption IN 2023, with projections indicating a rise to over 20 % by 2030 under sustainable development scenarios [45]. In the transport sector alone, advanced biofuels derived from lignocellulosic biomass are expected to meet 27 % of liquid fuel demand by 2050 [46]. This highlights the urgent need for intensified research in biomass valorisation through heterogeneous catalysis.

1.2.2.1. Biomass as a source of clean energy. Biomass, which includes plant-derived products such as crops, algae, and wood, has emerged as a significant potential source of energy and chemicals that can compete with traditional fossil fuels. Cellulose, hemicellulose, and lignin are the main components of biomass. Lignin, an essential component of plant cell walls, acts as a binder within the lignocellulose matrix and provides strength and rigidity by cross-linking with carbohydrate polymers [56]. It performs this function by filling the voids between cellulose and hemicellulose. In recent years, biomass has surpassed hydroelectric energy as the primary domestic renewable energy source in the United States, while the European Union derives approximately 66 % of its renewable energy from biomass, surpassing the contribution of other renewable sources. In addition, biomass is the only renewable source of liquid fuels for transport, making its chemical production essential [57]. Over the last three decades, three generations of biomass products have emerged, each defined by its type. In the 21st century, new renewable forms of energy are expected, especially bioenergy, to replace petroleum as the primary energy source [56].

Although the petroleum refinery of the 20th century and the biorefinery of the 21st century have similarities, there are notable differences. Originally, the petroleum refinery produced a limited range of products and had a limited number of chemical and energy components. It took considerable effort over decades to develop the oil refinery into the highly efficient and interconnected system it is today, with catalytic innovations enabling many breakthroughs. Similarly, today's biorefineries are nascent, producing a limited number of chemicals, mainly ethanol or bio-oils, with minimal integration of energy and chemistry. However, advances in catalyst technology promise to transform biorefineries into efficient, integrated systems capable of meeting the demand for chemicals and fuels in the 21st century. To achieve this transformation, catalytic processes for lignin, a biomass waste product, must be developed to extract high-value feedstocks for bulk and speciality chemicals. This conversion is critical as lignin is the only renewable source from which to produce aromatic chemicals essential to society [56].

Different types of biomass feedstocks and energy requirements can be met using several technologies to convert biomass into energy. Fig. 4 shows some common biomass-to-energy conversion technologies and their derivatives. Several aspects, including the type and accessibility of the biomass feedstock, energy demand, environmental concerns, and economic feasibility, influence the choice of biomass conversion technology [58]. The valorisation of biomass for bioenergy production involves three strategies: gasification to produce synthesis gas, pyrolysis to produce small molecules that can be used for chemical production, and the extensive removal of functional groups from lignin monomers, leading to the production of simple aromatic compounds. Catalyst technologies originally developed for petroleum refineries convert these platform chemicals into bulk and fine chemicals. In addition, biomass can be converted directly into useful chemicals using highly selective catalysts, facilitating the synthesis of complex aromatics that are not easily accessible by standard petrochemical methods. Separation of products is critical in any process to accurately assess the environmental impact. By integrating several biomass conversion technologies or merging biomass plants with other industrial processes, efficiency and sustainability can be further improved [59].

Biomass thus promises to become a major component in future energy systems, particularly through the development of advanced technologies that maximize the utilisation of its raw materials.

2. Catalyst study and feedstock compatibility for energy production

2.1. Advances in heterogeneous catalyst development and application for renewable energy production

From the Stone Age to the present, humanity has tried to produce and utilize various materials. The development of civilisations was closely linked to the materials they used, as the Stone Age, Bronze Age, and Iron Age show. Dealing with this constant need for new materials is the domain of materials science, which is crucial for progress in all industries and technologies. According to the International Union of Pure and Applied Chemistry (IUPAC) definition, catalysts accelerate reactions without altering the standard Gibbs energy change [60]. In catalysis, the acceleration of reactions is driven by catalysts that serve as

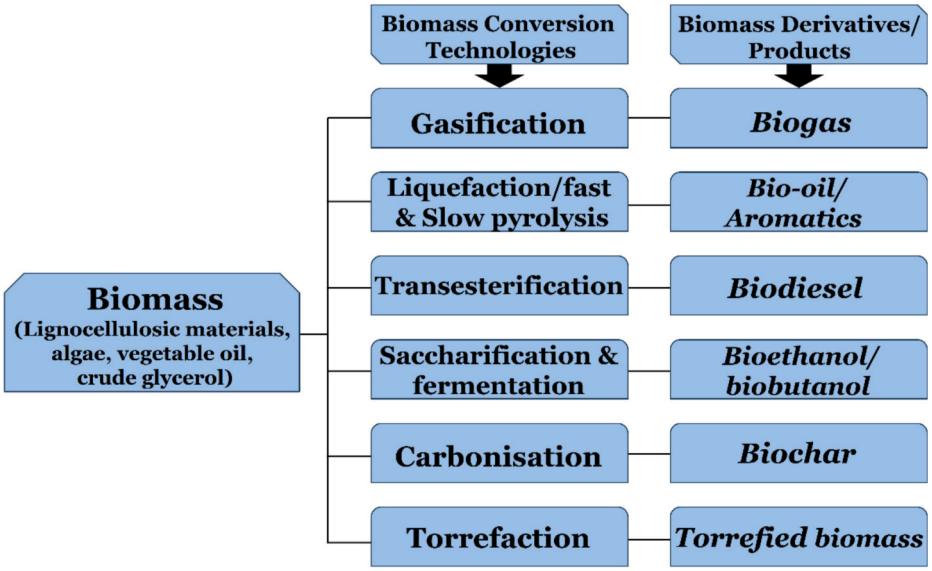

Fig. 4. Biomass conversion routes to energy.

intermediaries, facilitating the conversion of reactants into products without being consumed themselves in the process. Importantly, catalysts do not affect the thermodynamic equilibrium after the complete reaction. It is crucial to improve both performance and selectivity to optimize catalytic processes. The catalytic materials must be customised to have the required structures and distribution of active sites to achieve this. A range of materials such as zeolites, Aluminophosphate (AlPO), Silicoaluminophosphate (SAPO), mesoporous materials, Pillared Interlayered Clays (PILCs), and Metal-Organic Framework (MOFs) enables this level of customisation. These materials provide a controlled, large surface area for catalysis and ensure easy access to the active sites without needing individual fine particles. An important application of these porous solid catalysts is the replacement of environmentally harmful and corrosive homogeneous catalysts used in liquid-phase chemical synthesis [61].

Unlike most heterogeneous catalysts, homogeneous catalysts can be dissolved in the reaction medium, creating a uniform dispersion that enhances catalytic performance. In addition, homogeneous catalysts have high activity, selectivity, adaptability, and reproductivity with low reaction temperature and reaction time to promote catalytic activities [62,63]. However, the low thermodynamic and pressure stability, difficult separation, and recoverability of homogenous catalysts make heterogeneous catalysts advantageous for enduring high temperatures and pressure with easy separation and recyclability after a reaction [64]. Homogeneous catalysts, such as mineral and Lewis acids, organic and inorganic bases, and toxic metal compounds, are difficult to separate and dispose of [65,66]. Table 2 shows the comparative evaluation of homogeneous and heterogeneous catalysts.

Solid heterogeneous catalysts come in various families, such as metals, oxides, sulphides, and carbons, either in bulk form or as supports on catalytically active materials like silica, alumina, zirconia, and titanium [67,68]. These materials can have specific chemical properties such as acid, redox, dehydrogenation, hydrogenation, or oxidation capacity and physical properties such as porosity, large surface area, attrition resistance, and thermal or electrical conductivity. Among the variety of solid catalysts, zeolites, clays, mesoporous materials, and mixed oxides (Fig. 5) are usually employed in biofuel production [69]. Oxides are versatile and act as both catalysts and supports. Porous materials offer several unique properties essential for catalytic applications, including biofuel production [57]. Heterogeneous catalysis is vital in various chemical processes, offering distinct benefits such as selectivity and reusability [70,71]. Its pivotal role extends across various industrial operations, enhancing economic efficiencies and yielding environmental advantages surpassing traditional methods. Heterogeneous catalysis drives economic advantages through improved process efficiency, reduced energy consumption, and lowered production costs. Heterogeneous catalysts with high activity and selectivity contribute to increased yields and superior product quality, leading to enhanced profitability. Moreover, the recyclability and durability of heterogeneous catalysts can reduce operational expenses by minimising the need for frequent catalyst replacement [71].

Materials science has driven human progress, from the Stone Age to modern times. Catalysts accelerate reactions without altering their equilibrium and are critical in advancing industrial processes. Porous solid catalysts like zeolites and mixed oxides offer superior performance over traditional, harmful homogeneous catalysts, boosting efficiency and sustainability. Heterogeneous catalysis enhances process efficiency, reduces energy consumption, and provides economic and environmental benefits by improving product yields and lowering costs. This makes it essential for both the industry and sustainable energy solutions.

As efforts are made to develop environmentally friendly and efficient renewable energy sources, catalysts have become an indispensable part of this pursuit. To advance the development of renewable energy technologies, it is crucial to thoroughly investigate the catalytic performance and potential contribution of various catalysts, including zeolite catalysts, hierarchical zeolites, carbon materials, metal-organic frameworks (MOFs), and mesoporous materials. By comprehensively analysing these catalysts' properties, mechanisms, and performance metrics, valuable insights can be gained into their potential application in sustainable energy solutions. This will, therefore, contribute to the ongoing global transition to renewable energy sources.

2.1.1. Zeolite catalysts

Zeolites are a group of microporous crystalline aluminosilicate materials with catalytic properties that can be modified. These materials contain heteroatom-containing active sites arranged in homogeneous environments as delineated by the framework consisting of microspores intersections and channels [72]. Their porous structure acts like millions of test tubes enclosing molecules and atoms to enable chemical reactions. The diverse catalytic capabilities of zeolites are due to their ion exchange properties, pore size structure, and chemical composition [73]. Zeolites are crystalline aluminosilicates that occur in nature. They comprise oxygen, silicon (Si), and aluminium (Al). With an increasing Si/Al ratio, the structure becomes more stable and retains its stability even at higher temperatures. A representative structure of several typical zeolites is illustrated in Fig. 6a-d [74].

Hierarchical zeolites are formed by alkali treatment, which improves the pore structure and the accessibility of large molecular oxygen molecules to the active sites. This process creates secondary pores within the crystal lines by selectively removing Si atoms from the zeolite framework [75]. By adhering to this principle, mesoporosity can be generated in zeolites or metal oxide particles. It has been suggested that a combination of microporous and mesoporous materials offers advantages over only microporous or mesoporous materials. The reactant molecules are expected to diffuse more easily through these openings to reach the active zeolite sites [76]. The materials mentioned above exhibit improved hydrothermal stability [77], greater versatility in processing a wide range of feedstocks, better control over leaching rates to ensure consistent and progressive discharge of active components, and better ability to encapsulate waste within the micropores [78,79]. In recent years, numerous porous materials with a combination of micropores and mesopores have been developed, including zeolites, mesoporous titanium silicates (MTS), mesoporous aluminium silicates (MAS), plugged hexagonal templated silica (PHTS), and SBA-15.

Table 2
Comparative merits and demerits of homogeneous and heterogeneous catalysts [62].

Parameter	Homogenous catalysts	Heterogeneous catalysts
Solubility of the catalyst	Soluble	Insoluble
Physical nature of the catalyst during the reaction	Liquid phase, however insensitive to fatty acid and water content	Usually, a distinct solid phase
Optimal operating pH	Very active in acidic medium	Active in a wide range
Reusability of the catalyst	Difficult to recover and reuse	Possible recovery and reusability
Separation of catalysts from the aqueous phase	Expensive and difficult to separate	Readily separated
Reaction phase and time	Occurs in the liquid phase with a short life, which requires an extensive purification step	Generally, occurs on the catalyst surface, with long life and fewer purification steps.

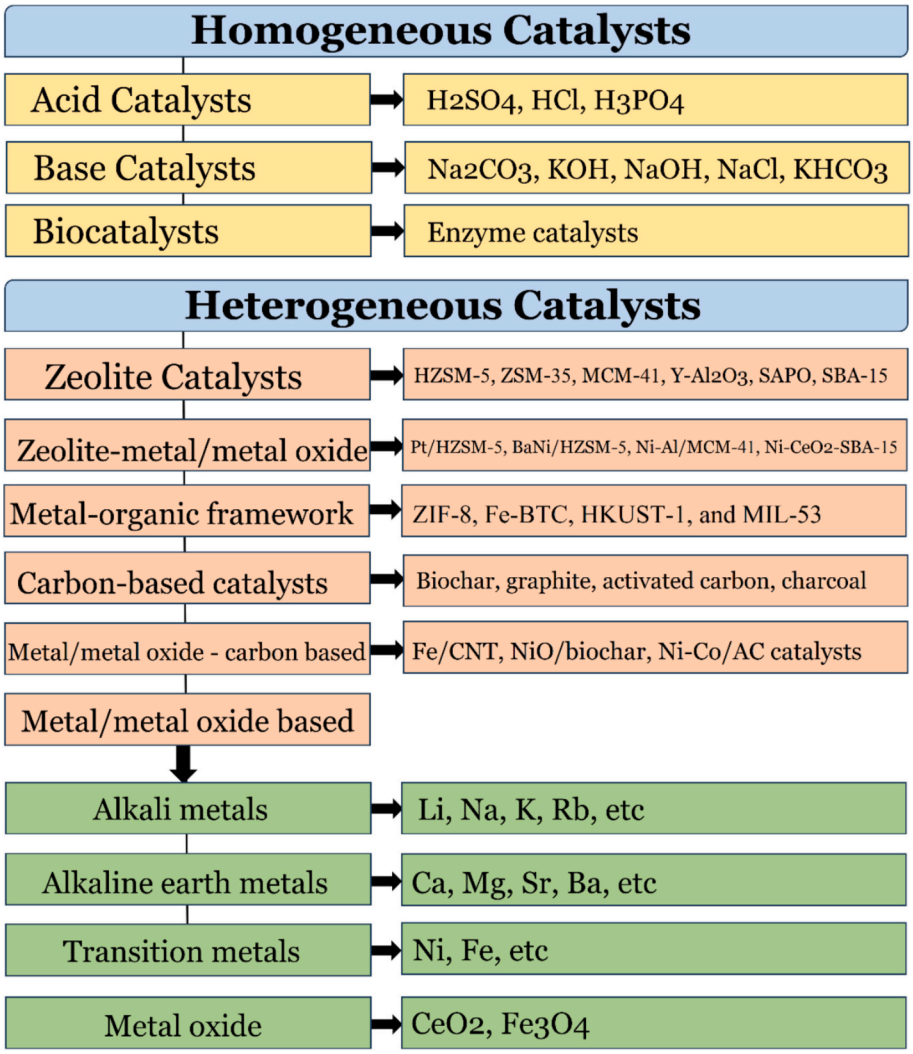

Fig. 5. Classification of homogeneous and heterogeneous catalysts for energy production.

Zeolite catalysts, particularly hierarchical zeolites, show great promise in biomass conversion to fuels and chemicals due to their structural and catalytic properties. Zeolites like ZSM-5, SAPO-34, and SAPO-11 have effectively converted biomass derivatives into valuable products such as BTX (benzene, toluene, xylenes). Zhang et al. [80] demonstrated the catalytic pyrolysis of corn cobs using HZSM-5, which produced bio-oil with a 25 % reduction in oxygen content and a high heating value (34.6 MJ/kg), comparable to diesel and heavy fuel oil. Similarly, Hernando et al. [81] showed that MgO-loaded hierarchical HZSM-5 produced bio-oil with higher energy yields and lower oxygen content. Hierarchical zeolites, with micropores and mesopores, enhance performance in processes like thermochemical and catalytic fast pyrolysis (CFP) of biomass. Anekwe, et al. [82] evaluated hierarchical Co/HZSM-5 and Fe/HZSM-5 for bioethanol conversion into fuel blendstocks and petrochemicals, achieving over 97 % bioethanol conversion. Lower space velocities (5 h^{-1}) favoured gaseous hydrocarbons (C_1-C_4), while higher velocities (12h^{-1}) increased liquid fuel blendstocks (C_5+), with metal-doped catalysts showing higher selectivity (>79 %) and enhanced aromatic production, particularly benzene. Luo, et al. [83] found that catalytic conversion of acetone, butanol, and ethanol using 2 % Ni/HBET led to excessive ether formation, reducing bio-jet fuel quality and selectivity. However, a dual catalyst bed (HSAPO-34 and Ni/HBET) improved bio-jet fuel production, achieving a 95.3 % conversion rate and 83.0 % selectivity for C_9-C_{16} hydrocarbons by reducing ether formation and increasing lighter olefin selectivity.

In addition, zeolite-based catalysts have also been employed in biomass conversion to petrochemicals. Deng et al. [84] explored various zeolite catalysts (HZSM-5, NaZSM-5, HY, ReY) for biomass conversion into aromatic compounds, with HZSM-5 showing the highest activity. Qiao, et al. [85] synthesised hierarchical ZSM-5 by alkali treatment with TPAOH, Na_2CO_3, and NaOH. The structure exhibited a greater number of strongly acidic sites, which was due to more regulated desilication by Na_2CO_3 (0.4 M - 0.8 M). Micro- and mesoporosity were also observed. Hierarchical ZSM-5 treated with Na_2CO_3 (0.6 M) exhibited increased selectivity towards BTX (benzene, toluene, and xylenes), which reduced the amount of polyaromatic hydrocarbons produced. After the treatment of hierarchical HZSM-5 with NaOH solution, the yield and physical properties of the organic phase were improved, and a significant reduction in coke formation on the catalyst surface was observed [86]. After desilicating hierarchical HZSM-5 with 0.3 M NaOH [87], the carbon yield of BTX had increased, and the micropores and mesopores formed had been preserved. This process was carried out for the catalytic cracking of cardboard waste. Due to the improved adsorption and diffusion, the intermediates in the hierarchical pores have an extended lifetime of up to 120 h. Consequently, the conversion of methanol to aromatics resulted in a higher yield of aromatics when hierarchical Zn/ZSM-5 was treated with 0.2 M NaOH. Lower NaOH concentrations (≤0.4) had a remarkable effect on the catalytic activity, namely on the lifespan of hierarchical HZSM-5 and its selectivity towards BTX in the aromatisation of glycerol [88]. Recently, improved mass transfer via

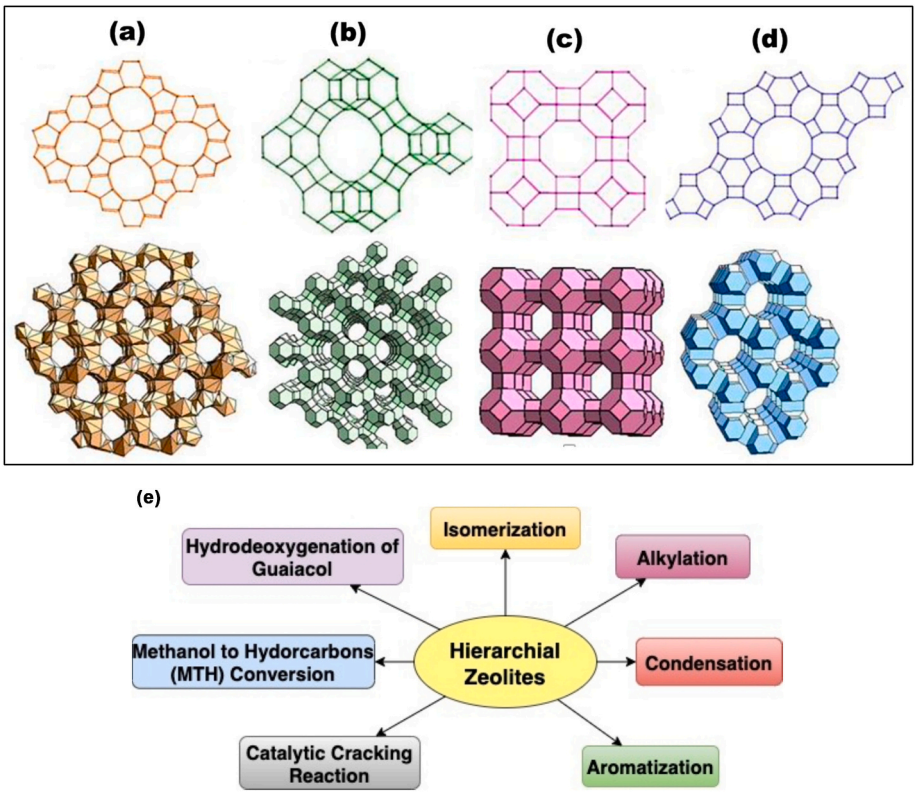

Fig. 6. a. Representative structures of various zeolite frameworks, illustrating their pore openings and dimensionalities: (a) Zeolite L with a one-dimensional (1D) channel system and a pore opening of 7.1 Å; (b) Zeolite Y featuring a three-dimensional (3D) pore network with 7.4 Å openings; (c) Zeolite A, also with a three-dimensional channel structure and 4.2 Å pore openings; (d) ZSM-5 (silicalite), exhibiting a two-dimensional (2D) channel system with pore openings of 5.3 × 5.6 Å and 5.1 × 5.5 Å. These frameworks demonstrate the diversity of zeolite pore structures, which are key to their catalytic performance in various applications. Adapted from Ref. [92]. e. Hierarchical zeolites and their applications in catalytic reactions.

hierarchical zeolites treated with NaOH has been associated with higher production of heavy hydrocarbons [88,89]. Fig. 6e shows the application of hierarchical zeolites in various catalytic reactions [90,91].

Zeolites are widely valued for their catalytic properties, which can be enhanced through ion exchange, pore size adjustment, and chemical composition modifications. Hierarchical zeolites, produced through alkali treatment, create secondary mesopores that improve molecular diffusion and accessibility to active sites, enhancing their performance in catalytic reactions. These materials exhibit superior hydrothermal stability and process versatility. Research shows that hierarchical zeolites, like ZSM-5, significantly improve desired product yields while reducing by-products like coke during reactions. These studies

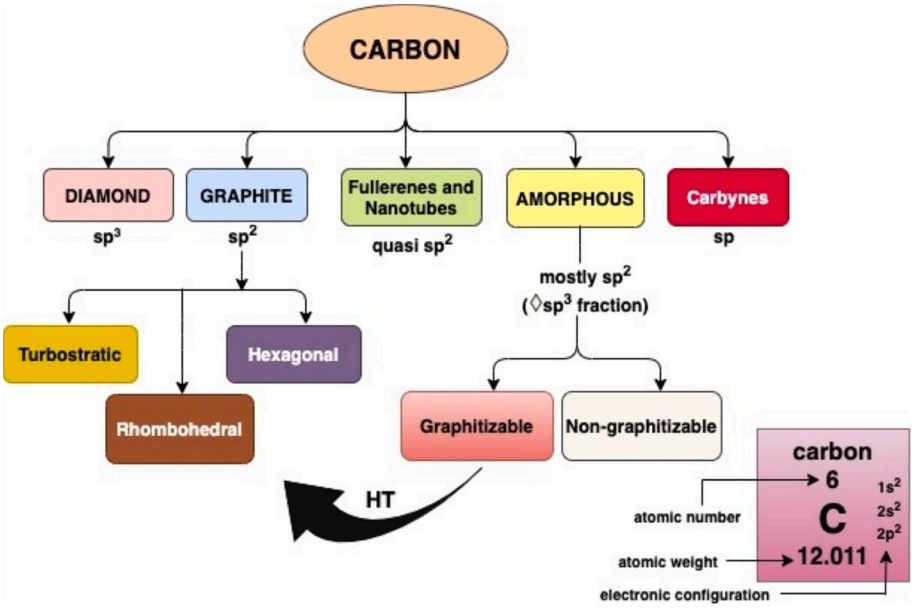

Fig. 7. Allotropes of the element carbon. Adapted and modified from Ref. [103].

collectively highlight the versatility and efficiency of zeolite catalysts, particularly hierarchical zeolites, in biomass conversion processes for producing fuels and valuable chemicals, making them indispensable in sustainable energy and chemical production.

2.1.2. Carbon materials

Carbon-based materials are the most adaptable materials used in modern environmental science/engineering, as well as sustainable energy. Conventional carbon materials, including activated carbon (AC), carbon cloth (CC), and graphite, are inexpensive, readily available, and easy to produce. Conversely, carbon nanotubes (CNTs) and graphene (GA) stand out as nanocarbon materials widely employed in heterogeneous catalysis owing to their expansive specific surface area, exceptional electrical conductivity, and intricately crafted porous structures [93–96]. Carbon materials are categorized based on their pore size into microporous (<2 nm), macroporous (>50 nm), or mesoporous (2–50 nm). All three levels of pores are present in trimodal porous materials. Diamond, graphite, and charcoal are known carbonaceous materials occurring naturally. An overview of the primary carbon allotropes, ordered by atomic arrangement and hybridisation state, can be found in Fig. 7.

Carbon black and activated carbons with a large surface area are the preferred materials for carbon-based catalysts due to their widespread availability and cost-effectiveness. At around 1500 °C, amorphous carbon is converted into carbon black through the pyrolysis of hydrocarbon precursors or organic polymers. The remaining basic carbon atoms, randomly cross-linked with unbound interstices, reorganise into layers of flat aromatic sheets. The resulting carbon materials consist of almost planar layers of sp^2-hybridised carbons. The substances have a crystalline architecture, but their range is limited, so there is no stacking direction. Activated carbon is produced through either physical or chemical activation processes. Physical activation at temperatures of 600–900 °C is used to pyrolyse carbon compounds without the presence of oxygen. When carbonised substances are subjected to oxidizing atmospheres such as steam or oxygen within the temperature range of 600–1200 °C, they undergo oxidation. Following carbonisation at 450–900 °C, chemical activation occurs by impregnating the raw material with an acid, a strong base, or a salt ($ZnCl_2$ or $CaCl_2$). This method is favoured due to the lower temperature and time required for material activation. The structure cross-linked by aliphatic bridging groups can most accurately describe an intricate network of defective carbon layers. In the form of an amorphous solid, activated carbon is characterized by a large pore volume and an exceptionally high internal surface area.

Liu and Wu [97] developed cost-effective nitrogen-doped carbon materials with a graphene-like structure through pyrolysis in a tube furnace, using waste lignin and Ni powder as starting materials. These properties make them promising candidates for applications such as oxygen reduction reaction catalysts, catalyst carriers, and hydrogen fuel cells. Kong, et al. [98] synthesised biochar-based catalysts (Fe-MEC, Ni-MEC, and Co-MEC) by loading nano-sized Fe, Ni, and Co onto biochar derived from sequoia wood chips via microwave heating. These catalysts were used for the catalytic pyrolysis of polystyrene powder. The results indicated that all three catalysts had a large specific surface area and well-developed pore structures. The Fe, Ni, and Co nanoparticles on the bio-char surface showed high catalytic activity in breaking C—C and C—H bonds in the bio-oil, significantly increasing bio-oil yields (91 %, 82 %, and 90 % for Fe-MEC, Ni-MEC, and Co-MEC, respectively) and enhancing bio-oil quality. Additionally, the catalysts demonstrated excellent stability, with no significant reduction in bio-oil yield even after five cycles of reuse [98].

Sulphonated CMK-3 (ordered mesoporous carbon) was used for cellulose hydrolysis and achieved a conversion rate of 94.4 % and a glucose yield of 74.5 % [99]. Increasing the temperature from 150 to 300 °C increases the acid density, but the specific surface area reaches its maximum at 250 °C. Mesoporosity influences glucan adsorption, as seen with mesoporous carbon nanoparticles (MCN) [100]. Cellulose can also be converted to C_2–C_6 polyols with a Ru/CNT catalyst in the presence of hydrogen. [101]. This process takes two steps: First, cellulose is hydrolysed by acid-functionalised CNTs to reducing sugars, which Ru then hydrogenates to sugar alcohols. The yield of sorbitol improves as the crystallinity of the carbon carrier decreases. Another example of a multifunctional catalyst is tungsten carbide nanoparticles on three-dimensional mesoporous carbon (MC), which achieve an efficiency of 72.9 % in the direct conversion of cellulose to ethylene glycol [102].

Carbon-based materials, particularly activated carbon and nanomaterials, offer versatile and efficient solutions for environmental and energy applications, owing to their structural and functional properties. Conventional materials like activated carbon, carbon cloth, and graphite are widely used for their ease of production and affordability, while nanocarbon materials like carbon nanotubes and graphene are highly valued in catalysis for their large surface area, high electrical conductivity, and porous structures.

2.1.3. Metal-organic frameworks (MOF)

Metal-organic frameworks (MOFs), or porous coordination polymers (PCPs), are crystalline materials exhibiting porosity in two or three dimensions. The synthesis of secondary building units (SBUs), comprised of metal cation compounds or clusters and polydentate organic ligands forming coordination-like bonds, yields materials characterized by infinite lattices [104–107]. Their structure is malleable and can be altered after synthesis by post-synthesis modification (PSM) and by varying the character of the metal cations and linkers [108]. MOFs combine mesoporous and microporous materials and have extremely large surface areas, which, according to BET, are up to 10,000 m^2/g and thus significantly larger than the surface areas of zeolites and activated carbon. In the 1990s, the research groups of Hoskins [109], Gardner [110], Yaghi [111], Munakata [112] and Riou [113] promoted and emphasised the continuous development and use of MOF structures and applications. To date, over 20,000 MOF structures have been documented. BASF has successfully produced MOFs on a tonne scale, now available through MOF Technologies, Sigma-Aldrich, and Strem Chemical. Among the most widely utilized MOFs are ZIF-8, Fe-BTC, HKUST-1, and MIL-53. In addition to gas storage, catalysis, proton conductivity, drug delivery, chemical sensing, and energy conversion, these materials are used in the textile industry and oleochemistry, food packaging, electric car prototypes, transportation, and respiratory systems [104–107,114].

MOFs serve as superb catalyst templates owing to their functional organic linkers, metal centres, remarkably large surface areas, well-defined porous structures, and uniform pore sizes and environments. After the thermal removal of water ligands, vacant coordination sites emerge within the metal nodes of the MOF structure, such as Cr [115], Mn [116], or Cu [117,118], with minimal alterations to the structure. When used individually or in conjunction with encapsulated NPs, coordinatively unsaturated metal sites exhibit exceptional Lewis acid catalytic activity. An alternative, highly effective method for integrating catalytically active metal sites into MOFs involves metallizing ligands positioned on the MOF linkers. This metallization process can occur either during the MOF synthesis or through post-synthesis modifications (PSM, Fig. 8a). MOFs are quite flexible when it comes to catalyst design due to their wide range of topologies. They can harbour different guests, such as semiconductor oxide NPs and metal. Finally, functional MOF groups can prevent the leaching of tiny cluster atoms. Pore confinement promotes the development of ultrafine nano-objects while hindering the growth of metal oxide and metal nanoparticles. As MOFs are insoluble, heterogeneous catalysis is ensured for easy regeneration, and their open channels favour the diffusion and transport of products and substrates with the lowest possible mass transfer limit. The uniform and variable pore configurations and dimensions of MOFs facilitate the ability to catalyse by size. MOFs can be combined with other nanostructures, such as nanotubes and graphene, to enhance conductivity. Calcination can also produce hybrid, catalytically active metal, carbon, and heteroatom

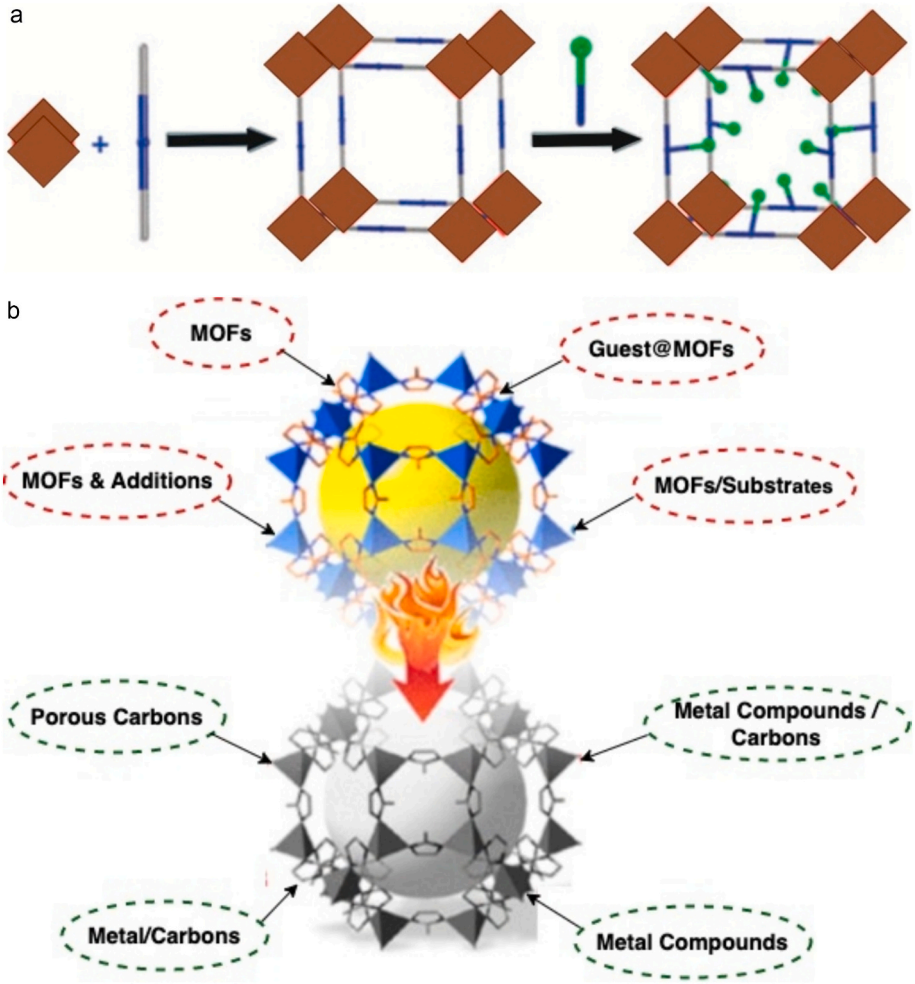

Fig. 8. a. The illustration of the Porous MOFs Postsynthetic Modification Principle. Adapted from Ref. [121]. b. Pyrolysis-based production of various porous materials from MOFs and MOF-based composites. Adapted and modified from Ref. [121].

nanocomposites (Fig. 8b) [119].

MOF-based catalysts, such as M/NC3 materials, have shown high activity in the liquid-phase conversion of model compounds and lignocellulosic biomass derivatives [120]. For example, benzyl alcohol, representing aromatic groups in lignin, was oxidised to benzaldehyde. Levulinic acid, a biomass-derived compound, was hydrogenated with various M/NC materials to γ-valerolactone and esterified to methyl levulinate. In all cases, M/NC3 materials obtained from the amino terephthalate IRMOF-3 performed better than M/NC1 materials from the terephthalate IRMOF-1, which was attributed to the smaller size of the M-NPs (M = Ru, W, V, Ti) [120]. The best results were obtained with Ru/NC3 for the hydrogenation of levulinic acid, where γ-valerolactone was obtained with 97 % yield and 100 % selectivity under the following conditions: Levulinic acid (1.36 mmol), H_2O (20 mL), 2 MPa N_2, 130 °C, 6 h, Ru/NC3 (Ru 8.64 μmol), with a catalyst-to-reactant ratio of 1:160 [120].

Metal-organic frameworks (MOFs), with their tunable porous structures and immense surface areas, represent a powerful platform for catalytic applications and energy solutions. Their ability to incorporate metal centers, functional linkers, and nanoscale guests within uniform pores makes them exceptional candidates for various industries, from environmental science to energy storage and conversion. The flexibility in MOF design allows for precise control over catalysis, offering significant advantages in reaction efficiency, selectivity, and catalyst regeneration.

2.1.4. *Mesoporous materials*

According to the IUPAC classification, materials featuring pores within the 2 to 50 nm range are designated as mesoporous [122–125]. Mesoporous materials are important in the world of materials due to their easily modifiable synthetic pore organization, adsorption capabilities, and catalytic and conductive properties [126–129]. Mesoporous materials are versatile for numerous applications, attributed to their substantial surface area and well-organized mesostructure. This characteristic facilitates the dispersion and adsorption of molecular particles, rendering them valuable across various domains [122,125]. Leveraging their structured support and extensive surface area, mesoporous materials afford control over the size and dispersion of supported metal particles, thus optimizing the utilisation of reactive metals. Following the identification of mesoporous materials, the need for improved separation and reaction capabilities led to considerable interest in silica-based and metal-substituted mesoporous materials. This was because of the potential applications in biomaterials, adsorption, separation, and nanoscale devices [130,131]. Hence, the possibility exists to generate a diverse array of isolated nanophase composites by manipulating the composition of chain architecture and the block copolymer species responsible for modifying and assembling the material. Various process variables such as pH, temperature, and environmental conditions control the complexation of the desired functional structures [126,132].

In 1992, researchers at Mobil Corporation introduced the pioneering discovery of mesoporous silica, marked by the identification of the M41S family of mesoporous materials [133–135]. Highly ordered mesoporous

silica has garnered significant attention in recent years owing to its substantial pore volume, tunable pore size (amenable to modification across a wide spectrum), controlled surface chemistry, and large surface area [136,137]. These properties render it an exceptionally favourable catalyst support or carrier, offering numerous advantageous applications in the fields of catalysis, separation, and adsorption. Since the discovery of mesoporous silica, substantial advancements have been achieved in composition variation, pore size modification, morphological manipulation, synthesis techniques, and applications [129,138]. In 1998, Zhao, et al. [133] conducted remarkable research in which they obtained "Santa Barbara Amorphous no. 15 (SBA-15)" mesostructured silica, which exhibited parallel hexagonal cylindrical pores and clustered pores. The range of pore sizes was 45–30 nm [139]. This shows that the research risk was worth it, as the material could be refined and further developed [128,133]. The channels are evenly arranged in a hexagonal pattern, which allows for narrow pore size distribution and adjustable pore size [140]. Since its discovery, SBA-15 has emerged as a promising support material for synthesizing novel catalytic materials [135].

Mesoporous oxides, bulk mixed oxides, microporous solids like zeolites, and metal-organic frameworks (MOFs) are widely used in heterogeneous catalysis, particularly in Fischer-Tropsch Synthesis (FTS) processes. These materials are critical in converting CO_2-rich syngas into valuable hydrocarbons and chemicals, offering sustainable pathways for synthetic fuel production and carbon utilisation. Zeolite catalysts such as HZSM-5 are known for their strong acidity and shape selectivity, facilitating the production of lower olefins and aromatic compounds. When combined with metals like Zinc, Cu, and Mn, Mesoporous oxides further enhance CO_2 conversion and hydrocarbon selectivity. Supported catalysts, such as cobalt or iron-based catalysts on oxide supports, are frequently employed in FTS due to their stability, high surface area, and ability to achieve high conversion rates of syngas to hydrocarbons [141]. Na-Fe_3O_4/HZSM-5, for example, showed a 73 % selectivity towards C_5–C_{11} hydrocarbons, including 40 % aromatics, at a CO_2 conversion rate of 33.6 % [142]. With their tunable porosity and high surface area, MOFs also show promise in CO_2 hydrogenation to methanol, which can be further processed into valuable hydrocarbons via zeolite-based systems. In addition, the combination of ZnZrOx and HZSM-5 achieved 74.7 % selectivity for aromatic compounds [143]. These catalysts improve hydrocarbon yields and contribute to more sustainable CO_2 utilisation in energy production.

Mesoporous materials, with their adaptable pore structures and high surface areas, are critical in catalysis and separation processes. Their ability to control metal particle dispersion and tailor pore sizes for specific applications makes them invaluable in material science. The evolution from M41S materials to SBA-15 has significantly expanded the possibilities for designing novel catalytic systems, showcasing the transformative potential of mesoporous silica in industrial applications.

2.1.5. Versatile heterogeneous catalytic systems

Recently, the combination of confinement and synergistic effects has been an effective method for creating heterogeneous catalytic systems that are adaptable and efficient. Thus, over the last 50 years, several studies have focused on immobilizing homogeneous catalysts on solid supports to produce heterogeneous catalysts [144]. This method allows easy separation of the catalyst from the reactants and products. To reduce the detrimental effects of the support surfaces on the catalytic sites and to preserve the homogeneous metal complex environment of the ligands with a long spacer and, consequently, the catalytic capabilities, the active sites were initially designed to be distant from the support surfaces [145]. Later, it was discovered that support could even favour the anchored homogeneous catalysts in various ways, including confinement [146] and synergistic effects [147]. This would allow the synthesis and study of heterogeneous bifunctional and even trifunctional catalysts, as synergies between multifunctional groups could occur under controlled conditions. Synthesizing heterogeneous catalysts with improved enantioselectivity after introducing chiral catalysts in confined regions was a crucial additional goal. Raja and Thomas [148], for example, have shown that chiral RhI complexes introduced into the channels of mesoporous silica increase the enantioselectivity (ee% 53–94 %) in asymmetric hydrogenation processes, in contrast to the racemic products formed during homogeneous catalysis. Furthermore, Yu, et al. [149] showed that incorporating the bifunctional catalyst 9-thiourea-epi-quinine into the channels of mesoporous silica SBA-15 significantly enhanced the selectivity and enantioselectivity of the heterogeneous catalyst (92.5 % selectivity and 99.2 % ee compared to 83.8 % selectivity and 93.2 % ee) in the asymmetric Friedel-Crafts reaction between indoles and imines.

Moreover, two-dimensional layered compounds with flexible interlayer areas offer intriguing possibilities as substrates for homogeneous catalyst immobilization. For instance, [150] discovered that immobilizing copper complexes in laponite clay increased the value in the reaction between methyl phenyldiazoacetate and tetrahydrofuran from nearly zero to approximately 40 %. Catalytically active substances should be grafted, anchored, or covalently bonded to mesoporous silica. Consequently, the proximity of anchored intrinsic functional groups and active sites on the support surface can provide a synergistic effect, particularly favourable for specific reactants within a confined space. This approach thus presents a pivotal avenue for exploring and discovering novel catalysts. Multifunctional catalysts have been synthesised by exploiting synergistic effects between two anchored functional groups within anchored bifunctional catalysts and between the hydroxyl and anchored groups on a solid surface. Nature also frequently utilises synergy effects. For example, some catalytic materials possessing minimal functional groups exhibit remarkable selectivity and activity across a diverse range of processes, even at temperatures close to room temperature [151].

Zeolites, mesoporous materials, MOFs, and carbon-based catalysts show significant potential as effective heterogeneous catalysts for substituting precious metal catalysts in renewable energy production. A summary of the review and performance evaluation of various heterogeneous catalysts and processes can be found in Table 6, which includes factors such as pore volume, surface area, operating parameters, catalytic performance/yield, and stability. The comparative evaluation of the three types of porous materials shown in Table 6: MIL-53 (a MOF material), MCM-41 (a mesoporous silica) and HZSM-5 (a conventional zeolite) in terms of various dimensions such as stability, surface area, structure and catalytic properties shows that each of them exhibits a wealth of catalytic chemical properties. This indicates that they have the potential to complement each other in heterogeneous catalysis. Zeolites, for example, exhibit superior stability, making them suitable for gas phase catalysis, particularly in industrial catalysis; mesoporous silica has the largest pores, allowing extensive substrates to enter the pores; and MOF materials have a larger surface area, corresponding to the highest density of active sites [152,153].

The combination of confinement and synergistic effects in heterogeneous catalysis has revolutionised the development of more adaptable and efficient catalysts. Researchers have significantly enhanced selectivity and overall catalytic performance by immobilizing homogeneous catalysts on solid supports and introducing multifunctional catalysts. Materials such as zeolites, mesoporous silica, and MOFs complement each other in catalysis, with each material offering unique advantages in terms of stability, surface area, and catalytic properties. These developments are crucial for advancing renewable energy production and reducing reliance on precious metal catalysts.

2.1.6. Emerging catalytic materials for energy production

2.1.6.1. Single-atom catalysts (SACs). Single-atom catalysts (SACs) have garnered significant attention in heterogeneous catalysis due to their distinct structural and functional advantages over conventional

catalysts. These systems are uniquely defined by the atomic-level dispersion of individual metal atoms on suitable support materials, enabling enhanced catalytic performance [154,155]. This unique atomic dispersion endows SACs with several notable advantages compared to conventional nanoparticle catalysts (1). Firstly, the absence of metal–metal bonds allows each metal atom to exhibit a well-defined coordination environment, resulting in unique electronic and physicochemical properties [156,157]. Furthermore, the strong interaction between the metal atoms and the isolated support material helps avoid catalytic deactivation brought on by metal atom aggregation [154,158]. Secondly, the minimal metal loading combined with strong chemical anchoring reduces catalyst costs and significantly lowers the risk of metal leaching [159]. As a result, SACs demonstrate superior catalytic efficiency, stability, and operational safety, making them a highly promising alternative to conventional nano-scale catalysts.

The breakthrough moment in SAC research was marked in 2011, when Qiao, et al. [160] introduced the concept by synthesizing Pt-based SACs on FeOx supports. Their study demonstrated that these Pt single-atom catalysts exhibited threefold higher CO oxidation activity than their nanoparticle counterparts. This pioneering work catalyzed extensive interest in SACs for heterogeneous catalysis, prompting the development of various metal–support combinations. A wide array of metal SACs, such as Fe, Co, Ni, Pd, Ru, and Pt have since been anchored on oxide supports, including SiO_2, TiO_2, FeOx, Co_3O_4, CeO_2, and ZnO [161]. For instance, Wang, et al. [162] utilized an impregnation method to disperse Rh on Co_3O_4 nanorods, successfully creating a catalyst where Rh atoms, uniformly distributed on the carrier, formed active sites via bonding with surface oxygen atoms. EXAFS analysis confirmed single-atom dispersion, and the resulting Rh-SACs demonstrated excellent performance in nitric oxide reduction using hydrogen, achieving 87 % selectivity for N_2 at 220 °C and 97 % at 300 °C.

Building upon these advancements, Ge, et al. [163] synthesised Co-SACs via complexation pyrolysis using lignin-derived carbon as the support (Fig. 9a-b) and confirmed the formation of Co–N_4 active sites

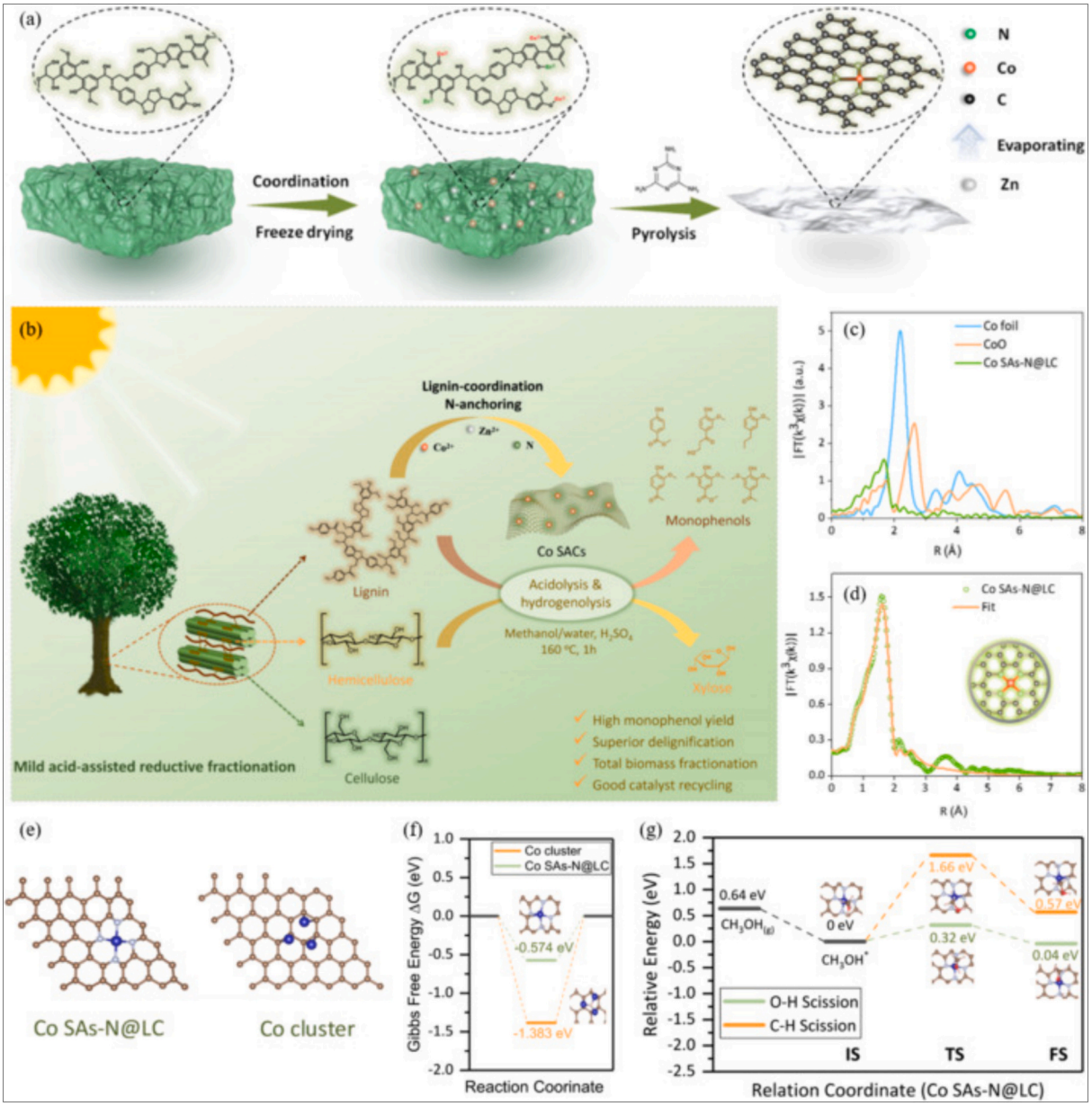

Fig. 9. (a) the synthesis pathway for Co-SACs derived from lignin; (b) depolymerization strategies for woody biomass employing Co-SACs; (c) EXAFS spectra and (d) corresponding fitting curves confirming the atomic structure of Co-SACs; (e) structural comparison between Co-SACs and Co cluster catalysts; (f) Gibbs free energy profiles; and (g) potential energy distribution during the initial decomposition process on Co-SACs. Adapted from Ref. [163].

through EXAFS and XANES analysis (Fig. 9c-d). Efficient separation of lignin, hemicellulose, and cellulose was achieved using Co-SACs in the acid-assisted lignin-first reductive fractionation of poplar biomass. The process achieved a high monophenol yield and nearly complete delignification (>99 %). Compared to Co cluster catalysts (Fig. 9f), the Co-SACs exhibited superior activity in lignin reductive depolymerization (Fig. 9e). DFT calculations revealed that the Co-SACs had lower Gibbs free energy for hydrogen adsorption and a higher tendency for hydrogen desorption, contributing to their enhanced catalytic performance. Moreover, methanol cleavage pathway analysis depicted in Fig. 1g indicated that Co-SACs were more effective in facilitating O—H bond scission than Co clusters. At 160 °C and 0.1 % sulfuric acid, the Co-SACs achieved a monophenol yield of 41.7 %, further validating their potential in biomass valorization processes.

2.1.6.2. Ionic liquid-based catalysts in biomass volarisation. To date, lignocellulose and its derivatives have been successfully converted using ionic liquids (ILs) into a range of value-added products, including formic acid, levulinic acid, HMF, and others, as illustrated in Fig. 3. ILs play a pivotal role in biomass conversion, functioning both as reaction media and, in many cases, as catalysts. Their effectiveness is further enhanced by optimizing process parameters such as temperature and reaction time to maximize product yield. Given the high oxygen content in lignocellulosic biomass, approximately 40–45 %, partial deoxygenation is necessary, typically through the release of CO_2 and H_2O, to facilitate the subsequent conversion of biomass into liquid biofuels.

In a notable study, Liu, et al. [164] demonstrated that hydrolyzed corn stalk diluted in [BMIM][HSO_4] and [BMIM]Cl achieved reducing sugar yields of approximately 68 % and 71 %, respectively. Further experimentation involved dissolving wheat straw in a solvent mixture comprising [BMIM]Cl, [EMIM][OAc], and several phosphate-based ILs, including 1-ethyl-3-methylimidazolium dibutyl phosphate ([EMIM][DBP]), −ethyl-3-methylbutylpyridinium diethyl phosphate ([EMBy][DEP]), and 1-ethyl-3-methylimidazolium diethyl phosphate ([EMIM][DEP]). Among these, [EMIM][DEP] produced the highest yield of reducing sugars, approximately 50 % after a 1-h pretreatment at 100 °C. However, it is important to note that excessive IL concentrations can inhibit enzyme activity during the subsequent fermentation process. An adequate water content must be maintained to support optimal enzymatic hydrolysis and fermentation. The conversion of cellulose to ethanol via the fermentation of reducing sugars remains a critical step in the pretreatment and valorization of biomass for biofuel production.

Hydroxymethylfurfural (5-HMF) has gained significant attention as a versatile platform chemical, primarily due to its potential for conversion into various biofuel precursors and value-added chemicals. One key transformation involves the hydrogenation of 5-HMF to produce 2,5-dimethylfuran (DMF), a promising biofuel candidate. Additionally, through condensation and hydrodeoxygenation reactions, 5-HMF can be upgraded into C_7–C_{15} liquid alkanes suitable for drop-in fuels. Ionic liquids (ILs) have proven to be highly effective solvents for the dehydration of monosaccharides into HMF by disrupting the intermolecular hydrogen bonds that stabilize sugar structures [165,166]. As illustrated in Fig. 10, ILs enhance the efficiency of monosaccharide-to-HMF conversion, improve product selectivity, and facilitate recovery. Despite its promising applications, large-scale industrial production of 5-HMF remains limited due to high production costs. Zhang, et al. [167] were among the first to demonstrate that metal halides, when used in combination with ILs such as [EMIM][Cl], act as effective catalysts for the dehydration of carbohydrates into 5-HMF. Their study explored the effects of various metal halides and ILs, including [BMIM][Cl], [EMIM][Cl], and [OMIM][Cl], on sugar dehydration reactions. The highest yields reported were 83 % for fructose and 70 % for glucose.

Levulinic acid (LA) is emerging as a critical platform chemical, effectively bridging the biomass and petroleum-based chemical industries. Derived from lignocellulosic biomass, LA is a precursor to several high-value compounds. Notably, it can be converted into γ-valerolactone (GVL), which, through hydrogenation, can be further transformed into liquid alkene compounds with significant potential as renewable biofuels. Beyond biofuels, LA is gaining recognition for its versatility across a wide range of industrial applications, including cosmetics, pharmaceutical intermediates, polymers, resins, and drug delivery systems [168]. Recent studies have explored using ionic liquids (ILs) as catalysts for LA synthesis from diverse biomass sources, including bamboo, maize stalk, pinewood, and rice straw. For example, Liu et al. (2020) reported that rice straw could be converted into LA via a one-pot reaction using an acidic IL, [C_3SO_3HMIM]HSO_4, at 180 °C for 30 min, achieving a yield of 21 %. This study highlighted the role of strong hydrogen bonding interactions between the IL and biomass components in enhancing the LA yield. Additionally, the IL catalyst demonstrated recyclability, retaining catalytic efficiency over five cycles.

In liquid membrane applications, ionic liquids (ILs) are functional supports coated or impregnated on the membrane surface. This integration offers several notable advantages, including low capital and operational costs, minimal solvent loss, reduced energy consumption, and, most importantly, ease of operation [169]. Due to its high

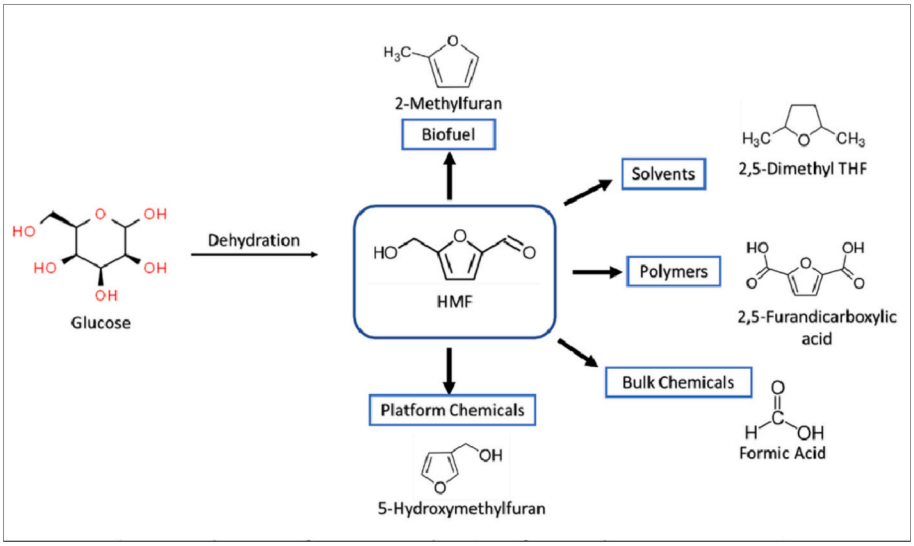

Fig. 10. Illustrative pathway for the conversion of glucose to HMF. Adapted from Ref. [170].

selectivity and stability, the supported liquid membrane (SLM) technique, enhanced by ILs, has demonstrated broad applicability in extracting various organic compounds, particularly those derived from biomass.

2.2. Integrated role of catalyst characterisation, mechanistic modeling, and catalyst regeneration in advancing heterogeneous catalysis for renewable energy applications

2.2.1. Catalyst characterisation and mechanistic insight

Significant progress has been made in developing heterogeneous catalysts for renewable energy and biomass-derived petrochemical production. However, to strengthen the understanding between catalyst structure and application, it is crucial to move beyond material description and explore the mechanisms governing catalyst activity, stability, and regeneration in greater detail. The superior performance of a catalyst in converting biomass to biofuels depends on the catalyst, structural remodelling, or surface reorganisation of the catalyst formed [171]. Ex-situ characterisation techniques are limited in understanding the transient behaviour or structural reorganisation that occurs under reaction conditions, leading to an incomplete understanding of catalyst behaviour. In-situ characterisation techniques therefore offer solutions to these challenges.

In-situ characterisation techniques provide information on the real-time detection of catalyst deactivation and reaction conditions. Li, et al. [172] reported on in-situ electron transmission microscopy for energy applications, which indicates reaction kinetics and catalyst stability in real time. Wang, et al. [171] reported that real-time monitoring of catalyst microstructure, especially when reaction conditions vary, and in-situ electron transmission microscopy are useful for understanding the reaction mechanism. In situ X-ray absorption spectroscopy (XAS) provides real-time insight into growth mechanisms, phase transitions, and surface restructuring during reaction processes, which is crucial for optimizing catalyst performance. In-situ Raman spectroscopy and in-situ Fourier transform infrared spectroscopy (FTIR) provide insight at the molecular level by identifying reaction intermediates, surface bonds, and products. Raman and infrared spectroscopy are complementary techniques that can effectively elucidate the properties and configurations of critical intermediates, favoured reaction pathways, selectivity, and the effects of the reaction environment [171]. In-situ X-ray diffraction (XRD) techniques give qualitative analysis of material crystallinity and crystal parameters, capturing the transformation process of the catalyst crystal during reaction.

In addition to in-situ characterisation, theoretical approaches have become essential for addressing limitations beyond experimental techniques' reach [173]. Methods such as molecular dynamics (MD) simulations, density functional theory (DFT), and machine learning (ML) models now serve as powerful mechanistic tools for predicting energy barriers, pinpointing active catalytic sites, and unraveling complex reaction mechanisms at the atomic level. To deepen the understanding of the catalytic mechanism, recent studies have applied in-situ techniques (e.g., atomic force microscopy (AFM), RAMAN, Diffuse Reflectance Infrared Fourier Transform Spectroscopy (DRIFTS), XPS, and XRD) and multi-scale simulations including Density Functional Theory (DFT) simulations and microkinetic modeling to monitor active species, intermediate formation, and electron transfer processes under reaction conditions [174,175]. These integrative approaches offer predictive insights into catalyst performance, enabling the design of systems that are not only mechanistically sound but also compatible with industrial-scale energy production. Density Functional Theory (DFT) is widely regarded as a foundational tool in catalysis research, providing valuable predictions of catalyst behaviour at the atomic scale. Celebrated for its optimal trade-off between computational efficiency and accuracy, DFT has become the method of choice for many computational investigations in this field [176]. Its strength lies in its capacity to model complex chemical systems under realistic conditions, making it particularly effective for probing catalytic mechanisms and surface interactions [175].

Researchers have gained improved control over the synthesis of HKUST-1 by fine-tuning synthesis parameters, which has allowed for targeted manipulation of crystallinity and defect concentrations. Mandemaker, et al. [177] employed advanced nanospectroscopy techniques, particularly AFM-IR, to investigate these structural variations in HKUST-1. Their study demonstrated that increasing synthesis temperature led to the desorption of self-assembled monolayers (SAMs), as indicated by the absence of characteristic carboxylate C═O stretching bands at 1700–1800 cm^{-1} in AFM-IR spectra (Fig. 11a–b). These findings were further supported by in-situ liquid-phase AFM, which showed suppression of nucleation at 50 °C. Additionally, a defect-rich, amorphous Cu_3BTC_2 layer referred to as a "carpet" was found to surround larger HKUST-1 crystals, raising questions about surface structure uniformity. In a complementary investigation, Weckhuysen, et al. [178] explored the relationship between structural defects and topological features in SURZIF-8(Zn) thin films. By integrating atomic force microscopy (AFM), Raman spectroscopy, principal component analysis (PCA), and density functional theory (DFT), the study identified intergrowths and variations in defect distribution. Specific spectral markers such as a distinct peak at 284 cm^{-1}, a high 675/686 cm^{-1} ratio, and diminished intensities in bands associated with Zn^{2+} coordination enabled precise quantification of defect density. Their findings revealed that thinner twenty-cycle films exhibited more pronounced phase barriers and heterogeneity, whereas thicker fifty-cycle films demonstrated improved chemical uniformity and structural consistency (Fig. 11c–d). These insights collectively advance the understanding of defect engineering in metal–organic frameworks and their impact on material performance. As such, the future of heterogeneous catalysis lies at the intersection of fundamental science and applied engineering, where materials are tailored with both reactivity and process viability in mind.

Molecular dynamics (MD) simulations have emerged as a powerful computational technique for investigating the behaviour of atoms and molecules in gaseous, liquid, and solid states at atomic resolution [179]. By numerically solving Newton's equations of motion, MD provides detailed insights into thermodynamic and kinetic properties, enabling accurate prediction of molecular behaviour and interactions [180]. These simulations allow researchers to monitor the time-dependent movement of individual atoms, offering a deeper understanding of bond formation and cleavage, molecular rearrangements, and catalyst–reactant interactions under various conditions [181]. As such, MD is a critical tool for predictive modeling, experimental planning, and mechanistic elucidation in catalytic processes. Table 3 summarizes selected studies highlighting the applications and key findings of molecular dynamics (MD) simulations in catalytic research. Incorporating these insights into catalyst development and studies bridges fundamental understanding and practical application and aids in tailoring catalytic systems for enhanced selectivity, stability, and sustainability in renewable energy processes.

2.2.2. Catalyst deactivation and regeneration

Catalyst deactivation, a major challenge in biomass valorisation, arises primarily from coke deposition, metal sintering, and poisoning by impurities [186]. For instance, coke formation blocks active sites and micropores of zeolites, reducing their activity. To mitigate this, regeneration methods such as oxidative calcination, steam reforming, and surface modification with coke-resistant promoters have been reported as effective strategies. Integrating metal–acid bifunctionality has also shown promise in reducing coke formation by facilitating hydrogen transfer reactions that stabilize reactive intermediates [187,188]. Table 4 shows the different catalyst deactivation mechanisms, causes, and regeneration methods.

The evolution of heterogeneous catalysis research for renewable energy and biomass valorisation has moved progressively towards bridging the gap between academic development and industrial

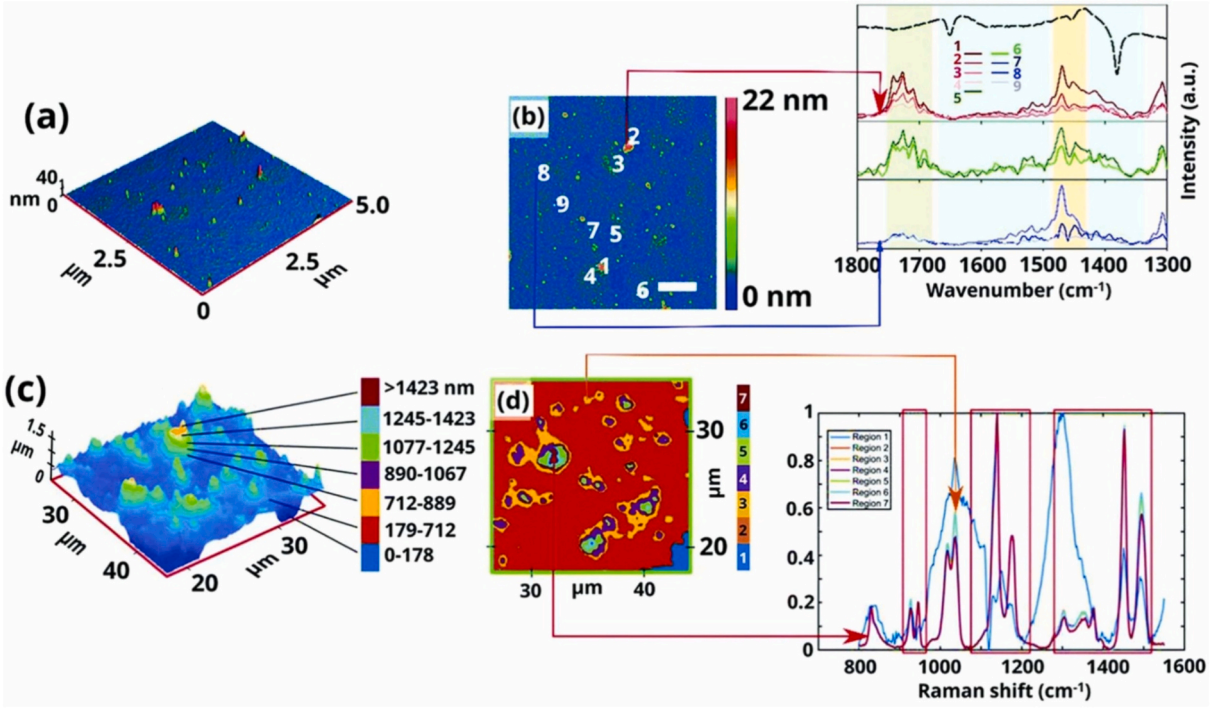

Fig. 11. (a) A three-dimensional AFM rendering and (b) an AFM micrograph paired with infrared spectra (right), annotated by numerical labels and categorized by morphological distinctions: red indicates grain structures, green represents circular or patch-like areas, and blue corresponds to the regions between patches. The absence of the C═O stretching band in the blue regions signifies the desorption/removal of the self-assembled monolayer. The scale bar in (b) denotes 1 μm. Figs (a) and (b) are adapted from Ref. [177]. (c) A 3D AFM image illustrating height-based segmentation, used in (d) to demarcate zones for Raman spectral averaging. These spectroscopic fingerprints provide chemical insight correlated with surface morphology. The Raman spectral colours directly correspond to the regional colour coding on the left. Figs. (c) and (d) are adapted from Ref. [178]. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Table 3
Applications of molecular dynamics simulations in catalysis study.

Application Area	Catalytic System	Simulation Details	Key Findings	Benefits	Limitations	Reference
Hydrocarbon configuration analysis	Cu@4A zeolite nanocatalyst	MD with energy minimization, NPT/NVT ensembles	C_3H_8 density peak dropped by 68.3 % at 300 °C; interaction energy decreases with temperature	Clarified catalytic mechanism and thermal behaviour	High reaction temperature and limited hydrocarbon recovery	[182]
Hydrocarbon cracking	Amorphous silica, hydrated amorphous silica, amorphous aluminosilicate	ReaxFF; T = 1477–1677 °C, P = 4–7 MPa	Hydrocarbon cracking via C—C scission and radical formation; yields H_2 and hydrocarbons.	Uncovered complex reaction networks	Computationally intensive at extreme conditions	[183]
Catalytic oxidation	Pd-based nanoparticles (with/without oxygen)	ReaxFF MD; T = 127–727 °C	CH_4 dissociates more readily on oxygen-coated Pd surfaces at lower temperatures	Mechanistic insight into CH_4 activation; impact of oxygen coverage	High computational cost; sensitive to force field accuracy	[184]
Hydrogen production	Mg nanoparticles	ReaxFF MD; T > 1727 °C	Mg–H bond formation initiates H_2 release above 927 °C	Revealed kinetic barriers and H_2 evolution pathways	High thermal input is required for effective hydrogen release	[185]

application. While early studies focused primarily on catalytic activity, surface properties, and selectivity under controlled laboratory conditions, recent research emphasizes the importance of incorporating operational parameters relevant to scale-up and large-scale deployment. Demonstration-scale initiatives such as those undertaken by the National Renewable Energy Laboratory (NREL) and the IEA Bioenergy Task 39 have revealed critical performance criteria such as catalyst deactivation rates, regeneration intervals, tolerance to feedstock variability, and compatibility with continuous processing systems [196–198]. These practical considerations are essential in evaluating the technological readiness of catalyst systems and their potential for integration into biorefineries. Comparative studies have also revealed that high laboratory performance does not always translate to industrial feasibility. For example, while zeolite-based catalysts such as Ni-modified ZSM-5 exhibited high selectivity towards aromatics, Fe-modified ZSM-5 favoured olefin production in the conversion of bioethanol to hydrocarbons [199], their regeneration efficiency and cost-effectiveness vary significantly under industrial conditions [200]. Moreover, techno-economic assessments indicate that the catalyst cost per cycle, coke suppression strategies, and scalability are pivotal in commercial viability [201]. Table 5 compares laboratory- and pilot-scale studies on heterogeneous catalysis for renewable energy production.

2.3. *Feedstock–catalyst–process compatibility*

The compatibility between the feedstock, the reaction catalyst, and

Table 4
Catalyst deactivation mechanisms and regeneration methods.

Deactivation Mechanism	Primary Cause	Typical Manifestation	Regeneration Method	**Remarks**	Ref.
Poisoning	Chemisorption of strongly bound impurities (e.g., S, P, Cl)	Loss of active sites; inhibition of reactant adsorption	Chemical washing, partial regeneration	Effectiveness depends on poison type; it may require pre-treatment protocols	[186,189–191]
Sintering	Prolonged exposure to high temperatures	Particle agglomeration; surface area reduction	Minimally reversible; designed with thermal stability	Nanoparticle sintering is often irreversible; it is mitigated via support interaction	[186,192]
Fouling (Coking)	Carbon deposition from unsaturated hydrocarbons	Pore blockage; reduced mass transfer	Oxidative regeneration at elevated temperature	Requires precise temperature control to avoid catalyst oxidation	[186,193]
Leaching	Solubilization of metal components in acidic/basic media	Loss of active metal species into the reaction phase	*Re*-impregnation followed by calcination and activation	Common in aqueous-phase reactions; leach-resistant supports may help	[186,194]
Mechanical Degradation	Attrition, crushing, or thermal stress	Loss of particle integrity; support fracture	Often irreversible; complete replacement recommended	Occurs in fixed-bed or fluidized systems; robust structural design advised	[186,195]

the operating conditions critically influences biomass conversion into petrochemical products and renewable energy. These interrelated factors together determine the nature and yield of the products produced. However, due to the inherent complexity and variability of biomass composition, which results in inconsistent catalyst performance and product yield, uniform catalytic processing remains a major challenge, ultimately limiting process optimisation [202]. To overcome this, a synergistic relationship between the physicochemical properties of the feedstock and the catalyst is essential for efficient biomass conversion.

Biomass feedstocks, which include industrial wastes, municipal organic wastes, lignocellulosic plant biomass, animal wastes and fats, and algae [203–205], have different physicochemical properties such as oxygen content, moisture content, aromaticity, and inorganic impurities. These properties have a major influence on the selection and effectiveness of heterogeneous catalysts, particularly with regard to catalyst selectivity, deactivation, and coking during the conversion processes. For example, lignocellulosic biomass, a complex matrix consisting mainly of cellulose (40–50 %), hemicellulose (25–30 %), and lignin (10–20 %) with a small amount of ash and extractives [206] poses a particular challenge. The rigid framework and the complex spatial organization of lignin during depolymerisation favour severe condensation reactions, forming complex products that prevent large-scale application [207]. In addition, lignin-rich raw materials generate phenolic intermediates that can poison acid catalysts or rapidly foul active sites [208]. Different types of biomass are better suited for certain conversion pathways (Fig. 12a). Ash-rich herbaceous feedstocks such as corn stover are favoured in biochemical processes such as ethanol fermentation, which mainly target cellulosic and hemicellulosic fractions [209].

Conversely, thermochemical conversion processes favour low-ash, lignin-rich woody biomass, which offers higher yields and a lower risk of catalyst deactivation. Biomass with high lignin content usually requires highly acidic catalysts that enable selective deoxygenation and controlled structural degradation to increase biofuel production [210]. Furthermore, biomass often contains varying amounts of impurities such as ash, water, and trace metals, depending on its origin and pretreatment. These impurities can severely impair catalytic performance. For example, high moisture content in the feedstock during bio-oil production can inhibit esterification or transesterification reactions by promoting hydrolysis or dilution of intermediates, leading to soap formation, deactivation of the catalyst, and lower conversion efficiency [211]. In such cases, using catalysts developed for raw materials with low FFA or moisture content is crucial. Alternatively, hydrophobic catalysts such as copper or zeolite-based systems, or pre-drying treatment of the feedstock, can be used. In addition, trace elements such as nitrogen, sulphur, and coke-forming species can be adsorbed onto the catalyst's active sites, leading to poisoning, fouling, or sintering, which ultimately reduces the lifetime and effectiveness of the catalyst [186,212]. Therefore, pretreatment processes aimed at reducing impurities are often necessary to ensure optimal compatibility between the feedstock and the sensitive catalysts and to support both the efficiency and durability of the biomass conversion processes.

Recent studies have shown that feedstocks from lipid-rich biomass sources such as microalgae, animal fats, and used cooking oils favour transesterification reactions and require catalysts with both basic and hydrophobic properties to achieve high biodiesel yields [213,214]. Therefore, the choice of catalyst must be optimized not only for the desired reaction pathway (e.g. hydrodeoxygenation, transesterification, reforming, or pyrolysis), but also for the specific properties of the feedstock. According to Naseef and Tulaimat [215], alkaline catalysts work well with oils with low free fatty acids (FFA), but tend to form soaps when used with raw materials with high FFA values. In contrast, acidic catalysts are more suitable for high FFA oils due to their ability to promote esterification reactions, although they are sensitive to the presence of water. In addition to chemical compatibility, the feedstock's physical properties, including viscosity and structure, must also be considered when developing or selecting catalysts. For example, bio-oils produced by fast pyrolysis are highly viscous and therefore require catalysts with hierarchical porous structures to enable efficient mass transfer and prevent pore clogging [216,217]. Mesoporous zeolites such as MCM-41, SBA-15, and hierarchical zeolites are particularly effective. They offer a large surface area and adjustable pore sizes that accommodate bulky biomass intermediates [218,219]. As summarised in Table 6, supported zeolite catalysts, including NiMo/zeolite and HZSM-5, show exceptional hydrothermal stability and high selectivity for aromatic hydrocarbons when used with palm oil and microalgae as feedstock, respectively [220,221].

In addition, hierarchical zeolites produced by desilication (e.g., ZSM-5, Hβ) have been shown to provide consistent aromatic yields and superior thermal stability, even over multiple regeneration cycles, an essential property for lignocellulosic biomass such as beechwood and kraft lignin [222,223]. Furthermore, carbonaceous catalysts such as $NiCe/AC_N$ and Cu–Ni/graphite have shown high selectivity for methane production and efficient syngas upgrading, emphasising the advantages of carbonaceous supports for gas-phase reforming reactions [224,225]. In liquid-phase conversion, MOF catalysts such as MOF-5/SBA-15 and ZIF-90-Gua exhibit excellent stability and high product yields, promising candidates for producing biodiesel and chemicals from oils and alcohols [226,227]. Similarly, mesoporous catalysts such as Ni–Mo/MCM-41 and Fe_3O_4@SBA-15@HPW have shown sustained activity and longevity, providing effective and sustainable options for syngas and biodiesel conversion [228,229]. These results emphasize that the interplay between the catalyst's physico-chemical properties and the feedstock's composition is crucial for the overall process's conversion efficiency, product selectivity, catalyst durability, and cost efficiency. This is illustrated in Fig. 12b, which shows the catalyst performance metric. Tailored catalyst design optimizing parameters such as surface area, porosity, acidity/basicity, and thermal stability is necessary for

Table 5
Comparative performance of laboratory- and pilot-scale studies in biomass conversion to renewable energy and their industrial upscaling potential.

Scale	Catalyst type	Feedstock/Product	Operational parameters	Catalyst performance	Practical remarks & upscaling potential	Ref.
Lab Scale	Heterogeneous catalysts (Modified HZM-5 with Ni, Cu and Ru)	Biomass/Lignin derived bio-oil (LDB)	Catalysts under supercritical ethanol conditions (320 °C, 14 MPa	28.95 % hydrocarbons conversion at a heating value of 35.22 MJ/kg	Hydrodeoxygenation of LDB of 80.40 % was upgraded to 96.32 % energy recovery with potential for upscaling	[230]
	Basic oxides (MgO, La_2O_3, MgO-La2O3, CaO and BaO_2) supported Cu—Zn bimetallic catalyst	Bioglycerol/ Propylene glycol	210 °C and 4.5 MPa	98.7 % conversion with 69.6 kJ mol- activation energy	High selectivity potential for upscaling	[231]
	Ni-Mo/Al_2O_3	Biomass/green diesel	325–375 °C, 35–70 bar, and H2/Oil ratio of 50 % at Liquid hour space velocity of 0.5–3 per hour	92 % conversion, cetane number of 75, and light weight gases (5 %) and green naphtha (15 %)	With a selectivity of 70–80 %, it has high potential for catalytic cracking at an industrial scale with less CO_2 emission	[232]
	Nanocatalysts eg K_2CO_3, Fe_3O_4	Biomass /bioenergy	260–300 °C, and 15–30 h	Improve yield and energy value	Potential for hydrothermal liquefaction and accelerated reaction rate in industrial applications	[233]
	CaO, HZSM-5, Fe/HZSM-5,	Biomass/biocrude	catalyst-to-feedstock ratio of 0.15 *w*/w, 250–550 °C, 5–24 h	Fe-HZSM-5 increased coke formation with CO2 adsorption and deposition. CaO has a low cost with high deoxygenation of acids. The metal-doped catalyst yielded a low oil of 25.9 wt%.	Decarbonisation potential of catalytic pyrolysis with synergistic effect of CaO, Fe and HZSM-5 for industrial production has long-term sustainable solutions.	[234]
	Heterogeneous-based catalysts (Fe/Ni /ZSM-5)	Biomass (Chinese herb residue)/bio-oil	320 °C, inert atmosphere for 10 min	High heat value (29.39 MJ/kg) and bio-oil yield (24.7 %) with reduced oxygenation and aliphatic compounds in the bio-oil with yield of 73 %	High recyclability potential of Fe-ZSM-5 recommended for industrial application	[235]
Pilot scale	Heterogeneous acid catalyst (CoMo and NiMo/Al_2O_3)	Biomass /Jet fuel	350–450 °C 3- 6 MPa, 100 h	High yield of 30–75 % and moderate cost	Ni-W/SiO2-Al20 has the potential for upscaling bio-jet fuel systems	[236]
	Ni/Cu/TiO_2	Glycerol/Proylene glycol	20 % wt. glycerol concentration, 200 °C–250 °C, and 3.5 MPa	83 % conversion with 7 % reduction of total cost and 71 % CO_2 emission reduction	With low cost and potential for next-generation bio-refineries. Modelled on a pilot plant, and operational conditions were validated	[237]
	Activated carbon derived from spent coconut shell with 90 % CaO	Biomass/green diesel	9000 kg/h federate, running time of 335 days/year, life span 20 years	Produced 3091 tons of green diesel, 862 activated carbon, 4953 tons of coconut meal and 269 tons of tar annually	Economically viable with a 14 % rate of return and a production efficiency of 47 % at a payback period of 7 years for refinery scale implementation	[238]
	Alkaline-based catalysts of order K_2CO_3 > KOH > NaOH and noble metals (Fe, Cu, Ni)	Municipal waste/ biocrude	300–500 °C, 10–15 MPa,	High yield with a profitability index of 5.5–6 and 31 % return on investment at 20 years payback	Hydrothermal liquefaction pilot plant of municipal waste with technoeconomic analysis and life cycle assessment.	[239]

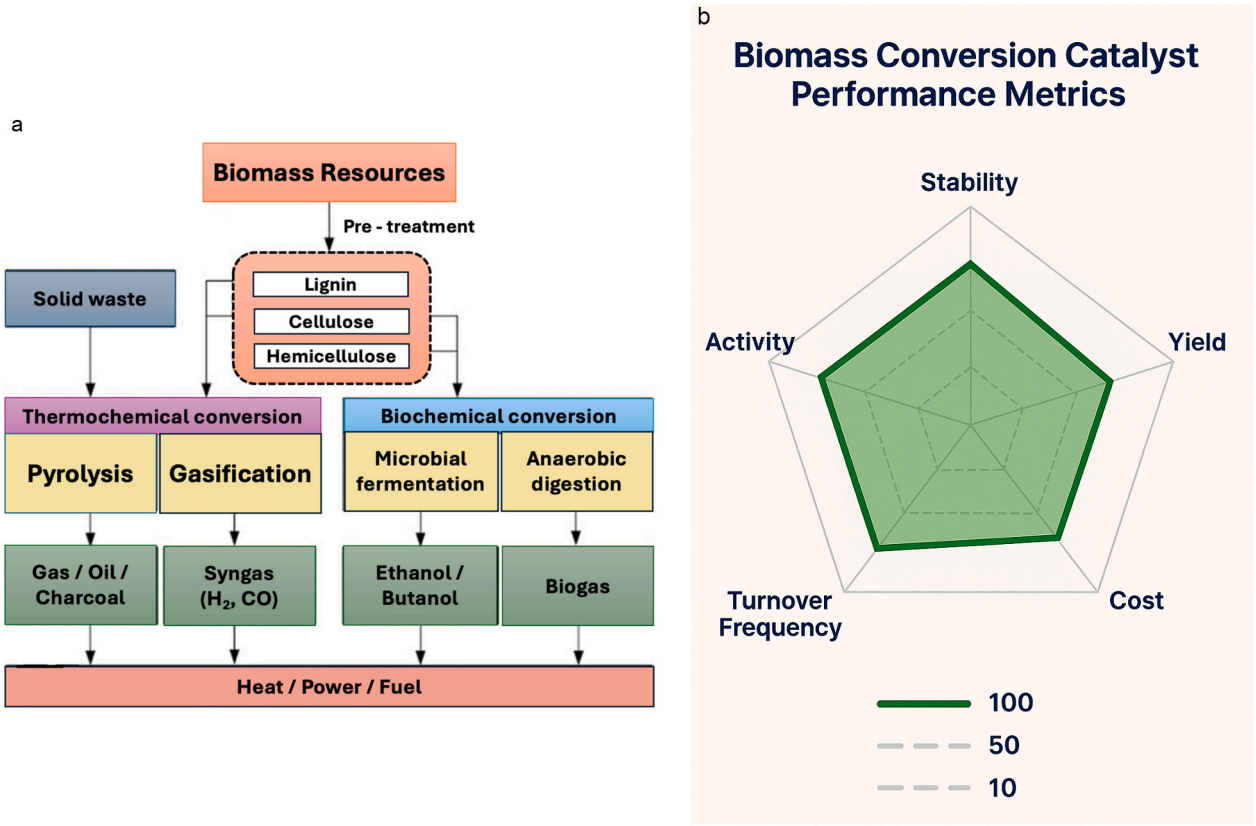

Fig. 12. a. Biomass conversion roadmap to renewable energy sources. b. Radar chart for the catalyst performance metric.

developing tailored catalytic systems suitable for specific biomass feedstocks. This approach is critical for the sustainable and economically viable valorisation of biomass into renewable chemicals and fuels.

3. Economic and environmental evaluation of heterogeneous catalysis

Extensive research highlights the economic and environmental advantages of heterogeneous catalysis across diverse sectors, encompassing pivotal areas like the production of biofuels from biomass and the generation of clean energy through catalytic mechanisms such as decarboxylation, hydrogenation, and oxidation.

3.1. Economic evaluation of different biomass conversion methods for energy production

The economic evaluation of catalytic conversion of biomass into biofuels encompasses various aspects, including catalyst synthesis costs, reactor design, and downstream processing efficiency, aimed at optimizing overall process economics. Several studies have provided insights into the technological and economic aspects of converting biomass into biofuels through catalytic processes. Alzate, et al. [255] showed that using several types of catalysts to make biorefineries more economically viable is possible. Through comparative techno-economic assessments, they showcased that incorporating catalytic processes in biorefineries is economically feasible and could improve the formation of different high-value products and fuel additives from lignocellulosic materials. Similarly, Hakeem, et al. [256] conducted a thorough analysis of the techno-economic factors related to biomass conversion using biochemical methods. They focused on important characteristics, which include production capacity, minimum selling price, conversion efficiency, and profitability metrics. Biochemical methods such as biomethanation and fermentation are widely used to convert biomass into bioethanol and biogas, which are regarded as the most economically feasible products derived from biomass processing. Although bioethanol and biogas have become economically viable products, generating other biofuels and chemicals still encounters obstacles like low conversion rates, microbial strain limitations, and refining complexities. Studies on ethanol production emphasize the crucial role of catalysts and biomass feedstock in production costs [257].

Over a decade ago, Alonso, et al. [258] provided insights into catalytic strategies for producing biofuels from biomass, highlighting the importance of reducing the oxygen content of feedstock and creating C—C bonds. Furthermore, suggestions like employing aldol condensation of ketones and oligomerisation of alkenes were proposed to facilitate the generation of hydrocarbons spanning gasoline, jet fuel, and diesel fuel ranges. Recently, Yan, et al. [259] assessed a new catalytic method for generating sustainable bio-gasoline from corn stover. Their economic evaluation revealed a return on investment of 15.8 %, affirming the economic viability and sustainability of waste biomass conversion. Sensitivity analysis showed that bio-gasoline prices and raw material costs significantly influence return on investment, emphasising the critical role of catalytic processes in enhancing the economic feasibility and efficiency of biomass conversion into biofuels. Similarly, Bagnato and Sanna [260] conducted a study to evaluate the economic feasibility of using catalytic hydrogenation to produce valuable chemicals and drop-in fuels from bio-oil obtained from lignocellulosic sources. When considering a plant's operational lifespan of 30 years, the techno-economic evaluation of the catalytic hydrogenation process revealed promising profitability, with biofuels priced at 22.22 $/GJ for gasoline and 18.87 $/GJ for diesel. Additionally, the analysis indicated a return on investment of 69.18 % and a payback period of 2.48 years.

Techno-economic analyses provide a framework to elucidate the intricate relationship between implementation strategies and economic considerations. The economic assessment of producing biofuel from agricultural and lipid-extracted algae via anaerobic digestion relies on

Table 6
Comparison of feedstock materials, characteristics, preparation methods, and the specific performance of heterogeneous catalysts.

Feedstocks	Catalysts	Catalyst Physicochemical Properties				Operating conditions for performance assessment	Reaction results / Inference	Ref.
		Synthesis method	Surface area (m^2/g)	Pore volume (cm^3/g)	Stability			
Zeolite materials								
Palm oil	NiMo/Zeolite	IEM	340	–	High hydrothermal stability The catalyst is stable at temperatures of up to 800 °C.	Rxn. T (°C) = 300–320 Time (h) = 1, 1.5, 2 Reactor = BR	% Yield of biogasoline = 11.93 %	[220]
Chlorella vulgaris	HZSM-5	–	425	–	–	Fixed-bed reactor at 510 ± 5 °C. Biomass-to-catalyst ratios of 1:1, 1:4, and 1:9 were used. Nitrogen flow rate of 30 mL/min.	Compared to non-catalytic pyrolysis, a larger quantity of aromatic hydrocarbons is extracted from the bio-oil. When the catalyst concentration increased from 0 to 9 times the biomass, the yield of aromatic hydrocarbons increased from 0.9 wt% to 25.8 wt%.	[221]
Methanol	KOH/4 A molecular sieve	IWI	–	–	The catalyst showed a sustained high selectivity towards DMC and the conversion of PO even after multiple uses. Complete conversion of PO was still possible, and the catalyst experienced at least a 10 % change in PC and DMC yield after eight recycling cycles.	Calcination T (°C) = 700 for 12 h Pressure (MPa) = 3, Rxn. T (°C) = 180 Reaction Time (h) = 6	Propylene carbonate (PC) yield (%) = 58.7 Dimethyl carbonate (DMC) yield (%) = 16.8 Selectivity of PO to DMC (S_{DMC}) = 16.8	[240]
Waste tire	Natural zeolite	–	590	–	–	T (°C) = 300–600 Time (min) = 25,30,60, 85 Reactor = BR	Light hidrocarbon (biogasoline, biodiesel) 12 %,	[241]
Cottonseed oil	Y-Zeolite, halloysite-Yzeolite	–	25.6	0.08	–	T (°C) = 480–540 Time (min) = 1 h Reactor = FBR	Bigasoline (46–55 %)	[242]
Hierarchical zeolites								
Beech wood	ZSM-5	Desilication by a solution of 0.1–0.5 M NaOH	406.8	0.058	The results also show that desilication has no significant effect on the thermal stability of ZSM-5 zeolite, allowing thermal regeneration and subsequent regeneration.	CTF =10	The study shows that the aromatic yield of both the parent zeolites and the desilicated zeolites did not change significantly throughout the three regeneration cycles.	[222]
Kraft lignin	Hβ	Desilication by Na_2CO_3 solution				T (°C) = 500 Pressure (bar) = 013 bar CTF = 10		[223]
Rice straw	HZSM5/MCM-41	Hybrid method in which ZSM-5 is desiccated with 2.0 M NaOH and the surfactant is CTAB.				T (°C) =650 Pressure (bar) =1.013 W/D = 1.0		[243]
Waste cardboard	HZSM-5	Desilication by 0.1–0.7 M NaOH solutions.				T (°C) = 600 Residence Time = 20 s CTF = 2.0		[87]
Kraft lignin (KL) and Pyrolytic lignin (PL)	ZSM-5	Hybrid approach comprising the dehydration of ZSM5 with 0.2 M NaOH and the surfactant with CTAB.				T (°C) = 600 Pressure (bar) =1.013 Residence Time (s) =30 s CTF = 3 and 5		[244]
Carbon materials								

(*continued on next page*)

Table 6 (*continued*)

Feedstocks	Catalysts	Catalyst Physicochemical Properties				Operating conditions for performance assessment	Reaction results / Inference	Ref.
		Synthesis method	Surface area (m^2/g)	Pore volume (cm^3/g)	Stability			
Cork wastes	$NiCe/AC_N$,	IWI	403	0.12	–	H_2/CO_2 = 4:1 Rxn. T (°C) = 200–450. PCO_2 = 0.16 bar GHSV = 86,100 $mL{\cdot}h^{-1}{\cdot}gcat^{-1}$	CH_4 (%) yield = 73 CH_4 selectivity (%) = 86–97	[224]
Natural graphite powder	Cu–Ni/graphite	IWI	107	0.43	The durability and activity of the catalyst developed in this study for the direct synthesis of DMC in less than 10 h were comparatively high.	Calcination T (°C) = 600 Pressure (MPa) = 1.2 Rxn. T (°C) =100 Time (h) = 3	Methanol conversion (%) = 10.13 DMC yield (%)/mmol = 0.91	[225]
Methanol and carbon dioxide	Cu–Ni/MWCNTs	IWI	107	0.43	The catalyst synthesised in this study showed good durability and activity in the direct synthesis of DMC in less than 10 h	Calcination T (°C) = 600 Pressure (MPa) = 1.2 Rxn. T (°C) =120 Time (h) = 3	Methanol conversion (%) = 4.3 DMC yield (%)/mmol = 3.74	[245]
Metal-Organic Frameworks (MOFs)								
Benzyl bromide and toluene	MOF-5/SBA-15	SG	571	0.68	The hydrostability of MOF-5 increases significantly when it is enclosed. It remains stable for up to 8 h under humid conditions, while MOF-5 collapses in the bulk in only 15 min.	Catalyst = 100 mg T (°C) = 80 Time = 3 h	100 % conversion	[226]
Soybean oil	ZIF-90-Gua	SG	830.4	0.42	The solid catalyst was easily recovered by filtering and retained its catalytic activity after five reuse cycles, indicating its good reusability.	Methanol/oil molar ratio Time = 15:1 T (°C) = 65 Catalyst amount = 1 wt %	Biodiesel yield (%) = 95.4	[227]
Furfural	M-MOF-808	IWI	1313	–	A slight decrease in catalytic activity was observed in the second cycle, with the conversion rate dropping from about 75 % in the first cycle to 64 % in the second cycle. During the following catalytic cycles, the conversion rate remained constant at around 64 %.	Calcination T (°C) = 600 Pressure (MPa) = 1.2 Rxn. T (°C) = 40 Time (h) = 24	X_{CO}/% = 96.5 S_{CH4}/% = 86.6 furfuryl (Fol) alcohol product was formed.	[246]
Carbon dioxide	MIL-53(Al)/Fe_2O_3	SG	1535	0.59	The catalysts were reported to be stable enough under the selected reaction conditions.	T (°C) = 300 Mass of catalyst (g) = 1 CO_2 Conversion (%) = 20	CO_2 Conversion (%) = 20 Selectivity (%) = CO = 20, CH_4 = 41, C_2-C_4^- = 34, C_2-C_4^- = 0, C^{5+} = 5	[247]
Carbon dioxide	ZIF-8(a)(Zn)/Fe_2O_3	SG	1900	0.89	The catalysts were reported to be stable enough under the selected reaction conditions.	T (°C) = 300 Mass of catalyst (g) = 1 CO_2 Conversion (%) = 20	CO_2 Conversion (%) = 20 Selectivity (%) = CO = 23, CH_4 = 21, C_2-C_4^- = 23, C_2-C_4^- = 21, $C5^+$ = 12	[247]
Mesoporous materials								
Syngas	Ni–3 %Mo/MCM-41	IWI	473	0.28	The CH4 selectivity over the Ni–3 %Mo/M catalyst gradually decreased from 93 % to 89 % in the first 50 h and remained stable at around 89 % for the next 50 h.	T (°C) = 280 WHSV (mL g^{-1} h^{-1}) = 12,000 h Pressure (P/MPa) = 0.1	X_{CO}/% = 100 S_{CH4}/% = 80	[228]
Carbon dioxide	Ni/MSN	IWI	879	0.79	The Ni/MSN catalyst prepared in this study showed no deactivation for the methanization process during up to 200 h of continuous operation. The Ni/MSN catalyst is	T (°C) = 280 WHSV (mL g^{-1} h^{-1}) = 12,000 h Pressure (P/MPa) = 0.1	X_{CO}/% = 64.1 S_{CH4}/% = 99.9	[248]

(*continued on next page*)

Table 6 (*continued*)

Feedstocks	Catalysts	Catalyst Physicochemical Properties				Operating conditions for performance assessment	Reaction results / Inference	Ref.
		Synthesis method	Surface area (m^2/g)	Pore volume (cm^3/g)	Stability			
					resistant to coke formation and has good stability under the reaction conditions.			
Palm oil	Fe_3O_4@SBA-15@HPW	IWI	374.329	0.85	The reusability of the catalysts was investigated. After six cycles, the grafting procedure produced Fe3O4@SBA-15-NH2-HPW with better reusability and a yield of more than 80 % biodiesel. This suggests good stability for this particular catalyst under the reaction conditions.	Molar ratio of methanol to oil: 20:1. Rxn. T: 150 °C. Catalyst amount: 4 wt%. Rxn. time: 5 h.	Fe_3O_4@SBA-15-NH2-HPW exhibited higher catalytic activity than Fe_3O_4@SBA-15@HPW. The yield of biodiesel reached over 91 %.	[229]
	Fe_3O_4@SBA-15-NH2-HPW	GM	290.517	0.56				
Ethanol	SBA-15 (Commercial)	SG	486	0.59	The coking deactivation led to a slight reduction in the catalytic activity of the fresh POC-SBA-15(5) catalyst after 105 h.	Reaction: Ethanol dehydration to ethylene. LHSV: 4–20 mL/g/h. Rxn. T: 200–400 °C. Initial ethanol concentration: 10–99.5 wt%.	At 400 °C and 50 % ethanol feed, the catalytic activity for ethanol dehydration was graded as follows: SBA-15(Comm.) < POC-SBA-15(3) < POC-SBA-15(7) < POC-SBA-15(5). The highest ethylene selectivity (84.70 %), and ethanol conversion (73.33 %) were achieved with POC-SBA-15(5) at 400 °C, 50 wt% ethanol feed, and LHSV of 16 mL/g/h.	[249]
	POC-SBA-15(3)	SG	508	0.63				
	POC-SBA-15(5)	SG	537	0.71				
	POC-SBA-15(7)	SG	642	0.83				
Soybean oil	SBA-15-pr-DCOG)	HM	267	0.48	The DCOG-functionalized SBA-15 catalyst exhibited good reusability for at least.	Rxn: Transesterification of soybean oil with methanol. Rxn Temperature: 65 °C. Methanol/oil molar ratio: 3:1 to 18:1. Catalyst amount: 1 to 10 wt%. Rxn. time: 1 to 18 h.	The conversion of soybean oil increased with increasing DCOG loading up to a DCOG/SBA-15 ratio of 5:2 (g/g). A maximum oil conversion of 93.5 % was achieved with a methanol/oil molar ratio of 15:1, a catalyst amount of 8 wt%, and a reaction time of 15 h.	[250]
Ionic Liquids								
Rice Straw	***IL:*** $[C_3SO_3HMIM][HSO_4]$ ***Catalyst:*** S_2O_{82}-/ZrO_2–SiO_2–Sm_2O_3	–	–	–	–	Time = 10 min T = 180 °C; Solvent: H_2O	LA, 21 % to 46 %	[251]
Bamboo	***IL:*** $[C_4(MIM)_2][(2HSO_4)(H_2SO_4)_4]$	–	–	–	–	Time = 60 min T = 100 °C; Solvent: H_2O	LA, 47,5 %	[251]
Paddy straw	***IL:*** $[C_3SO_3HMIM][HSO_4]$ ***Catalyst:*** HCl	–	–	–	–	Time = 45 min T = 220 °C; Solvent: H_2O	LA, 24 %	[251]
Pine Wood	***IL:*** $[C_2MIM]Cl$ ***Catalyst:*** $CrCl_3$	–	–	–	–	Time = 60 min T = 100 °C; Solvent: H_2O	5-HMF, 71.6 %	[252]
Cellulose	***IL:*** $[C_2MIM][Cl]$ ***Catalyst:*** $CrCl_3$	–	–	–	–	T = 120 °C; Solvent: H_2O	5-HMF, 10 %	[253]
Glucose	***IL:*** [BMIM]Cl [AMIM]Cl $[BMIM][BF_4]$	–	–	–	–	Time = 180 min T = 100 °C; Solvent: $IrCl_3$, $CrCl_3$	5-HMF, 78,8 %	[254]

(*continued on next page*)

Table 6 (*continued*)

Feedstocks	Catalysts	Catalyst Physicochemical Properties				Operating conditions for performance assessment	Reaction results / Inference	Ref.
		Synthesis method	Surface area (m^2/g)	Pore volume (cm^3/g)	Stability			
	Catalyst: Boric acid							
Fructose	***IL:*** [BMIM]Cl [BMIM]OH [CMIM][Cl]	–	–	–	–	Time = 120 min T = 160 °C; Solvent: DMSO, EtOH, Amberlyst-15	5-HMF, 92 %	[254]
Sucrose	***IL:*** [AMIM]Cl [BMIM]Br [EMIM]Br ***Catalyst:*** H_2SO_4	–	–	–	–	Time = 60 min T = 120 °C; Solvent: [NMP][HSO_4]	5-HMF, 72–80 %	[254]
Corn Stalk	***IL:*** [$C_4(MIM)_2$][(2HSO_4)(H_2SO_4)$_4$]	–	–	–	–	Time = 60 min T = 95 °C;	LA, 70 %	[167]
Sugarcane bagasse	***IL:*** [$BMIMSO_3H$][HSO_4] ***Catalyst:*** H_2SO_4	–	–	–	–	Time = 75 min T = 170 °C; Solvent: H_2O	LA, 55 %	[167]

IEM – Ion Exchange Method, IWI – Incipient Wetness Impregnation, CP - Co-Precipitation; SG = Sol-Gel, SM - Solvothermal method, HM – Hydrothermal method. SBA-15 – Santa Barbara amorphous type-material, HMS – Hexagonal mesoporous silica, MCM-41 – Mobil crystalline materials No 41, MSN – Mesostructured silica nanoparticles, POC – Palm oil clinker, ZIF - zeolitic imidazolate framework-8, MIL - Materials Institute Lavoisier.
Abbreviations: CTAB: hexadecyltrimethylammonium bromide; TPAOH: Tetrapropylammonium hydroxide; CFT: Catalyst-to-feed ratio; Liquid hourly space velocity (LHSV); HRTEM TEM (high-resolution transmission electron microscopy); IL: Ionic Liquid.

several factors, such as cultivation, harvesting, digester operation, purification costs, upscaling, and market rates for both the biofuel and byproduct obtained from the digestate. These evaluations are particularly significant given the projected rapid growth of the global biogas production industry, which is expected to reach a value of $50 billion by 2026 [261,262]. The economics of anaerobic digestion are strongly influenced by algae cultivation and harvesting expenses, from which harvesting constitutes roughly 25–30 % of the overall production expenses [263]. It is worth noting that many factors, including treatment facilities, product upgrading, and unit operations considerations, shape the feasibility of anaerobic digestion as a biomass conversion method. Gebremariam, et al. [264] did a study to examine the techno-economic performance of four catalyst technologies used in synthesizing biodiesel from low-cost acid oil through transesterification. The catalysts examined included ionic liquid, enzyme, bulk calcium oxide (CaO), and nano-calcium oxide. Out of these choices, the CaO-catalyzed method showed better economic efficiency, with a higher internal rate of return (IRR), return on investment (ROI), net present value (NPV), gross margin, and lower total capital investment expenses. In contrast, the method that utilises enzymes as catalysts was found to be economically impractical because of the excessively expensive enzyme catalyst and the need for a bigger reactor size. The enzyme catalyst had to be acquired at a cost of less than 60 US$/kg in order for the process to be financially viable. The method catalyzed by bulk CaO showed exceptional resistance to variations in biodiesel, oil, and catalyst prices, maintaining profitability even when biodiesel is priced as low as $0.74 per kilogram, oil prices as high as $0.70 per kilogram, and catalyst expenses reaching up to $7 per kilogram.

Advancing the understanding and application of catalysts in thermochemical conversion processes for biomass holds significant promise in the quest for renewable and carbon-neutral fuel sources. Ong, et al. [265] examined the catalytic roles within various thermochemical conversion methods such as carbonisation, pyrolysis, hydrothermal liquefaction, and gasification, elucidating their influence on reaction parameters and resultant product characteristics. In a complementary vein, Solarte-Toro, et al. [266] offer insights into energy-driven applications and catalytic enhancements for woody biomass utilisation. Their study provides a comparative analysis of various thermochemical pathways for converting woody biomass, focusing on techno-economic considerations. The findings emphasised the superior performance of gasification over combustion and pyrolysis in terms of techno-economic viability. Additionally, advanced biofuels produced through Fischer-Tropsch synthesis from biomass gasification have been evaluated for their economic viability. Utilizing the framework established by Veipa, et al. [267], a comprehensive techno-economic evaluation was conducted on developing a synthetic Fisher-Tropsch (FT) fuel using biomass gasification. Sixteen global studies on the production of FT fuel were analysed, collecting detailed data on capital expenditures, operational costs, revenue streams, raw material procurement, and product pricing. Through the analysis of parameters exhibiting robust correlations, it was deduced that higher production capacities of FT fuels corresponded to reduced relative production costs (EUR/MWh) and capital investments. Moreover, larger production capacities were associated with shorter investment payback periods and enhanced production efficiency. Notably, the cost of obtaining biomass emerged as the most significant contributor to production costs, constituting 46.6 % of the total expenditure.

These findings highlight the significance of integrating technical and economic aspects into the catalytic conversion of biomass for biofuel generation. Through thorough techno-economic evaluations, stakeholders can gain insights crucial for informed decision-making regarding investments, technology advancements, and optimization strategies for heterogeneous catalytic processes. Hence, there is a need for more research on the techno-economic evaluation of catalytic biomass conversion to biofuels, with particular emphasis on the impact of heterogeneous catalysts on the economic aspects of the conversion process. The use of heterogeneous catalysts holds significant promise for enhancing the economic viability of biomass conversion. Specifically, these catalysts can lower overall costs, enable catalyst reuse, and reduce the need for energy-intensive downstream purification processes. Table 7 summarizes the economic implications associated with various biomass conversion methods. From the data presented in Table 7, it can be inferred that anaerobic digestion and in-situ transesterification are generally more cost-effective for low-value biomass or waste streams,

Table 7
Economic evaluation of different biomass conversion methods (summary).

Conversion Methods	Techno-economic highlights	Inference	References
Anaerobic Digestion (Algae)	• Major expenditures include cultivation, harvesting, digester operation, purification, upscaling, and market rates. • - Harvesting: ~25–30 % of costs	Efficient for algae-based biofuel, rapid productivity, significant biofuel in 3.5 h compared to other substrates	[263]
Biodiesel from Microalgae	• Catalyst concentration impacts costs • 2 % KOH (optimum): $4.77/kg • In-situ transesterification: $9.92/kg • Enzymatic transesterification: $12.53/kg • Lipid content increase: costs decrease from $0.89 to $0.59 per litre	Cost-effective at optimal catalyst concentration, lipid content crucial for cost reduction	[268]
Lipid Cane for Biodiesel	• Biodiesel cost: $0.59 - $0.89/L for lipid (2–20 %), which is cheaper compared to soybean ($1.08/L) • Ethanol from lipid cane: $0.40 - $0.46/L • Soybean-based diesel: 15 % IRR • Lipid-cane diesel: 13.7 % - 24.0 % IRR	Lipid cane provides a cheaper alternative to soybeans, promising economic returns.	[269] [268]
Low-cost Acid Oil Biodiesel	• Catalysts: bulk CaO, nano-CaO • CaO: Better economic efficiency • Homogeneous catalyst impractical: high costs, larger reactor size	Bulk CaO catalyst offers the best economic performance; homogeneous (enzyme) catalysts are too costly	[264]
Anaerobic Digestion (Vinasse)	• Initial investment costs for digesters and treatment units • H2S removal cost: $20,797 • Rate of return: 11 %	Significant initial investment, moderate return rate	[270]
Biogas and Biomethane	• Net cost: $6.29 (biomethane), $4.68 (biogas) • Assumes 20-year lifespan, 11 % interest rate, 270 operational days/year	Biomethane production is more costly than biogas, and has substantial profit potential	[273]
Fischer-Tropsch (FT) process	• FT Net cost: $146/bbl, not comparable to: • Traditional fossil fuels: $115 - $206/bbl	Fischer-Tropsch synthesis faces competitiveness issues, but breakeven is achievable with careful planning.	[271]
Thermochemical conversion and anaerobic digestion process	• Breakeven cost of diesel via anaerobic digestion and thermochemical conversion: $1.30/L of diesel	Thermochemical conversion methods for transforming biomass into fuel are considered promising integrated solutions.	[272]
Synthetic Fuel from Biomass Gasification	• CAPEX, OPEX, revenue streams, raw material procurement, product pricing • Higher production capacities: reduced costs (EUR/MWh), shorter payback, enhanced efficiency	High production capacities and efficient resource use reduce costs, resulting in faster payback periods.	[267]
Thermochemical Pathways for Biofuels	• Comparison of biomass conversion to liquid biofuels • Economic evaluation of carbonisation, pyrolysis, hydrothermal liquefaction, gasification • Influence on reaction conditions and resultant product characteristics. • Economic challenges: competitiveness with fossil-derived fuels	Gasification is preferred over combustion and pyrolysis for economic viability.	[266]

particularly when capital investment is minimal, and co-product valorization is achievable [263,268–270]. In contrast, although catalytic hydrogenation and gasification require higher initial capital costs, they offer the advantage of long-term profitability by producing higher-value chemicals and advanced biofuels [267]. The considerable influence of harvesting costs in algae-based systems and the cost sensitivity to catalyst type in acid oil conversion demonstrate that the choice of feedstock and catalyst continues to be a crucial cost driver [263,264]. While enzymatic conversion methods are attractive from a green chemistry perspective, they face substantial financial hurdles due to their high material and operational costs [268]. Meanwhile, thermochemical processes such as the Fischer–Tropsch synthesis become economically favourable primarily at large production scales, where capital expenditures can be amortized and production efficiencies optimized [266,271,272]. According to these comparative insights, techno-economic viability depends heavily on context and necessitates compliance with end-use market conditions, catalyst technology, process scale, and feedstock type.

3.2. Environmental impacts and life cycle assessment (LCA) of different biomass conversion methods – comparative study

Environmental concerns related to bioenergy can be addressed by implementing emission control methods and source-reduction strategies [274,275]. Life cycle assessment (LCA) methodology offers a comprehensive approach to environmental analysis, focusing on key impact categories such as primary energy consumption (Net Energy Ratio, NER) and global warming potential, which measures greenhouse gas emissions [276]. The LCA analysis of biomass-to-biofuels conversion serves dual objectives: optimizing process platforms and operational conditions while assessing environmental impacts.

Sun, et al. [277] conducted a detailed Life cycle assessment (LCA) to evaluate microalgae processing for biofuel production. Their study explored five process platforms for producing biodiesel and biogas. Biodiesel production involves three distinct platforms: transesterification, hydrothermal liquefaction, and pyrolysis. Whereas biogas recovery employed two platforms: anaerobic digestion (AD) with and without pretreatment. Pyrolysis gave the maximum NER of 2.45 among

Table 8
Environmental aspects of biomass conversion technologies.

Aspect	Environmental Impact	Inference
Hazardous Chemical Risk	Reduces the risk of hazardous chemical spillage or leakage	Heterogeneous catalysts minimize the use of harmful chemicals, enhancing safety
Energy Consumption	Higher energy consumption compared to some processes	Requires more energy, potentially leading to fossil fuel depletion
Waste Generation	Minimizes waste production	Eliminates the need for energy-intensive purification steps
Greenhouse Gas Emissions	Potential for increased GHG emissions due to higher energy and methanol consumption	Must be carefully managed to avoid negative environmental impacts
Catalyst Recovery and Reuse	Enables recovery and reuse of catalysts, reducing by-product generation	Promotes resource efficiency and reduces waste
Process Efficiency	Higher biodiesel yield and improved glycerine purity	Results in better process efficiency and lower operating costs
Reaction Conditions	Operates under milder reaction conditions	Less energy-intensive and more environmentally friendly
Environmental Footprint (LCA)	Requires a comprehensive LCA to assess the overall environmental impact	Life Cycle Assessment is essential for a thorough evaluation.
Resource Efficiency	Promotes resource efficiency through catalyst recovery and minimal waste generation	Supports sustainable practices
Comparative Studies (Homogeneous vs. Heterogeneous)	Heterogeneous catalysts offer significant environmental advantages over homogeneous catalysts	More sustainable and cost-effective in the long term
Pollution Prevention	Effective in minimising pollution	Reduces reliance on hazardous substances, thus preventing pollution
Sustainability	Ongoing research aims to enhance performance, recyclability, and environmental compatibility.	Advances in catalyst technology are critical for sustainable development.

biodiesel production platforms, surpassing hydrothermal liquefaction (1.25) and transesterification (1.52). Furthermore, pyrolysis showed the highest greenhouse gas (GHG) emissions at 265.26 g CO_2 / MJ biofuel, while hydrothermal liquefaction and transesterification demonstrated lower emissions at −6.77 g CO_2 / MJ biofuel and − 10.37 g CO_2 / MJ biofuel, respectively. Regarding biogas production, AD without pretreatment reached the maximum net energy ratio (NER) of 1.27, whereas AD with pretreatment had an NER of 0.71. Greenhouse gas (GHG) emissions were approximately −60.83 g CO_2 / MJ biofuel for AD with pretreatment and − 173.02 g CO_2 / MJ biofuel for AD without pretreatment.

Biochemical methods such as fermentation and biomethanation are often praised for their environmental friendliness, attributed to their reduced energy demands and moderate operational parameters in contrast to thermochemical techniques [256]. However, certain comparative studies have unveiled instances where thermochemical processes exhibit reduced environmental footprints compared to biological methods, even under similar biomass, geographic location, and temporal conditions [278,279]. For instance, Aberilla, et al. [280] research shows that although thermochemical processes showed higher overall environmental impacts, gasification demonstrated lower greenhouse gas emissions than anaerobic digestion for rice and coconut residues.

When assessing bioenergy systems as viable alternatives to fossil fuels, measuring their environmental impacts using life cycle analysis (LCA) is crucial. Recently, Das, et al. [281] performed an extensive cradle-to-grave LCA, comparing fast pyrolysis combined with electrocatalytic hydrogenation followed by centralised hydro-processing (Py-ECH) with cellulosic fermentation. The study focused on key environmental impact categories such as climate change, water scarcity, and eutrophication. The findings revealed that liquid hydrocarbon production via Py-ECH had significantly lower eutrophication potential and water scarcity footprint than cellulosic ethanol production. Additionally, greater use of renewable electricity reduced greenhouse gas emissions in the Py-ECH process. Remarkably, when the renewable fraction of grid electricity exceeded 87 %, the Py-ECH process exhibited lower greenhouse gas emissions than cellulosic ethanol production. In a separate study, Masoumi and Dalai [282] conducted an LCA to evaluate algal biofuel production through a two-stage process involving hydrothermal liquefaction (HTL) and catalytic hydrodeoxygenation (HDO). Initially, microalgae were converted into bio-crude oil using HTL in a methanol-water system. This biocrude oil was then upgraded catalytically to produce algal biofuels. The application of HDO enhanced the bio-crude oil quality by reducing its oxygen content to 3.1 wt% and increasing the higher heating value (HHV) to 42 MJ per kilogram of biofuel. The LCA analysis showed that the greenhouse gas (GHG) emissions performance of the resulting algal biofuel was −1.13 $gCO_{2\text{-eq}}$ per MJ, indicating a significant reduction in GHG emissions compared to petroleum-based fuel production.

Heterogeneous catalyzed processes offer environmental benefits by reducing the risk of hazardous chemical spillage or leakage and eliminating the need for energy-intensive glycerine purification steps, thus minimising waste generation. However, It is important to note that these processes can inadvertently result in fossil fuel depletion and increased greenhouse gas emissions because of their higher energy and methanol consumption [283]. Despite the potential advantages of utilizing heterogeneous catalysts (such as biochar derived from biomass waste) in biodiesel production, there's a pressing need to assess their environmental impact through life cycle analysis (LCA). Such an analysis is essential for establishing the environmental benefits of waste-derived heterogeneous catalysts over conventional ones [284]. The work conducted by anak Erison, et al. [285] aimed to perform a life cycle assessment (LCA) of palm-based cooking oil for biodiesel generation. This was achieved using impregnated magnetic biochar derived from waste palm kernel shell (PKS) as a catalyst. Their research aimed to assess the environmental efficiency of biodiesel production using impregnated magnetic biochar generated from waste PKS through two LCA case studies. In Case 1, the primary focus of raw material processing was the extraction of PKS from palm fruit bunches, whereas the manufacturing of refined palm cooking oil was not included and had to be bought separately. In contrast, Case 2 involved the extraction of PKS and the manufacturing of refined palm cooking oil from fruit palm bunches. Afterwards, the LCA case study with the minimal environmental impact was determined. The findings of LCA results showed that Case 1 (6.64×10^2 Pt) had significantly lower environmental impacts compared to Case 2 (1.83×10^3 Pt). This implies that buying refined palm oil for biodiesel production could reduce environmental impacts by 64 % compared to producing biodiesel directly from raw fruit bunches.

Although Life Cycle Assessment (LCA) is a reliable tool for assessing the environmental impact of processes, there are still notable differences in the studies analysed. These discrepancies can be attributed to several interrelated factors. Firstly, defining system boundaries is crucial in shaping the assessment results. While some studies limit their assessment to the production phase, others take a broader perspective that encompasses the entire life cycle from material extraction to waste

disposal. As a result, inconsistent methodological approaches make direct comparison between the studies difficult, as they each measure different areas of emissions, resource utilisation, and environmental impacts. In addition, the environmental performance of a process is strongly influenced by the specification and characteristics of the biomass feedstock. Factors such as moisture content, chemical composition, and the energy required to process the biomass significantly impact emissions, process efficiency, and overall sustainability outcomes. The reliability of the data further complicates comparisons, as variations in the measurement of process efficiency, geographical conditions, and energy source assumptions lead to significant fluctuations. For example, using renewable electricity in the Py-ECH process reported by Das, et al. [281] directly impacted the greenhouse gas (GHG) emissions profile. Furthermore, studies often prioritise different categories of environmental impacts, with GHG emissions, water use, and energy efficiency usually emerging as primary metrics. Consequently, a process such as pyrolysis might be considered optimal based on energy recovery metrics, but performs less well when assessed on emissions-related criteria. Given this complexity, it is important to critically evaluate the scope, impact prioritisation, and data quality underpinning any LCA study. Such contextual awareness is crucial to accurately interpret the results and draw meaningful conclusions from comparative environmental assessments.

Hence, heterogeneous catalysis stands out for its significant environmental advantages over traditional methods. It effectively minimizes waste production and pollution by enabling milder reaction conditions and reducing reliance on hazardous substances. Moreover, the ability to recover and reuse catalysts reduces by-product generation, fostering resource efficiency and pollution prevention. Adopting environmentally benign catalysts and sustainable solvents will further boost the eco-friendliness of heterogeneous catalytic processes. Also, comprehensive evaluations like life cycle analyses (LCA) could offer a thorough assessment of the environmental impact of heterogeneous catalysis, covering aspects like waste generation, greenhouse gas emissions, and energy consumption throughout the process lifecycle. Ongoing research and development efforts to enhance catalyst performance, recyclability, and environmental compatibility will further propel the role of heterogeneous catalysis in advancing sustainable development. Table 8 presents a summary of the environmental impact of the biomass conversion process.

4. Challenges and prospects of heterogeneous catalysis

4.1. Challenges of heterogeneous catalysis

The economic drive by anthropogenic and industrial activities, mounting the demand for fossil fuel, makes environmental challenges and carbon footprint inevitable in the conventional energy sector [286]. Herein, the pragmatic approach of replacing traditional fuels with renewable energy is being hindered by various obstacles, especially in developing countries. These setbacks include insufficient capital and feedstocks, equipment design, and complex operational processes impeded by limited resources [287,288]. In recent years, catalysis science and technology have presented opportunities for directly using catalysts for renewable energy production with net-zero emissions [286,289,290]. However, homogeneous catalysts, being the most widely used catalysts, are reportedly driven by high energy with low reaction rates and are costly [291]. This signpost, heterogeneous catalysis, is advantageous in offering sustainability and high production yield with a quick reaction rate at lower temperatures and pressure [35,292]. Despite the high yields, the inability to separate heterogeneous catalysts from the product streams based on the sensitivity to recycling or reusing the catalyst makes it very challenging [293]. Notwithstanding, heterogeneous catalysts can be acidic, basic, or bifunctional (exhibiting both acidic and basic properties) [294]. Whereby the feedstock matrices and the morphological structure of the catalyst challenge the catalyst selectivity, product quality, yield, and reusability of the catalyst [288,294,295]. This has intensified research to improve the stability of the catalyst active sites by controlling the surface properties to favour their infusibility and affinity [296]. This involves trapping the active molecules with supports such as iron, silica, or alumina to promote the pores of the catalysts.

In essence, acidic-based heterogeneous catalysts require long reaction times and high temperatures, influencing their hydrophobicity [297]. Meanwhile, the bifunctional heterogeneous catalysis, being non-corrosive and cost-effective, can occur under mild conditions (biodiesel production) [294,296]. The mixed or waste material-based heterogeneous catalysts can exhibit different phases than their reactants by adhering to their surface. The reactant adsorbed onto the active phase of the catalyst then creates chemical affinity, which affects the catalyst's efficacy and regeneration for reuse. However, modifying heterogeneous catalysts has underlying mechanisms that can affect their performance and product quality [288]. This has become very sensitive to engineering highly active, cost-effective, and stable catalysts in the renewable energy sector. Meanwhile, the synergistic effect of radicals, excited molecules, and charged species to reconcile with a stable heterogeneous catalyst can influence its performance in accelerated reaction conditions [35,288,297]. This affects the catalyst chemistry or characteristics, especially its regeneration ability via electromagnetic induction or by coating and immobilization of the catalysts placed in a microchannel [35,294].

Furthermore, the applicability of heterogeneous catalysts can be combined with the scavenging material of the reaction products, which becomes very difficult to remove. This is critical in terms of catalyst placement techniques that can facilitate the mass transfer within a short period by either coating with beads or immobilizing with support [287,288]. However, heterogeneous catalysis faces the challenge of suitable support to form a packed bed, such as covalent support, self-support, adsorbent, H-bonding, ionic interaction, polymer resin, and non-conventional media [288]. However, using heterogeneous catalysts in photocatalysis requires various electrochemical redox potentials. This causes mass transport setbacks on the separation phase by adsorption onto the solid surface, restricting the photons' reaction with the catalyst. Also, to enhance the reaction rate with scale-up product quality, the chemistry of heterogeneous catalysis is very sensitive to high temperature, high pressure, and equipment design [296,298,299]. Therefore, the process augmentation requires equipment integration with extra capital investment. Likewise, activating the heterogeneous catalysts by either photo-, microwave- or ultrasound-induced flow chemistry hastens the interface construction is costly [300,301]. Ideally, the catalyst's surface area depends on the catalyst's load or amount, whereby the volume ratio requires a moderate catalyst load owing to the catalyst's active sites to propagate the reaction [300].

Moreover, the industrial-scale application of heterogeneous catalysts is also limited by the parametric conditions of operation. The parametric conditions, such as temperature, moisture quantity of the feedstock, amount of the catalyst, and reaction time, affect the overall conversion and reaction rate [35,288]. The morphological and molecular compositions are also significantly influenced by calcination temperature for both acidic and basic heterogeneous catalysts [295,301]. Thus, the amount of catalyst load required depends on the surface area owing to the presence of active sites, which can influence the reaction rate and product quality [287,301]. Generally, the primary properties of the catalysts include the surface area, pore size, pore volume, and the active sites that significantly influence catalytic activity [296,298,301]. A study done at calcined temperatures between 600 and 700 °C of zirconia (ZrO_2), improved biodiesel yield from 77 % to 88 %, whereby at 800 °C the yield reduced to 60 % [296]. This suggests that the catalyst structure can be disintegrated at high temperatures, whereby the thermal treatment restricts the gaseous dispersion and pores on the catalyst surface. So, the development of a structural or morphological predictive model via computational modeling and optimization of parametric conditions

requires intensive research in catalyst synthesis and application [302].

4.2. Current perspective and prospects of heterogeneous catalysis

The prospects of heterogeneous catalysts via photo-, electro-, and thermal-catalysis in converting CO_2 into valuable products come in handy to achieve a carbon-neutral economy. This offers multidisciplinary research interest in advancing heterogeneous catalytic technologies and engineering active sites and molecular level of the catalysts via doping heteroatoms, morphological control, and surface functionalization [35,301,302]. These factors indicate that CO_2 will continue to be abundant as long as fossil fuels remain the primary energy sources and can be used as feedstock for conversion into hydrocarbons. In this light, converting CO_2 into fuels and petrochemicals must be explored as a sustainable alternative [303–306]. Various approaches for CO_2 conversion have been investigated, including thermochemical, photoelectrochemical, biochemical, and electrochemical processes, with electrochemical strategies based on nanomaterials showing promise in terms of conversion efficiency [303]. Xu, et al. [306] reported novel carbon-supported Sn electrocatalysts with a tin size ranging from single atoms to ultrasmall clusters to nanocrystallites for the conversion of CO_2 to acetate, ethanol, and formate with a selectivity of over 90 % for each of these chemicals. Using CO2 as a feedstock for fuel production not only helps minimize global warming but also contributes to a circular carbon economy that aligns with the concepts of green chemistry and sustainable development. Integrating biotechnology and catalysis is critical in harnessing CO_2 for energy products to reduce reliance on fossil carbon and carbon emissions into the atmosphere.

With an emphasis on considering heterogeneous catalysts for industrial applications, key factors such as catalytic activity, selectivity, loading, reusability, and the ability to foster renewable energy production play essential roles. Herein, boron-based catalysts, waste material-based catalysts, carbon-based catalysts, acid and basic-based heterogeneous catalysts, transitional metal oxides, derivatives, mixed oxides and derivatives, and alkaline metal oxides and derivatives are gaining attention in heterogeneous catalysis research. Moreover, heterogeneous catalysts supported with metal oxides can improve the surface area, tunability, and morphology for remarkable product selectivity and catalytic activities [294,296]. Emerging catalytic materials such as single-atom catalysts (SACs) and ionic liquids (ILs) revolutionise heterogeneous catalysis for energy production. SACs offer high atom efficiency and well-defined active sites, enabling superior selectivity and activity in reactions like CO_2 hydrogenation and biomass conversion. Ionic liquids improve catalyst performance with tunable properties and thermal stability by enhancing mass transfer and suppressing deactivation. When integrated into solid supports, these materials boost recyclability and reaction efficiency. Their continued development offers transformative potential for next-generation, scalable, and carbon-neutral energy technologies.

A modified heterogeneous catalyst, especially with natural composites or metal oxides, makes separation easier and is eco-friendly with less environmental impact [288,296,298]. In addition, the transition from a carbon-based economy towards a sustainable green economy requires the development of catalytic technologies coupled with renewable energy [307]. This has more sustainability and environmental prospects than conventional thermal technologies that utilize fossil fuels. For this reason, exploiting photo- and electro-heterogeneity catalysis with renewable energy (solar, hydro, wind, etc) offers considerable research interest [288,299,302]. These include but are not limited to (i) the synthesis and application of heterogeneous catalysis with renewable energy sources and (ii) the technological advancement of plasma catalysis and the use of electromagnetic fields to modulate catalytic activity [296,298]. Also, integrating heterogeneous catalysis with renewable technologies provides hope for the transition from photocatalytic reforming to sustainable energy development (e.g. green hydrogen) [287,292,299]. The energy drive of heterogeneous catalysis in photocatalytic and electrocatalytic processes can be hindered by the suitability of band gaps [308]. This has garnered significant attention to modification techniques such as sulfonation, organic functionalization, and post-transition metal grafting with either alkaline or calcined natural composites [308–310].

Furthermore, microalgae-derived biochar produced via pyrolysis with high surface area, pore size, and presence of inorganics and functional groups has been demonstrated to be a promising catalyst for biodiesel production via the transesterification process [35,295,308,309]. This presents a sustainable solution over conventional catalysis to mitigate the current energy demand. Also, to enhance the physicochemical properties, the microalgae-derived biochar catalyst can be regenerated by either physical (steam treatment, CO_2 treatment) or chemical activation (acidic, basic, or oxidation treatment) [288,295,299]. Therefore, the prospect of developing a heterogeneous catalyst such as biochar derivatives from biomass or microalgae for biodiesel technology offers economic benefits for a sustainable environment and carbon neutrality.

5. Conclusion and outlook

Heterogeneous catalysis has become a promising method for converting biomass resources into clean, renewable energy. Heterogeneous catalysis offers advantages over conventional techniques, such as selectivity, reusability, and lower waste generation. The use of heterogeneous catalysts significantly improves the conversion efficiency, product yield and quality of this process. Catalysts such as advanced materials, including zeolites, MOF and mesoporous materials, improve process efficiency and environmental sustainability by minimising hazardous chemicals and energy consumption. Emerging catalytic materials, such as single-atom catalysts and ionic liquids, are transforming heterogeneous catalysis by offering enhanced selectivity, greater stability, and superior atom efficiency. Their integration enhances performance in key energy reactions such as CO_2 reduction and biomass conversion. These materials hold strong potential for future scalable and sustainable energy solutions. Analysing different catalysts for biomass conversion shows that selecting the right heterogeneous catalysts is crucial for the overall performance. In addition, optimisation of the operating conditions is essential to achieve the desired conversion rates and product distribution. Advancements in in-situ characterisation and theoretical modeling have significantly deepened the mechanistic understanding of heterogeneous catalysis for renewable energy. These tools enable real-time tracking of active species, structural evolution, and reaction pathways under operational conditions. Coupled with insights into catalyst deactivation and regeneration, they inform the rational design of robust and scalable catalytic systems. Such integrated approaches are essential for translating catalytic innovations into industrial bioenergy applications.

The economic and environmental assessment of biomass conversion methods highlights their complexity and varying impacts. Anaerobic digestion offers rapid biofuel yields, especially from algae, but faces high cultivation and harvesting costs. Biodiesel production from microalgae is viable with optimal catalyst use and sufficient lipid content, while lipid cane presents a cost-effective alternative to traditional sources like soybeans. Catalyst choice significantly influences economic feasibility, with heterogeneous calcium oxide outperforming costly enzyme-based options. Techno-economic factors such as catalyst cost, production scale, and biofuel market value shape process viability. For instance, Fischer-Tropsch synthesis can become profitable with strategic planning, and biomass gasification yields cost advantages at larger scales. Environmentally, anaerobic digestion without pre-treatment offers the highest net energy output and lowest emissions, while gasification has lower emissions for certain biomasses. Catalysts play a key role in optimizing both economic and ecological performance. Integrated assessments and continued research are essential to advance biomass conversion technologies for sustainable energy production.

Catalytic conversion of biomass holds great potential for promoting sustainable development and reducing GHG emissions. Catalytic processes are crucial in capturing CO_2 and converting it into useful products like fuels or chemicals. This carbon regeneration into valuable resources helps reduce greenhouse gas emissions and regenerates energy from what would otherwise be waste. The conversion of CO_2 into hydrocarbons presents a promising pathway towards achieving carbon neutrality and advancing a sustainable circular economy. Furthermore, considering factors such as catalyst performance, production capacity, and market dynamics to make informed decisions is critical to an effective and improved biofuel production process. Continued research and development efforts to improve catalyst performance, recyclability, and environmental performance will be critical to advancing sustainable biomass conversion and achieving carbon-neutral energy solutions. Through comprehensive assessments and innovative approaches, the potential of biomass as a renewable energy source can be fully realised and contribute to global sustainability goals.

CRediT authorship contribution statement

Ifeanyi Michael Smarte Anekwe: Writing – review & editing, Writing – original draft, Visualization, Validation, Supervision, Software, Resources, Project administration, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Stephen Okiemute Akpasi:** Writing – original draft, Investigation, Formal analysis, Data curation. **Emmanuel Kweinor Tetteh:** Writing – original draft, Investigation, Formal analysis, Data curation. **Atuman Samaila Joel:** Writing – original draft, Investigation, Formal analysis, Data curation. **Sherif Ishola Mustapha:** Writing – original draft, Investigation, Formal analysis, Data curation. **Yusuf Makarfi Isa:** Writing – review & editing, Supervision, Resources.

Declaration of competing interest

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

Data availability

Data will be made available on request.

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