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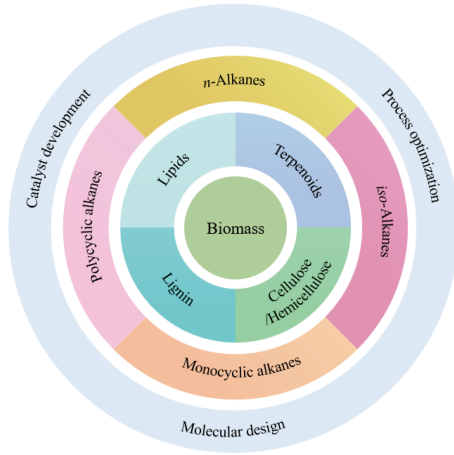
REVIEW

Research progress on chemical synthesis of biomass-based hydrocarbon fuels

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Abstract: Biomass-based hydrocarbon fuels, as one of the alternatives to traditional fossil fuels, have attracted considerable attention in the energy field due to their renewability and environmental benefits. This article provides a systematic review of recent research progress in the chemical synthesis of biomass-based hydrocarbon fuels. It outlines the conversion pathways using feedstocks such as lipids, terpenoids, cellulose/hemicellulose, and lignin. Depending on the feedstock, various products with distinct structural characteristics can be prepared through reactions such as cyclization, condensation, and catalytic hydrogenation. Throughout the synthesis process, three key factors play a critical role: efficient catalyst development, production process optimization, and computational-chemistry-based molecular design. Finally, the article discusses future perspectives for biomass-based hydrocarbon fuel synthesis research.



Key words: biomass; hydrocarbon fuel; catalyst development; process optimization; molecular design; computational chemistry

The energy crisis and environmental issues represent significant challenges confronting humanity in the 21st century. Amidst continuously growing global energy demands and excessive consumption of fossil fuels, the development of renewable, clean, and highly efficient alternative energy sources has become a focal point of international attention[1]. In the transportation sector, particularly in specialized applications such as aviation and aerospace, the non-renewable nature and high carbon emission characteristics of conventional petroleum-based fuels have prompted active exploration of sustainable alternatives. Against this backdrop, the synthesis of biomass-derived hydrocarbon fuels has garnered widespread interest due to their renewable feedstocks, carbon neutrality, and high design flexibility, positioning them as one of the most promising substitutes for petroleum-based fuels[2−3].

Biomass resources are abundant and diverse, with the primary feedstocks for hydrocarbon fuel production comprising lipids, terpenoids, cellulose/hemicellulose, and lignin[3−5]. These feedstocks can be converted via specific chemical pathways to synthesize hydrocarbon fuels characterized by varying energy densities, excellent low-temperature performance, and high thermal stability. Lipids—derived from sources such as plants, animals, and microalgae—represent a significant category of biomass. They first undergo hydrodeoxygenation to yield *n*-alkanes within the aviation kerosene distillation range[6], followed by an isomerization process that converts these *n*-alkanes into *iso*-alkanes with superior low-temperature properties[7]. Terpenoids (such as α-pinene and β-caryophyllene), which are plant secondary metabolites and often possess natural cyclic structures, can be directly converted into cycloalkane-based fuels through reactions including dimerization, hydrogenation, and isomerization. These compounds exhibit densities falling within the range of high-density fuels[8−9]. Cellulose and hemicellulose, as the primary constituents of plant cell walls, represent the most abundant and widely available biomass components. Through hydrolysis and dehydration processes, they yield

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platform compounds such as furfural and cyclopentanone, which subsequently serve as precursors for the synthesis of linear[10], branched[11], or cyclic alkane[12] fuels via aldol condensation and hydrodeoxygenation steps. Lignin, owing to its abundant aromatic structure[13−14], can be transformed into cycloalkane-based fuels through catalytic hydrodeoxygenation and intramolecular cyclization reactions.

This review systematically summarizes recent advances in the chemical synthesis of hydrocarbon fuels from biomass. It examines conversion pathways utilizing lipids, terpenoids, cellulose/hemicellulose, and lignin as feedstocks, and provides a thorough analysis of the ways in which catalyst development, process optimization, and computational chemistry-assisted molecular design have advanced fuel synthesis. Future research directions in this field are also discussed.

1 Progress in the synthesis of hydrocarbon fuels from lipids

Lipids, primarily comprising animal/vegetable fats and waste cooking oils, exhibit carbon chain lengths (C_{12}–C_{18}) that closely match the carbon number range of conventional middle distillate fuels such as diesel and aviation kerosene, demonstrating significant advantages in carbon chain compatibility. The core of their conversion lies in the removal of oxygen-containing functional groups and the modulation of carbon chain structures, with the main products consisting of *n*-alkanes and *iso*-alkanes.

1.1 Synthesis of *n*-alkane fuels from lipids

In the synthesis of biomass-derived hydrocarbon fuels, unsaturated fatty acids can be catalytically hydrogenated into saturated fatty acids, which subsequently undergo decarbonylation/decarboxylation reactions to yield C_{15}–C_{18} *n*-alkanes. Commonly employed catalytic systems include noble metals, transition metals, and bimetallic catalysts.

Chen et al.[6] developed a $PtWO_x/SiO_2$-Air catalyst prepared by calcination in air, which was applied to the decarboxylation of stearic acid, achieving a conversion rate of 99% and a heptadecane selectivity of 85%, as shown in Figure 1. The study revealed that tungsten existed in the form of amorphous WO_x on the support surface and engaged in a strong interaction with platinum, facilitating the formation of diverse Pt-WO_x interfacial structures, which significantly enhanced the decarboxylation performance.

Given the high cost associated with noble metal catalysts, the development of cost-effective transition metal and bimetallic catalysts has become highly significant. For example, the bimetallic nitride Ni_3Mo_3N, which exhibits a reduction decomposition temperature of 600 °C, demonstrated excellent catalytic performance in the hydrodeoxygenation of palmitic acid at 270 °C, achieving complete conversion (100%) with a selectivity toward C_{15}/C_{16} alkanes exceeding 90%[15] (Figure 2).

Although conventional nickel-based catalysts exhibit excellent catalytic performance, they typically require elevated reaction temperatures. Research has revealed that nickel alloys and metallic compounds can maintain high activity and selectivity under relatively mild conditions[16−17].

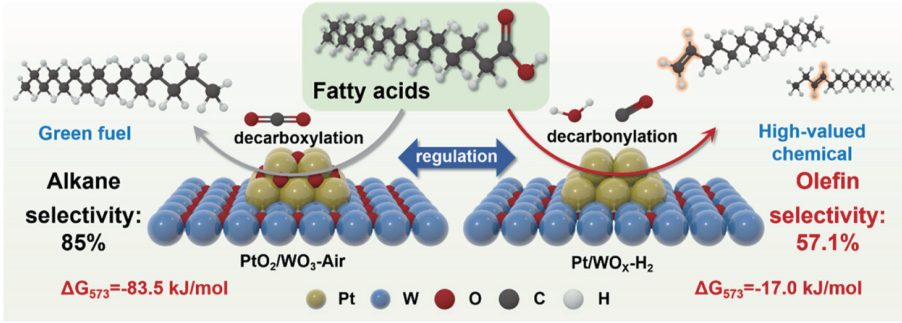


Fig. 1 Decarboxylation of stearic acid to heptadecane over $PtWO_x/SiO_2$-Air catalyst[6] (with permission from ACS Publications)

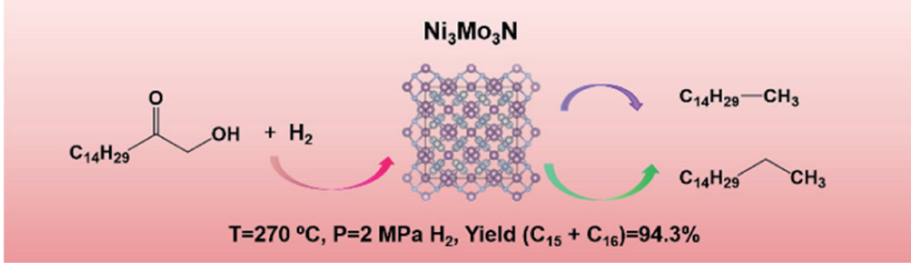


Fig. 2 Reduction of palmitic acid to C_{15}/C_{16} alkanes over bimetallic nitride Ni_3Mo_3N[15] (with permission from ACS Publications)

Zhao et al.[18] reported that the $Re_1Ni_1@SiO_2$ catalyst achieved 100% conversion in the hydrodeoxygenation of methyl stearate under mild conditions (170 °C, 2.5 MPa H_2), with a total selectivity of 96.3% toward C_{18} and C_{17} alkanes. When applied to the hydrodeoxygenation of soybean oil, this catalyst attained a conversion rate of 99%, successfully yielding a mixture of C_{15}–C_{18} alkanes, demonstrating promising potential for industrial applications.

In the optimization of production processes, Sudiyarmanto's group[19] employed a Ni@ZIF-8 catalyst under solvent-free conditions to catalyze the hydrodeoxygenation of palmitic acid and palm oil, achieving a 100% hydrocarbon yield with diesel-range hydrocarbon selectivities of 74% and 92%, respectively. This process, characterized by minimal side reactions and high environmental efficiency, offered a novel approach for the application of non-noble metal catalysts in biomass conversion and demonstrates considerable potential for industrial implementation.

Beyond this, waste cooking oil was also utilized to produce renewable fuels. Through hydroprocessing technology with Pd/C or NiMo/γ-Al_2O_3 catalysts, waste cooking oil was efficiently converted into C_{15}–C_{18} *n*-alkanes[20]. Among these, C_{15} and C_{17} alkanes were primarily generated via decarboxylation/decarbonylation pathways, whereas C_{16} and C_{18} alkanes were mainly produced through hydrodeoxygenation.

Although *n*-alkanes can serve as diesel substitutes or blending components, their low-temperature flow properties are relatively poor. To expand the application of biofuels in cryogenic environments, further isomerization modification of the carbon chain structure of *n*-alkanes is required.

1.2 Synthesis of *iso*-alkane fuels from lipids

Supported by carriers such as activated carbon, Al_2O_3, and molecular sieves, Pt- and Ni-based catalysts can further catalyze the cracking and isomerization of lipids, converting *n*-alkanes into *iso*-alkane mixtures with higher degrees of branching to improve their low-temperature performance.

Ju et al.[21] employed an ethanol-hexane fractional extraction method to selectively isolate neutral lipids from wet algae paste (achieving a lipid recovery rate of 90%), followed by direct hydroconversion using a Pt/Meso-ZSM-5 catalyst to produce renewable jet fuel. The hydroconversion process yielded 38% of jet fuel from the neutral lipids, featuring a uniform carbon number distribution and a high content of *iso*-alkanes. The resulting fuel exhibited a freezing point of −57 °C, a flash point of 42 °C, and an energy density of 45 MJ/kg, fully compliant with the ASTM D7566 standard.

In contrast to noble metal catalysts, Yan et al.[22] synthesized a Ni-based catalyst supported on nanocrystal ZSM-22 for the conversion of biomass into *iso*-alkanes. During the deoxygenation and hydroisomerization of palmitic acid at 270 °C, the 3.0Ni/N-ZSM-22 catalyst with a nickel loading of 3.0% exhibited optimal performance, achieving a total selectivity of 81.8% for *iso*-hexadecane and *iso*-pentadecane—significantly higher than that of the 3.0Ni/C-ZSM-22 catalyst (58.4%). This superior performance was attributed to its well-developed mesoporous structure, abundant 10-membered ring openings, and effective synergy between acid sites and metal centers.

In the field of process optimization, Tan's team[7] developed a pressurized CO_2–hexane–water functionalized green solvent system and employed a bifunctional Ni-Pd@Al-MCF catalyst for jet fuel production (Figure 3). When applied to a C_{18} model compound, this system achieved a conversion rate of 99.4%, a selectivity of 98.2% toward C_7–C_{17} liquid jet fuel products (LJFPs), and an *iso*-alkane to *n*-alkane ratio of 1.1, demonstrating the highly efficient catalytic performance of the bifunctional catalyst. Additionally, pressurized CO_2 reduced the system viscosity to enhance mass transfer efficiency and facilitated the reaction by regulating the pH value. Under these optimized conditions applied to the processing of castor oil derivatives, complete feedstock conversion (100%) and 98.8% selectivity toward LJFPs were achieved, indicating strong potential for industrial application.

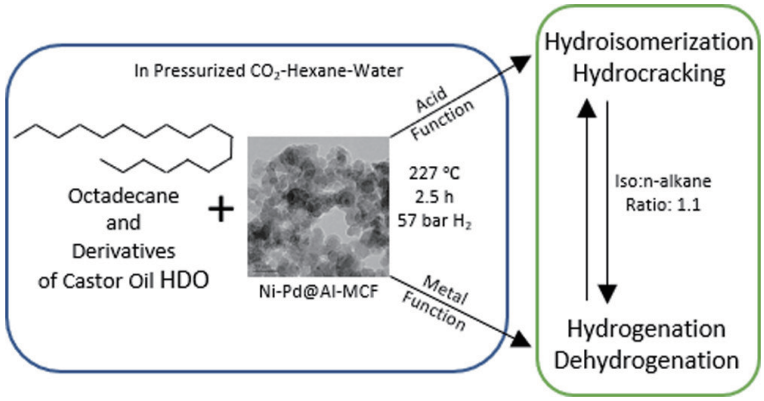


Fig. 3 Dual-functional Ni–Pd@Al-MCF-catalyzed jet-fuel production in a pressurized CO_2–hexane–water green solvent system[7] (with permission from ACS Publications)

Using palm kernel oil as the feedstock, a novel bilayer catalyst Pt/Cl-Al_2O_3@Ni/ZSM-5 enabled efficient production of bio-aviation fuel via a one-step tandem catalytic process in a single reactor[23]. Compared to the conventional two-step process (sequential hydrodeoxygenation and isomerization-cracking), this process achieved 96% feedstock conversion under optimal conditions. The resulting bio-jet fuel components consisted predominantly of C_8–C_{16} alkanes, with an *iso*-/*n*-alkane ratio of 2 and a freezing point as low as –57 °C—significantly superior to that of the two-step product (–36 °C). The catalyst exhibited excellent stability and reusability, while the streamlined process substantially reduced equipment complexity and energy consumption, demonstrating strong potential for industrial scalability.

Given that hydrocarbon fuels derived from lipids primarily consist of *n*-alkanes and *iso*-alkanes, their density is relatively low. To enhance volumetric energy density, increasing the proportion of cycloalkanes in the fuel by selecting alternative feedstocks has emerged as a critical strategy for improving fuel performance.

2 Progress in the synthesis of hydrocarbon fuels from terpenoids

Terpenoids, as plant secondary metabolites, are widely distributed in nature and are mainly derived from plant extracts such as turpentine oil, citrus essential oil, and peppermint oil. These compounds exhibit unique molecular structural characteristics, featuring polycyclic skeletons and abundant carbon−carbon double bonds, which enable their transformation into cycloalkane-dominated hydrocarbon fuels via C−C coupling reactions.

2.1 Synthesis of monocyclic alkane fuels from terpenoids

Terpenoid compounds, characterized by their high structural tunability, can undergo selective catalytic conversion to generate specific cycloalkane skeletons, thereby meeting the requirements for fuel performance. Among these, monocycloalkanes are considered ideal components for hydrocarbon fuels due to their moderate ring strain and relatively low kinematic viscosity. As a typical monoterpene, myrcene, with its conjugated diene and terminal alkene in the structure, is an ideal substrate for Diels-Alder reactions.

Staples et al.[24] utilized 2,2'-methylenebis(6-*tert*-butyl-4-methylphenol) as a radical inhibitor to dimerize myrcene via Diels-Alder reaction into a mixture of camphorene isomers, which was subsequently catalytically hydrogenated over Ni/SiO_2-Al_2O_3 to yield a fuel blend predominantly composed of camphorane isomers (Figure 4). This blended fuel exhibited a flash point of 155 °C, a boiling range of 318–332 °C, and an exceptionally low melting point (–96 °C). However, its kinematic viscosity at 40 °C was 9.32 mm^2/s, exceeding the ASTM D975 specification limit of 4 mm^2/s for diesel fuels, thus rendering it unsuitable for direct use as a diesel substitute. When blended with commercial diesel at a 50% *v*/*v* ratio, the resulting mixture demonstrates a kinematic viscosity of 3.91 mm^2/s at 40 °C, achieving favorable low-temperature performance without significantly compromising energy density.

However, the aforementioned stepwise synthesis approach exhibited significant limitations: Firstly, the Diels-Alder reaction and hydrogenation steps had to be performed sequentially, requiring intermediate separation via vacuum distillation (e.g., enrichment of camphorene isomers), resulting in complex processing and high energy consumption. Secondly, high-temperature reactions tended to induce side reactions (such as myrcene radical polymerization), necessitating the addition of radical inhibitors to improve selectivity, which further increased costs. Additionally, the hydrogenation step required a high-loading Ni catalyst (62%) with a reaction duration of approximately 48 h, demonstrating low efficiency. These factors collectively constrained the industrial applicability of this route.

Compared to the stepwise method, the biphasic tandem process not only retains the advantages of facile catalyst recovery and product separation, but also enables the coupling of multiple reactions in a “one-pot” system.

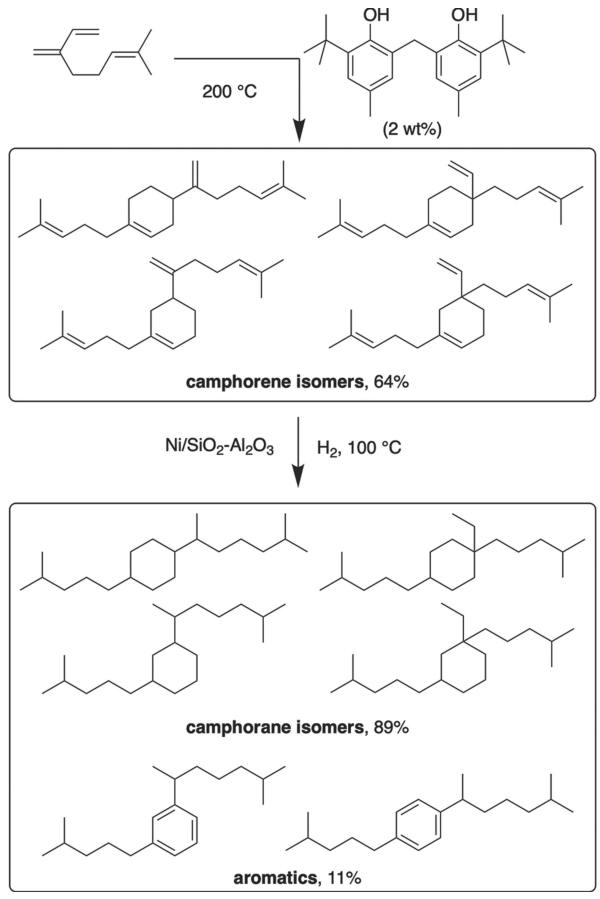


Fig. 4 Synthesis of camphorane isomers from myrcene[24] (with permission from ACS Publications)

Yang et al.[25] proposed a biphasic tandem catalytic process (biTCP) for the conversion of renewable terpenoid biomass 1,8-cineole into *p*-menthane in high yield (>99%) under mild conditions. In their approach, a "one-pot" strategy was employed to integrate multiple tandem reactions—including hydrolytic ring-opening (C–O bond cleavage), dehydration, and hydrogenation—thus reducing energy consumption and production costs.

2.2 Synthesis of polycyclic alkane fuels from terpenoids

Although monocyclic alkane fuels (such as camphane) have demonstrated favorable fuel characteristics, their relatively low energy density fails to meet the requirements for future miniaturized and long-range aircraft. Research indicates that increasing the number of rings in the molecular structure to form polycyclic configurations can significantly enhance the energy density of fuels. This improvement is attributed to the higher carbon-to-hydrogen ratio and more compact molecular packing inherent in polycyclic alkanes. Within the class of monoterpenes, compounds such as pinene, camphene, and limonene serve as critical precursors for synthesizing polycyclic alkane hydrocarbon fuels. Additionally, the principal constituents of cedarwood oil—namely, α-cedrene, and β-cedrene—also hold significant application value. Direct hydrogenation of cedarwood oil yielded a hydrocarbon fuel mixture with a density of 0.917 g/mL and a volumetric heating value of approximately 39.13 MJ/L. Through dehydration followed by hydrogenation, α-cedrol was converted into cedrane, which exhibited an even higher volumetric heating value. Furthermore, via isomerization, cedrane was transformed into a mixed fuel predominantly composed of 1-ethyl-3,5,7-trimethyladamantane (ETMA)[8], as illustrated in Figure 5. Sesquiterpenes (C_{15}) serve as premium fuel precursors for jet fuels and diesel due to their high carbon number. Molecules such as valencene, premnaspirodiene, and β-caryophyllene are ideal feedstocks for synthesizing military-grade jet fuels owing to their bicyclic molecular structures[26].

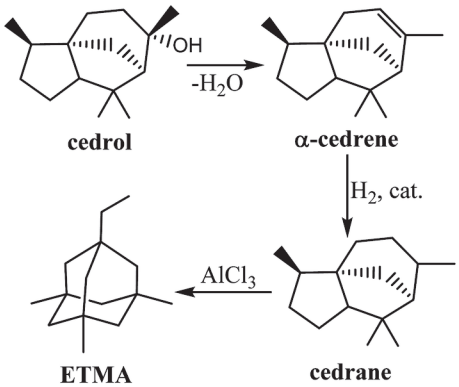


Fig. 5 Conversion of α-cedrol to 1-ethyl-3,5,7-trimethyladamantane (ETMA)[8]
(with permission from RSC Publications)

After hydrogenation, these three hydrocarbon fuels exhibited densities exceeding 0.85 g/cm^3, volumetric heating values greater than 37 MJ/L, and favorable kinematic viscosity properties at low temperatures (below 60.5 mm^2/s at –20 °C). To further enhance fuel density, dimerization reactions can be employed to increase the number of molecular rings. For instance, the dimerization product of β-pinene (C_{20}) achieves a density of 0.938 g/cm^3, comparable to that of the aviation fuel JP-10 (*exo*-tetrahydrodicyclopentadiene, *exo*-THDCPD)[27].

It is noteworthy that the pinene dimerization process is often accompanied by isomerization side reactions, and the design and development of catalysts directly influence the product distribution and fuel properties. Yuan et al.[9] developed a novel Brönsted-Lewis acidic heteropoly inorganic-organic salt catalyst, $Mn_{0.5}[MIMPS]_2PW_{12}O_{40}$, which enabled selective dimerization/isomerization of α-pinene, yielding a product mixture comprising approximately 60% dimers and 40% isomers. This hybrid hydrocarbon fuel exhibited outstanding overall performance: a density of 0.90 g/mL (20 °C), a freezing point of –66 °C, and a volumetric heating value of 39.7 MJ/L. Furthermore, catalytic systems such as MCM-22 and methyltrimethoxysilane-modified silica-alumina aerogel were also demonstrated to effectively regulate the selectivity of pinene dimerization[28−29].

The introduction of highly strained rings into olefin molecules represents an effective strategy for enhancing fuel energy density. For instance, utilizing longifolene and α-cedrene as feedstocks, Wang et al.[30] successfully synthesized biomass-derived fuels via Simmons-Smith reaction (Figure 6), achieving products with densities ranging from 0.925 to 0.965 g/mL and volumetric heating values between 39.45 and 41.51 MJ/L.

In addition to cyclic monoterpenes, acyclic monoterpene compounds, such as linalool (a type of acyclic monoterpene alcohol), are also important fuel precursors. The primary component of conventional RJ-4 fuel (tetrahydrodimethyldicyclopentadienes) was synthesized from linalool via a five-step reaction sequence, encompassing intramolecular cyclization, dehydration, Diels-Alder cycloaddition, hydrogenation, and isomerization[31]. However, the complex route and low overall yield limited its industrial viability.

In addition, Geiselman et al.[32] used poplar as a raw material and synthesized two tricyclic sesquiterpenes (epi-isozizaene and prespatane) through biological fermentation. After the hydrogenation reaction, the energy densities of the products were 40.69 and 41.46 MJ/L, which were 16.6% and 18.8% higher than that of Jet A respectively, while exhibiting relatively low kinematic viscosities. However, their excessively high melting points restricted their individual use as aviation fuels. When used as additives, they could improve the viscosity of Jet A and enhance its energy density.

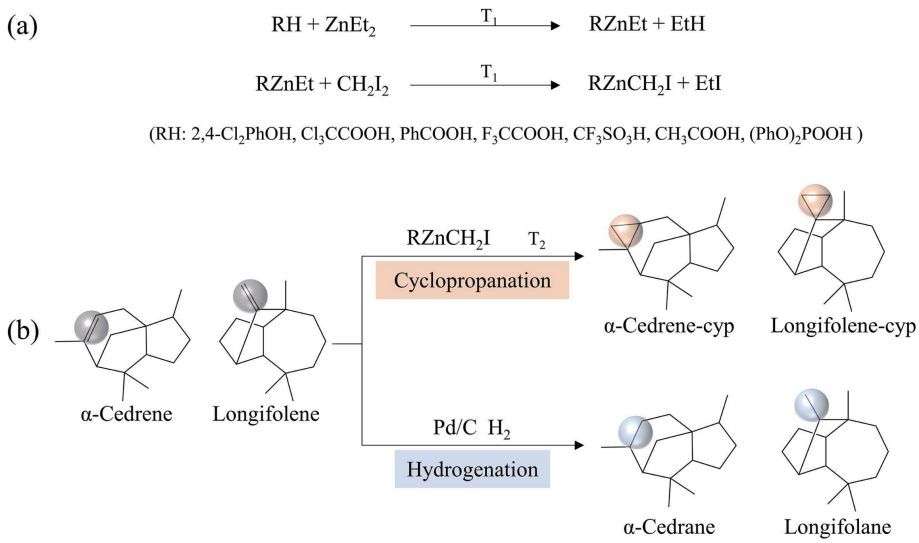


Fig. 6 Synthesis of zinc carbenoids (a) and cyclopropanation or hydrogenation of α-cedrene and longifolene (b)[30] (with permission from Elsevier)

2.3 Molecular design of terpenoid-derived hydrocarbon fuels

While conventional chemical synthesis methods for direct production of terpenoid-derived hydrocarbon fuels remain feasible, they exhibit notable limitations in rapidly screening optimal fuel molecules. In recent years, the rapid advancement of computational chemistry has prompted researchers to adopt an integrated strategy combining computational prediction with experimental validation. This approach has substantially reduced trial-and-error costs while significantly enhancing the screening efficiency for target products.

Pahima et al.[33] employed density functional theory and *ab initio* quantum chemical methods to computationally determine a series of thermochemical and combustion-related properties—including enthalpy of combustion, enthalpy of vaporization, enthalpy of formation, cetane number, boiling point, and vapor pressure—for various terpenes with high accuracy (Figure 7). The study proposed a strategy for identifying suitable petroleum alternatives while circumventing costly experimental trial-and-error processes. Huang et al.[34] integrated the group contribution method with Gaussian quantum chemical computations to establish a comprehensive database of 122 sesquiterpene skeleton molecules. They estimated key performance parameters including energy density, heat of combustion, freezing point, flash point, and density.

Based on structural characteristics and predicted properties, 17 compounds were selected, with 9 subsequently synthesized using metabolic engineering strategies. Furthermore, by comparing the experimental measurements and predicted values of representative products, the reliability of the model was verified, and its applicable boundaries and optimization directions were identified. This research proposed a methodological foundation for the targeted design of terpenoid fuel molecules and fully demonstrated the great potential of the integration of computational chemistry and experimental verification in the development of high-energy liquid fuels.

Terpenoid compounds (such as terpenes or oxygenated terpenes) can be used to synthesize biomass-based hydrocarbon fuels through steps such as catalytic hydrogenation/hydrodeoxygenation and cyclization reactions. However, terpene compounds like pinene usually need to be extracted from specific woods, and their sources are relatively limited. Therefore, the development of a synthetic method based on widely available feedstocks and simple processes is more valuable for practical applications.

3 Progress in the synthesis of hydrocarbon fuels from cellulose/hemicellulose

Cellulose and hemicellulose, as the primary structural polysaccharides in plant cell walls, are interconnected via glycosidic bonds and share similar physicochemical properties. They represent the most widely distributed and abundant renewable biomass resources in nature. Owing to their broad availability and low cost, these polysaccharides exhibit significant application advantages. Under specific reaction conditions, both can be converted into various key platform compounds through hydrolysis or biodegradation pathways[35−37]. Complete hydrolysis of cellulose yields glucose monomers, while hemicellulose hydrolysis produces various monosaccharides such as pentoses and hexoses. Notably, after cellulose undergoes thermochemical conversion (such as fast pyrolysis), its products still need to be processed through techniques like hydrodeoxygenation and catalytic cracking before they can be used as fuels. Through systematic degradation and transformation, these platform compound (Table 1) can be further processed into hydrocarbon fuels via steps such as aldol condensation and hydrodeoxygenation[38−40]. Among them, furfural and 5-hydroxymethylfurfural are the most mainstream platform compounds for preparing hydrocarbon fuels, owing to their abundant raw materials and mature conversion pathways.

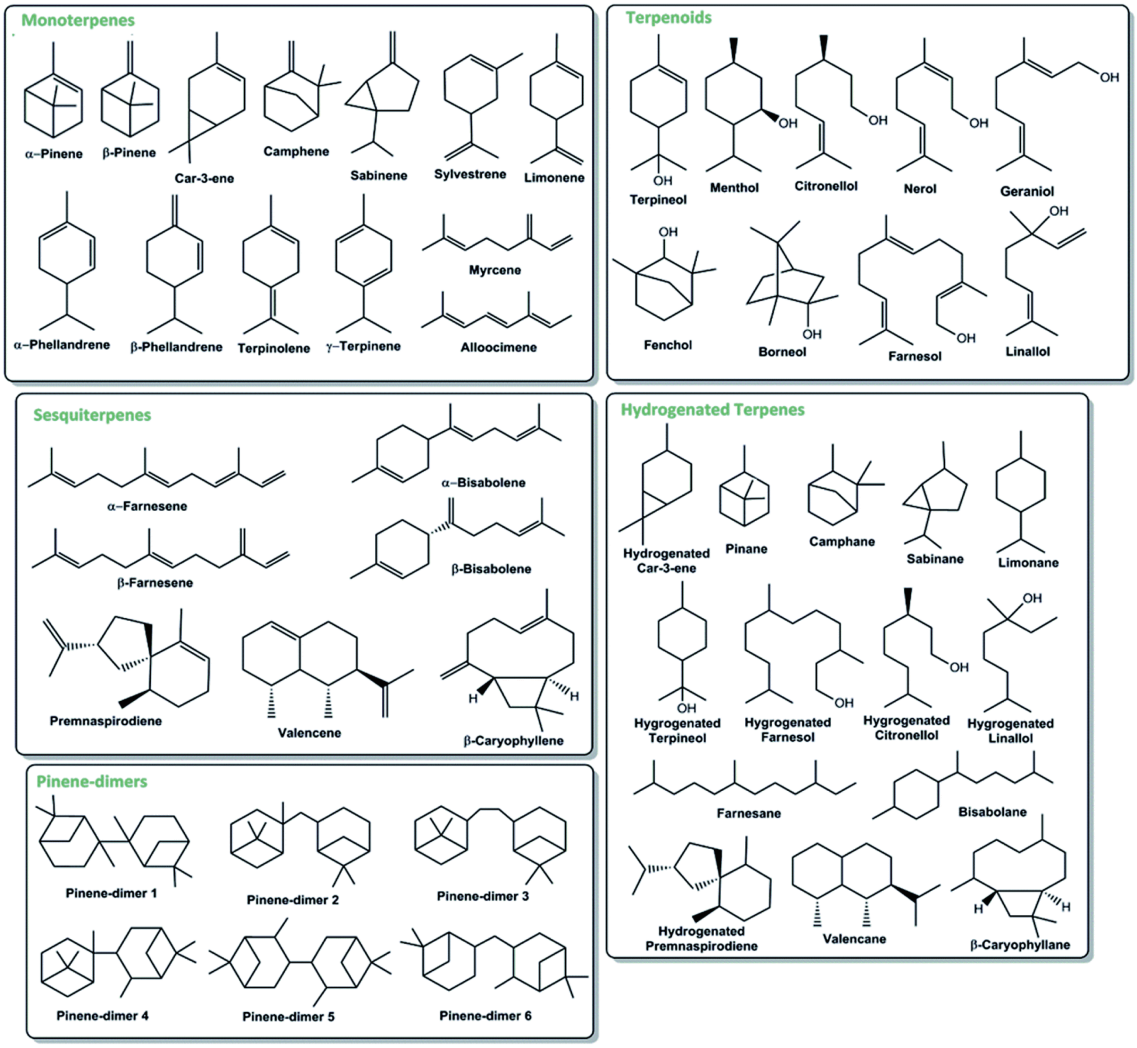


Fig. 7 Terpenes and terpenoids evaluated by density functional theory and *ab initio* quantum chemical methods[33] (with permission from RSC Publications)

Table 1 Platform compounds derived from cellulose and hemicellulose

Classification	Platform compounds
Sugars	glucose, fructose, xylose, etc.[41−42]
Alcohols	ethanol, hexanol, octanol, cyclohexanol, etc.[43−44]
Esters	ethyl levulinate, γ-valerolactone, angelica lactone, etc.[45−51]
Furans	2-methylfuran, 2,5-dimethylfuran, 5-hydroxymethylfurfural, furfural, etc.[52−56]
Acids	levulinic acid, lactic acid, formic acid, 2,5-dihydroxypentanoic acid, etc.[57−58]
Ketones	2,5-hexanedione, 1-hydroxy-2-hexanone, cyclopentanone, etc.[59−61]

3.1 Synthesis of *n*-alkane fuels from cellulose/hemicellulose

Platform compounds derived from cellulose and hemicellulose typically possess abundant oxygen-containing functional groups. These compounds can undergo chain elongation via condensation or polymerization reactions, thereby enabling their utilization in the production of *n*-alkane fuels.

In 2005, Huber et al.[62] pioneered the use of intermolecular aldol condensation reaction and hydrodeoxygenation reaction to convert biomass-derived acetone and furfural (at a specific ratio) into long-carbon-chain liquid alkanes dominated by *n*-alkanes, opening up a new route for obtaining hydrocarbon components at the aviation fuel grade. Another classical route employed levulinic acid as the feedstock, which was first converted to γ-valerolactone over a Ru/C catalyst (150 °C, 35 bar H_2), then transformed into pentanoic acid via Pd/Nb_2O_5-catalyzed reactions, and finally underwent ketonization to yield 5-nonanone—a key precursor for C_9 *n*-alkane[63]. Liu et al.[10] developed a strategy integrating N-heterocyclic carbene (NHC) organocatalysis with metal-acid cooperative catalysis for the conversion of 5-hydroxymethylfurfural into *n*-alkanes. The initial step ininvolved a solvent-free, NHC-catalyzed efficient and highly selective coupling of two 5-hydroxymethylfurfural molecules to form a C_{12} dimer intermediate. Subsequently, a bifunctional Pt/C+$TaOPO_4$ catalytic system was employed to achieve

hydrodeoxygenation of the intermediate in an aqueous phase, yielding C_{10}–C_{12} *n*-alkanes with 96% selectivity. This approach provided a novel pathway for the production of cellulose-derived hydrocarbon fuels.

Notwithstanding the exceptional performance of the aforementioned strategies in terms of product selectivity and functional group compatibility, conventional multi-step synthesis processes are generally plagued by issues such as operational complexity, high separation costs, and inefficient mass transfer, which collectively impede their scalability. Consequently, the development of highly efficient multifunctional catalysts and the advancement of reaction step integration coupled with process simplification are of paramount significance.

Faba et al.[64] achieved the "one-pot" coupling of aldol condensation and hydrodeoxygenation of furfural and acetone in the aqueous phase using a Pt/MgZr bifunctional catalyst. The reaction was carried out at 493 K and 4.5 MPa H_2, resulting in a total yield of *n*-alkanes (*n*-octane and *n*-tridecane) exceeding 50%. Moreover, after the reaction, the alkane products spontaneously separated from the aqueous phase, eliminating the need for solvent switching and product extraction. This provided a simplified example for the preparation of hydrocarbon fuels from furfural derived from hemicellulose.

3.2 Synthesis of *iso*-alkane fuels from cellulose/hemicellulose

Although the production process of *n*-alkanes is relatively straightforward and involves low feedstock costs, their inherent low-temperature performance limitations—such as a high freezing point—restrict their direct application in the field of jet fuels.

To improve the low-temperature performance of chain hydrocarbon fuels, researchers have systematically investigated methods for synthesizing *iso*-alkanes[65–67]. Yang et al.[11] developed a novel route for synthesizing alkanes within the jet fuel range from furfural and methyl isobutyl ketone (MIBK) under solvent-free conditions. The first stage of this pathway involved an aldol condensation reaction catalyzed by solid base catalysts (e.g., CaO or Mg-Al hydrotalcite) to generate intermediate compounds. Subsequently, the intermediates underwent hydrodeoxygenation in the second stage using a Pd-Fe/C catalyst, yielding jet fuel-range alkanes primarily composed of 2-methyldecane and 2-methylnonane. Both components are *iso*-alkanes, whose low freezing points (approximately −49.7 and −74.9 °C, respectively) demonstrated that incorporating branched structures effectively improves the low-temperature fluidity of biomass-derived fuels. Bond et al.[68] developed an integrated catalytic system that converts cellulose-derived γ-valerolactone (GVL) into fuel precursors such as liquid olefins suitable for transportation fuels, without relying on external hydrogen sources. Mascal et al.[69] synthesized C_7–C_{10} *iso*-alkanes from biomass-derived levulinic acid under relatively mild reaction conditions, as illustrated in Figure 8. Similarly, Ayodele et al.[70] employed a Ni/SiO_2-Al_2O_3 bifunctional catalyst to achieve selective conversion of angelica lactone dimers/trimers into C_8–C_{12} *iso*-alkanes. These studies provided novel technical pathways for synthesizing *iso*-alkanes from cellulose.

To address the carbon emission reduction challenges in the aviation industry, a highly promising technological approach involves producing syngas through the gasification of biomass such as cellulose and hemicellulose, followed by the production of sustainable aviation fuels via the Fischer-Tropsch synthesis process. The core challenge of this technology lies in how to selectively convert syngas into liquid hydrocarbons. Yang et al.[71] found that using a Y^{3+}-modified Co/H-β catalyst can effectively regulate the reaction selectivity. By optimizing the catalyst's acidity and metal dispersion, a mixture predominantly composed of *iso*-alkanes and *n*-alkanes can be obtained with a selectivity of 41.2% for hydrocarbons within the jet fuel range and a yield of 34.5%. This provided a crucial strategy for the efficient synthesis of biomass-based hydrocarbon fuels. Furthermore, Li et al.[72] developed a cobalt-based catalyst supported on hierarchical micro-meso-macroporous Beta zeolite. The multilevel pore structure concurrently enhanced mass transfer efficiency and acidic functionality, facilitating the highly selective direct conversion of syngas to *iso*-alkanes while maintaining low methane selectivity.

Employing concentrated acetone-butanol-ethanol (ABE) fermentation broth, Xie et al.[73] catalyzed the alkylation of acetone with ethanol and 1-butanol using palladium. By modulating the reaction conditions, they obtained fuel precursors with tunable proportions of C_5–C_7 (monoalkylation) and C_9–C_{11} (double alkylation) compounds, achieving an overall yield of 82%. These precursors could then be converted into alkanes via reduction reactions for use as liquid transportation fuels.

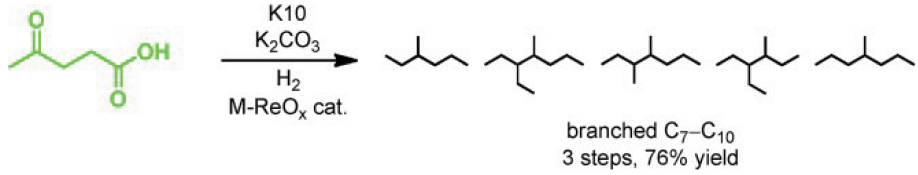


Fig. 8 Synthesis of C_7–C_{10} *iso*-alkanes using levulinic acid as the feedstock[69]
(with permission from Wiley Publications)

In the field of production process optimization, Zhang's research team[74−75] innovatively employed a dual-bed catalyst system to couple aldol condensation with hydrodeoxygenation reactions. This approach successfully converted cellulose fermentation products—acetone and its derivative (methyl isobutyl ketone)—into *iso*-alkanes, achieving carbon yields of 80% and 70%, respectively. This technological breakthrough not only significantly streamlined reaction steps, optimized the synthesis pathway, and reduced energy consumption, but also demonstrated exceptional operational stability, underscoring its substantial industrial applicability.

3.3 Synthesis of monocyclic alkane fuels from cellulose/hemicellulose

To further enhance fuel energy density, cyclic hydrocarbon structures can be introduced into fuel molecules. Heterocyclic compounds derived from cellulose/hemicellulose (such as 2-methylfuran and furfural) can undergo condensation reactions with carbonyl derivatives like cyclohexanone and cyclopentanone. Subsequent hydrogenation and hydrodeoxygenation treatments yield branched monocyclic saturated alkanes.

Under various solid-acid-catalyzed conditions, the reaction of 2-methylfuran with cyclopentanone or cyclohexanone enabled the selective synthesis of branched monocyclic alkanes[76−77]. Notably, due to its stronger electrophilicity compared to cyclopentanone, cyclohexane exhibited higher reactivity toward 2-methylfuran, yielding fuel molecules with greater density. Experimental measurements show that the two fuels produced from the reaction of cyclohexanone and 2-methylfuran—one consisting mainly of pentylcyclohexane and its isomers, the other mainly of 1,1-dipentylcyclohexane and its isomers—have densities of 0.804 and 0.825 g/mL, respectively. The freezing point of the former was lower than −60.0 °C, while that of the latter was −26.4 °C[77]. Further research revealed that utilizing hydrophobic mesoporous resins functionalized with sulfonic acid group (PS) and fluoride sulfonic acid group (PCS) acid groups as catalysts during this reaction process effectively mitigated the adverse effects of water—a byproduct of biomass conversion—on acid catalysts, while simultaneously suppressing undesirable side reactions. These catalysts demonstrated high activity, exceptional selectivity, and superior stability[78].

In the field of reaction process optimization, Deng et al.[12] developed an innovative solvent-free condensation process (Figure 9), which was applied to the reaction between cyclopentanone/cyclohexanone and furfural/5-hydroxymethylfurfural, yielding fuels with outstanding comprehensive performance. For instance, utilizing cyclohexanone and furfural as feedstocks successfully produced a fuel with a density of 0.822 g/mL, a freezing point of −21.7 °C, and a kinematic viscosity of 18.9 mm^2/s at −20 °C. In the field of catalyst design, the utilization of a Pt/HZSM-5 bifunctional catalyst enabled efficient hydrodeoxygenation of aldol condensation products derived from isophorone and furfural compounds. This approach facilitated the synthesis of multi-substituted cyclohexanes with densities of 0.813 and 0.846 g/mL, respectively, both exhibiting freezing points below −75 °C, offering a novel approach for the molecular design of biomass-derived hydrocarbon fuels[79].

In addition to the strategy of side-chain functionalization of cyclic molecules, intramolecular aldol condensation cyclization offers another significant pathway for constructing branched cycloalkanes. Under base-catalyzed conditions, 5-hydroxymethylfurfural first underwent an aldol condensation reaction with carbonyl compounds such as acetone, 2-pentanone, and methyl isobutyl ketone. After selective hydrogenation, a tricarbonyl intermediate was obtained. This intermediate further underwent intramolecular aldol condensation under base catalysis. Finally, through catalytic reduction, branched cycloalkane-rich fuels with a density in the range of 0.81−0.82 g/mL were obtained[80] (Figure 10).

Furthermore, intermolecular cycloaddition reactions demonstrate considerable potential for constructing branched monocyclic alkanes. Chen et al.[81] developed a route for synthesizing branched cycloalkanes using diacetone alcohol derived from lignocellulose as the feedstock. First, it was catalytically hydrogenated to 2-methyl-2,4-pentanediol.

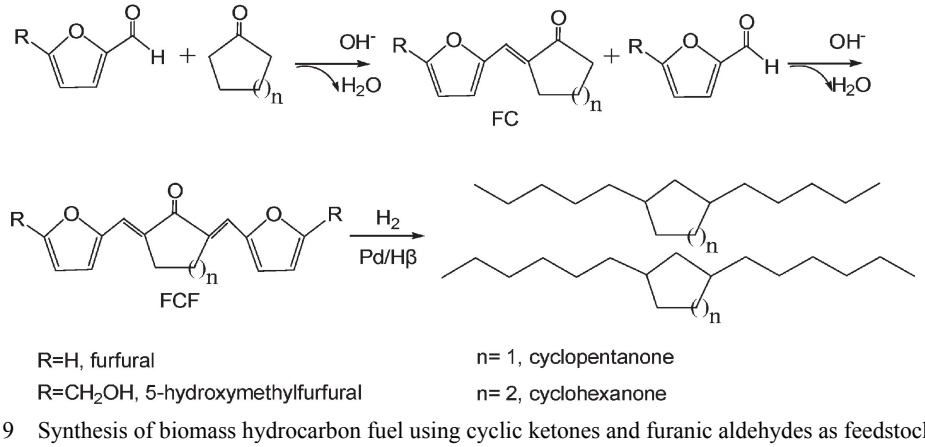


Fig. 9 Synthesis of biomass hydrocarbon fuel using cyclic ketones and furanic aldehydes as feedstocks[12] (with permission from Elsevier)

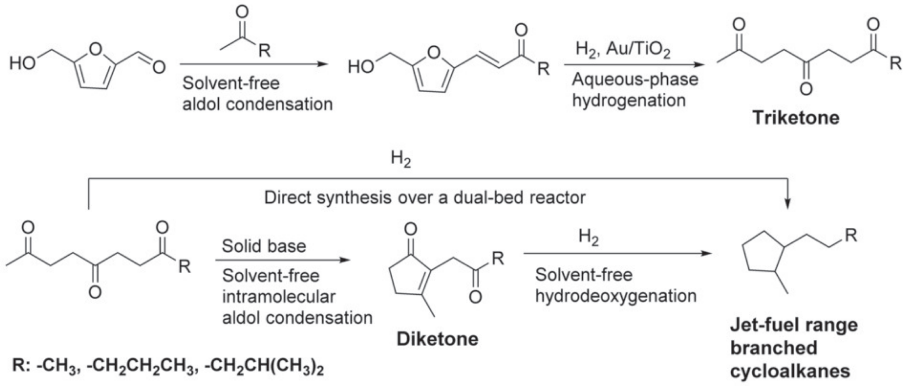


Fig. 10 Branched monocyclic hydrocarbon fuel synthesized from 5-hydroxymethylfurfural[80] (with permission from Wiley-VCH Publications)

Subsequently, through steps such as acid-catalyzed dehydration, Diels-Alder reaction, and final hydrogenation, a mixture of C_{12} and C_{10} branched monocyclic alkanes with a density of 0.83 g/mL and a freezing point of approximately −56.7 °C was obtained. This process featured relatively mild reaction conditions and excellent product performance characteristics.

3.4 Synthesis of polycyclic hydrocarbon fuels from cellulose/hemicellulose

Currently, research on biomass-based high-density fuels primarily focuses on polycyclic alkane structures such as fused rings, linked rings, and bridged rings. Their high energy density and excellent combustion performance endow them with application prospects in the field of aerospace propulsion.

The synthesis of such fuels predominantly utilizes platform compounds like cyclopentanone, cyclopentanol and 5-methylfurfural. As an important aldol condensation reaction, the self-condensation reaction of cyclic ketones can achieve expansion in terms of carbon chain and structural dimensions. By regulating the reaction conditions, fuel precursors with different carbon numbers and ring structures can be obtained, which provides a controllable pathway for the synthesis of polycyclic fuels. Among them, cyclopentanone can be obtained through the selective hydrogenation of furfural in the aqueous phase[82−85].

A C_{10} and C_{15} polycyclic alkane mixture predominantly composed of decalin was synthesized from cyclopentanol as the feedstock[86]. This hydrocarbon fuel blend exhibited a density of 0.896 g/mL and a freezing point of approximately −37 °C. When catalyzed by 98% concentrated sulfuric acid[87], cyclic alcohols (cyclopentanol and cyclohexanol) and cycloalkanes (methylcyclopentane and methylcyclohexane) underwent a series of consecutive reactions including dehydration, alkylation, rearrangement, and hydrogen transfer, yielding branched decalin derivatives. The resulting product exhibited a density ranging from 0.88 to 0.89 g/mL, a freezing point between −51 and −110 °C, and a kinematic viscosity of 2.4–2.7 mm^2/s at 20 °C. The key steps in this reaction pathway involve the sulfuric acid-catalyzed dehydration of cyclopentanol and carbocation rearrangement of alkylation intermediates. Owing to lower steric hindrance, five-membered rings facilitate hydrogen transfer more readily compared to six-membered rings.

In addition, through the reaction of 2-methylbenzaldehyde or 4-methylbenzaldehyde with cyclohexanone, the fused-ring alkanes, namely 1-methyldodecahydro-1*H*-fluorene and 3-methyldodecahydro-1*H*-fluorene, were synthesized via a two-step method[88]. The densities of these two compounds were 0.99 and 0.96 g/mL at 298 K, significantly higher than those of traditional aviation fuel components, indicating promising application prospects.

In the synthesis of linked-ring compounds, cyclopentanone underwent solvent-free self-aldol condensation catalyzed by solid base catalysts such as magnesium-aluminum hydrotalcite and lithium-aluminium hydrotalcite, followed by one-step hydrodeoxygenation to yield bi(cyclopentane)[89]. With a density of 0.866 g/mL and a volumetric heating value of 37.0 MJ/L, it could be utilized as an additive to conventional jet fuels to enhance energy density. It is noteworthy that cyclopentanone was converted into 2-cyclopentylidenecyclopentanone via a solvent-free reaction catalyzed by the ionic liquid ethanolamine acetate (EAOAc). This intermediate underwent hydrodeoxygenation catalyzed by a physical mixture of Ru/C and H-β zeolite to yield bi(cyclopentane), which was subsequently isomerized to decalin in the presence of La-Y zeolite. Furthermore, this catalytic system was applicable to the synthesis of alkyl decalins starting from cyclohexanone, as illustrated in Figure 11[90]. Compared to conventional metal oxide catalysts, EAOAc exhibited lower activation and operating temperatures, thereby reducing energy consumption. Similarly, ethanolamine lactate ionic liquid (LAIL) leveraged the synergistic interaction between the amine group of ethanolamine and the hydroxyl group of lactic acid to efficiently catalyze the aldol condensation reaction between cyclopentanone and vanillin. The resulting intermediate was subsequently subjected to hydrodeoxygenation catalyzed by a 5%Pd/Nb_2O_5 catalyst, yielding polycyclic alkane fuels[91].

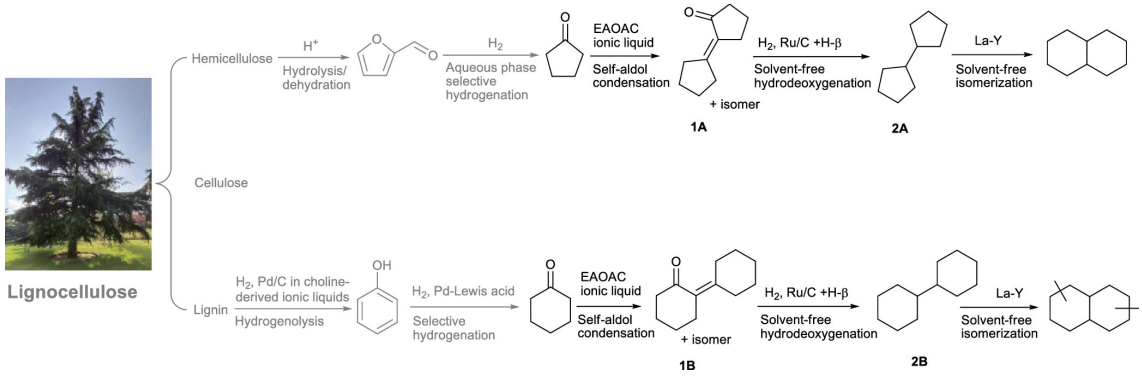


Fig. 11 Strategy for the synthesis of decalins from lignocellulose[90]
(with permission from ACS Publications)

Deng et al.[92] innovatively employed an emulsification-demulsification and dry-gel transformation approach to synthesize a bifunctional catalyst in which palladium nanoparticles were encapsulated within mesoporous ZSM-5 (Pd@meso-ZSM-5) under mild reaction conditions—low temperature and low template usage. This multifunctional catalyst exhibited exceptional performance in the "one-pot", multistep tandem conversion of lignocellulose-derived cyclic ketones (cyclopentanone and cyclohexanone) into bicyclic alkanes (bicyclopentane and bicyclohexane).

The study revealed that the unique mesoporous architecture of the catalyst provided ideal mass transfer pathways for reactive intermediates, while the intimate interface between acidic sites and metallic active centers effectively promoted the transformation of intermediates into target bicyclic alkanes. This synergistic structure–property relationship endows the catalyst with high levels of both activity and selectivity.

In the optimization of production processes, Liu et al.[93] employed a dual-bed catalyst system to directly convert 2,5-hexanedione—obtained from cellulose hydrogenolysis—into a mixture of C_{12} and C_{18} branched polycycloalkanes via aldol condensation-hydrogenation and hydrodeoxygenation reactions. The resulting fuel blend exhibited outstanding properties, including a high density (0.88 g/mL) and a low freezing point (−48.15 °C), making it suitable as an aviation fuel additive to enhance the volumetric heating value of conventional jet fuels.

JP-10 and RJ-4, as representative bridged-ring fuels, exhibit superior density characteristics owing to their highly compact molecular configurations. Among them, RJ-4 is a blended fuel composed of *endo*-tetrahydrodimethyldicyclopentadiene (*endo*-THDMCPD) and *exo*-tetrahydrodimethyldicyclopentadiene (*exo*-THDMCPD), whereas JP-10 is a single-component fuel consisting exclusively of *exo*-tetrahydrodicyclopentadiene (*exo*-THDCPD). Nie et al.[94] proposed a novel synthetic approach for methylcyclopentadiene-based fuels (dimer and trimer) using 5-methylfurfural as the starting material. Through a series of reactions including reductive ring-opening, aldol condensation, selective reduction, dehydration, and oligomerization, RJ-4 (Fuel 1) and a blended fuel (Fuel 2) with high thermal stability and energy density were successfully synthesized, achieving overall yields of 74.4% and 68.4%, respectively. This study presented a potentially viable pathway for the large-scale production of high-performance jet fuels from biomass (Figure 12). Li et al.[95] achieved the green synthesis of biomass-derived JP-10 fuel using furfuryl alcohol as the starting material through a series of steps including rearrangement, hydrogenation, dehydration, dimerization, and isomerization. This approach significantly reduced production costs and provided a sustainable pathway for the synthesis of this high-performance military-grade high-density fuel. On the other hand, Zhang's team[96] proposed a two-step synthetic route utilizing xylose or extracted hemicellulose to produce cyclopentadiene (CPD) and methylcyclopentadiene (MCPD).

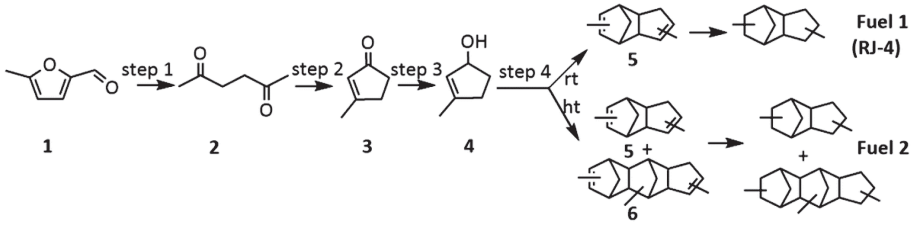


Fig. 12 Route for the synthesis of methylcyclopentadiene dimer and trimer derived fuels from 5-methyl furfural (rt: room temperature; ht: high temperature)[94]
(with permission from RSC Publications)

This biomass-based strategy offers a more sustainable source of key intermediates for the synthesis of high-density fuels such as JP-10 and RJ-4, thereby broadening the available synthetic pathways.

3.5 Molecular design of cellulose/hemicellulose-derived hydrocarbon fuels

The synthesis of biomass-derived hydrocarbon fuels currently faces bottlenecks such as complex processes, low selectivity, and high production costs. Conventional trial-and-error research paradigms exhibit inefficiency and prove inadequate for precisely regulating critical performance metrics of fuel, including cetane number, oxidation stability, and low-temperature fluidity.

To address these bottlenecks, researchers are adopting innovative interdisciplinary strategies: On one hand, computational approaches such as molecular dynamics (MD) simulations and density functional theory (DFT) are employed to elucidate reaction mechanisms at the molecular level, providing a theoretical foundation for catalyst design and process optimization; on the other hand, machine learning and data-driven techniques are leveraged to construct structure-performance prediction models, which substantially narrow the experimental screening scope and enable the targeted synthesis of high-performance, low-emission biomass-based fuels.

Ma et al.[97] employed density functional theory (DFT) and molecular dynamics (MD) simulations to predict and evaluate the properties of adamantane derivatives, systematically investigating the effects of various substituents and isomers on fuel density, net heat value, specific impulse, thermal stability, and oxidation stability. Research findings indicated that the C/H ratio could serve as a descriptor for both density and net heat value of adamantane derivatives, while the number of secondary carbon atoms attached by side chains and the HOMO-LUMO gap could function as descriptors for density (gravimetric net heating value) and volumetric net heating value, respectively. Based on the aforementioned descriptors, researchers screened alkyl-substituted adamantane derivatives—specifically ethyladamantane, propyladamantane, and butyladamantane compounds—demonstrating superior performance, and further predicted the molecular structures of high-performance pentyladamantane derivatives. Furthermore, some of the selected adamantane derivatives exhibited thermal and oxidative stability comparable to JP-10, demonstrating their potential as components for aviation fuels.

Li et al.[98] developed a machine learning-based high-throughput screening approach to evaluate 319895 hydrocarbon molecules, identifying 28 potential polycyclic alkane candidates for high-energy-density fuels. These candidates exhibited superior properties including high net heat of combustion, high specific impulse, high density, and low melting point, as illustrated in Figure 13. In addition, Wen et al.[99] employed the maximum sub-structure search in the ZINC20 database to obtain the common sub-structures of molecules with high strain energy and combustion heat values. Based on these findings, they designed 20 polycyclic alkane fuel candidates (ZD-1 to ZD-20). Among these, ZD-6 emerged as a particularly promising candidate due to its superior volumetric net heating of combustion, high specific impulse, low melting point, and acceptable flash point. By constructing a comprehensive database integrating molecular structures and properties, the researchers leveraged machine learning models to elucidate structure-property relationships, thereby enabling rapid performance prediction and high-throughput screening of fuel candidates.

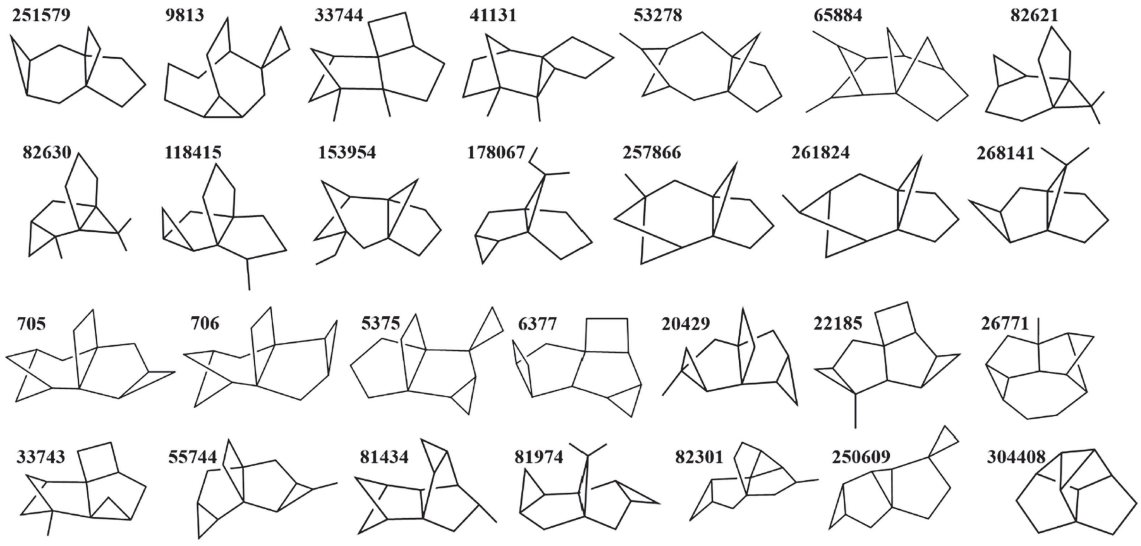


Fig. 13 The numbered codes and molecular structures of the 28 hydrocarbon molecules that have been selected[98] (with permission from Elsevier)

With the escalating demand for high-density hydrocarbon fuels, the design of such fuels through investigating the relationships between molecular structures and properties, integrated with advanced methodologies including theoretical computation, simulation, and machine learning, has progressively emerged as a prominent research focus.

4 Progress in the synthesis of hydrocarbon fuels from lignin

Lignin, as the second most abundant renewable polymer in the plant kingdom after cellulose, is primarily composed of three structural units—guaiacylpropane, syringylpropane, and *p*-hydroxyphenylpropane—interconnected via C–O bonds (such as β-O-4, α-O-4 and 4-O-5) and C–C bonds (including β-5, 5-5, β-1 and β-β) [13−14]. Owing to the abundant aromatic rings within its molecular structure, lignin can be converted into cycloalkane-based hydrocarbons through thermochemical processes such as depolymerization and hydrodeoxygenation.

Depending on the molecular structure of the resulting products, lignin-derived hydrocarbon fuels can be broadly categorized into two classes: monocyclic alkanes and polycyclic alkanes.

4.1 Synthesis of monocyclic alkane fuels from lignin

Lin et al.[100] developed a highly dispersed Pt/Al_2O_3-TiO_2 composite catalyst capable of efficiently catalyzing the hydrodeoxygenation of lignin-derived phenolic compounds. At 260 °C, this catalyst achieved nearly complete conversion (100%) and excellent selectivity (99.9%) toward cyclohexane from guaiacol (Figure 14). The superiority of this catalyst stemmed from the composite support, which successfully integrated the high specific surface area of Al_2O_3 with the abundant acidic sites and oxygen vacancies of TiO_2, leading to a significant enhancement in catalytic performance. Furthermore, the catalyst exhibited high activity in the hydrodeoxygenation of various lignin-derived phenolic compounds—including *p*-cresol, propylphenol, anisole, and eugenol—demonstrating broad applicability and considerable potential for practical use.

Han et al.[101] developed a two-step strategy involving Friedel-Crafts alkylation followed by hydrodeoxygenation to synthesize mono-substituted cyclohexane-based biofuels with excellent low-temperature properties. These compounds were produced from lignin-derived aromatics—such as anisole, guaiacol, and phenol—and furanic substrates like furfuryl alcohol or 5-hydroxymethylfurfural. In the alkylation stage, $FeCl_3$ and $AlCl_3$ exhibited high catalytic activity and selectivity for different substrates, respectively. Meanwhile, a semi-continuous feeding strategy was employed to enhance the selectivity toward the monoalkylated product while suppressing side reactions. During the hydrodeoxygenation stage, a bifunctional catalyst system consisting of Pd/C and HZSM-5 enabled efficient deoxygenation in aqueous phase, yielding pentylcyclohexane as the predominant final product. Notably, the fuel synthesized from guaiacol and furfuryl alcohol exhibited a density of 0.804 g/cm^3 at 20 °C, a kinematic viscosity of only 34.4 mm^2/s at −60 °C and a freezing point below −80 °C.

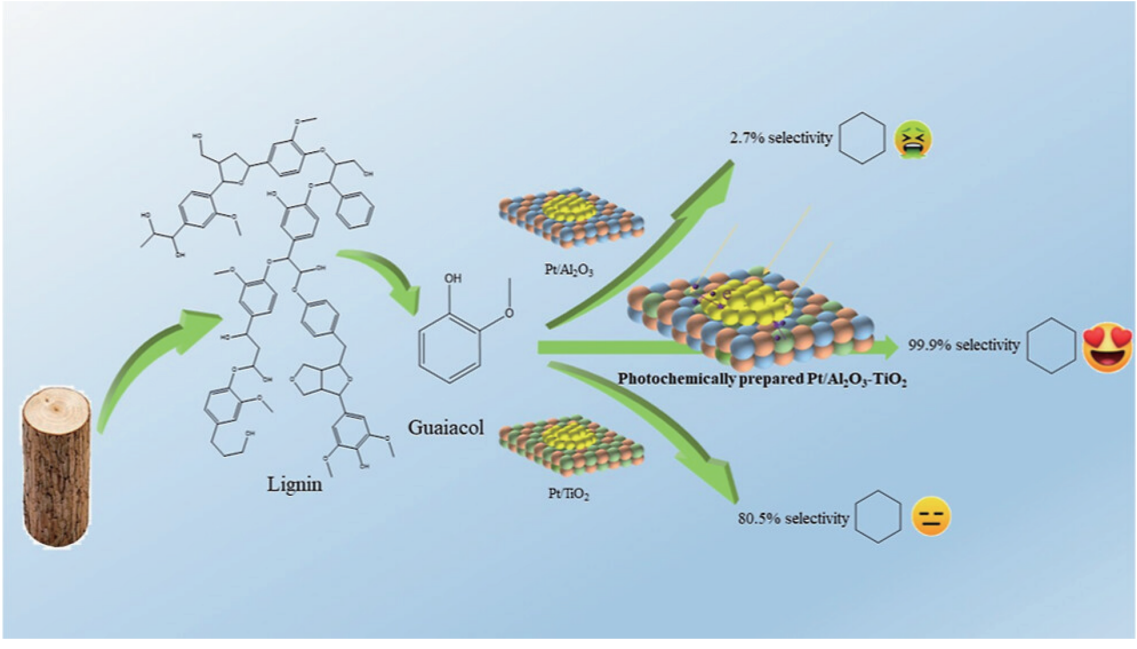


Fig. 14 The high-dispersed Pt/Al_2O_3-TiO_2 composite catalyst catalyzed the generation of cyclohexane from lignin-derived phenolic compounds[100]
(with permission from ACS Publications)

These properties indicated outstanding low-temperature fluidity and stability, highlighting its potential as an aviation fuel additive. Overall, this study offered a green and efficient route for the targeted production of high-value biofuels from lignin-derived feedstocks.

Although monocyclic alkane fuels exhibit favorable low-temperature performance, their energy density remains relatively limited. To achieve biofuels with higher energy density, research focus has progressively shifted toward the synthesis of polycyclic alkanes.

4.2 Synthesis of polycyclic hydrocarbon fuels from lignin

Under relatively mild conditions (120−200 °C, 4−6 h), selective depolymerization of biomass-derived lignin and lignin model compounds in high-concentration $ZnCl_2$ solutions enabled the production of alkyl-substituted phenolic compounds. These phenolic intermediates were subsequently converted into monocyclic and bicyclic saturated alkanes via hydrodeoxygenation reactions catalyzed by a Ru/C catalyst[102].

Yang et al.[103] reported a route for producing sustainable aviation fuel from corn stover lignin. The process involved initial separation of lignin through dilute alkali pretreatment, followed by hydrodeoxygenation catalyzed by Ru/Al_2O_3 coupled with zeolite CBV 400. The resulting product primarily consisted of C_6–C_{18} monocyclic, bicyclic, and tricyclic cycloalkanes, which could serve as blending components for conventional jet fuel.

To enhance the yield of lignin-derived polycyclic alkanes, Wang et al.[104] employed DFT calculations as a guiding strategy to design and synthesize a non-noble metal Ni-MoO_{3-x} catalyst via a hydrothermal-low-temperature reduction method. The catalyst exhibited excellent performance in the hydrodeoxygenation of crude lignin oil, achieving a deoxygenation degree of 99% and a 69.4% total carbon yield of cycloalkanes. The resulting product was a mixture of mono- and bicyclic cycloalkanes ranging from C_6 to C_{18}, making it a promising candidate for use as a high-density fuel additive in jet fuel. Mechanistic investigations revealed that the "metal-vacancy interface" formed by Ni clusters adjacent to oxygen vacancies serves as the key active site for efficient hydrodeoxygenation. Furthermore, the catalyst can be readily regenerated and is applicable to a variety of lignin-derived substrates.

Yang et al.[105] innovatively developed a novel two-step process for producing high-density fuels through alkylation and hydrodeoxygenation using lignin oil and cyclopentanol as feedstocks, as illustrated in Figure 15. Through systematic screening, the research team identified HY zeolite with a SiO_2/Al_2O_3 molar ratio of 5.3 as the optimal alkylation catalyst, and precisely optimized the reaction conditions to achieve effective control over reactant conversion and product selectivity. To validate the feasibility of the process, the researchers constructed a model system of phenolic compounds simulating the composition of typical lignin oil, conducting an in-depth analysis of the competitive reaction mechanisms among various components in the complex system. Practical application tests demonstrated the strong applicability of this process to lignin oil derived from beech powder depolymerization. A fuel precursor was obtained at 80% conversion, and the resulting hydrocarbon fuel mixture produced via hydrodeoxygenation exhibited outstanding properties: a density of 0.91 g/mL (20 °C), a freezing point below −60 °C, and promising potential for practical applications.

In addition, lignin-derived monomers can be utilized for synthesizing polycyclic alkane fuels. Using 4-ethylphenol and benzyl alcohol as feedstocks, a monoalkylated intermediate is first generated via alkylation. This intermediate was then selectively converted into ethyl-substituted dicyclohexylmethane (Figure 16) under a Pd/C-HZSM-5 composite catalytic system[106].

The resulting product exhibited excellent fuel properties, including a density of 0.873 g/cm^3 at 20 °C, a net heating value of 42.7 MJ/kg, and a freezing point of −42 °C, fully meeting the requirements for aviation fuel additives.

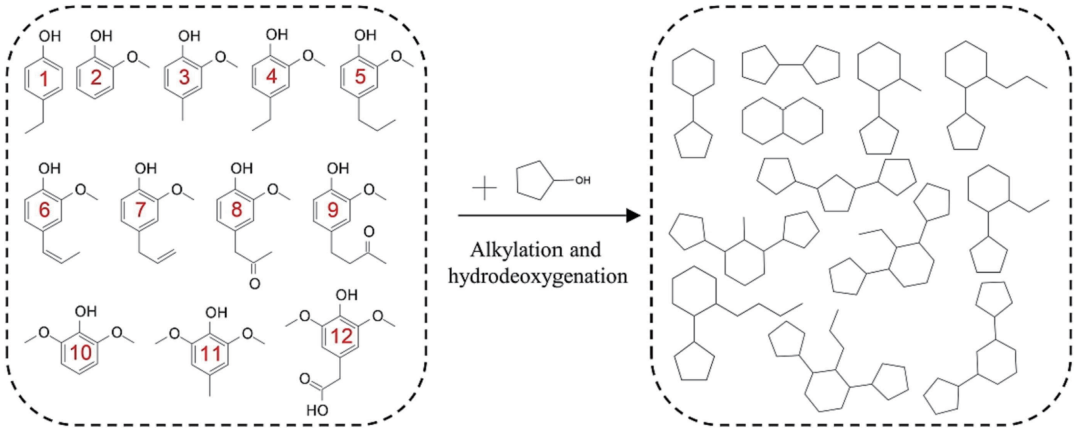


Fig. 15 Co-conversion of cyclopentanol and phenolic mixtures to jet fuel blend[105]
(with permission from Elsevier)

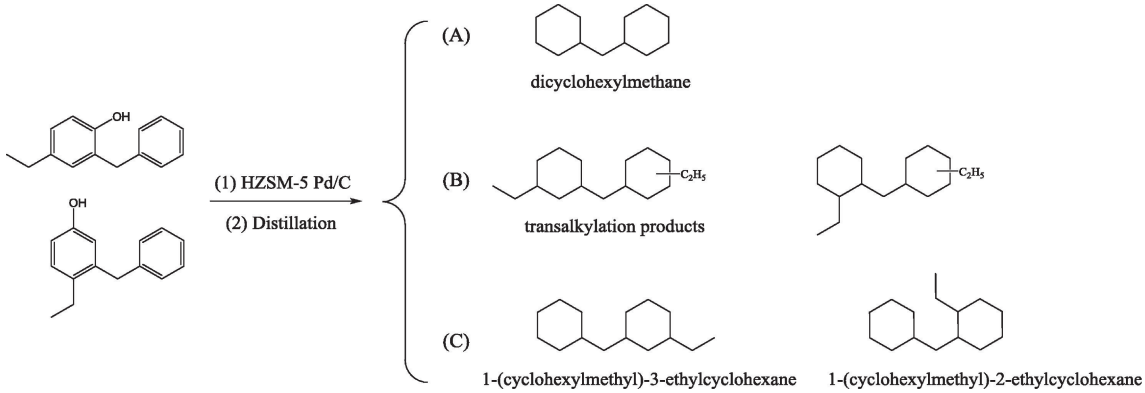


Fig. 16 Conversion of the monoalkylated intermediate into mixed hydrocarbon fuels via hydrodeoxygenation[106]
(with permission from Elsevier)

Although the separation and subsequent conversion of intermediate products can achieve high yields, the multi-step reaction process leads to operational complexity and elevated production costs. In this context, Shen et al.[107] developed a "one-pot" Pt/Hβ-catalyzed system converting lignin-derived phenol and cyclohexanol to polycyclic alkanes in 83.42% yield via a well-designed tandem reaction. This provided a novel strategy for the green synthesis of biomass-based fuels. Subsequently, leveraging the broad applicability of such bifunctional catalysts, the authors expanded the substrate scope to include various biomass-derived compounds. As shown in Figure 17, the catalyst was applied in reactions between phenol and benzyl alcohol, as well as between cyclohexanone and cyclopentanone, affording polycyclic alkane mixtures in 81.86% and 82.14% yields, respectively.

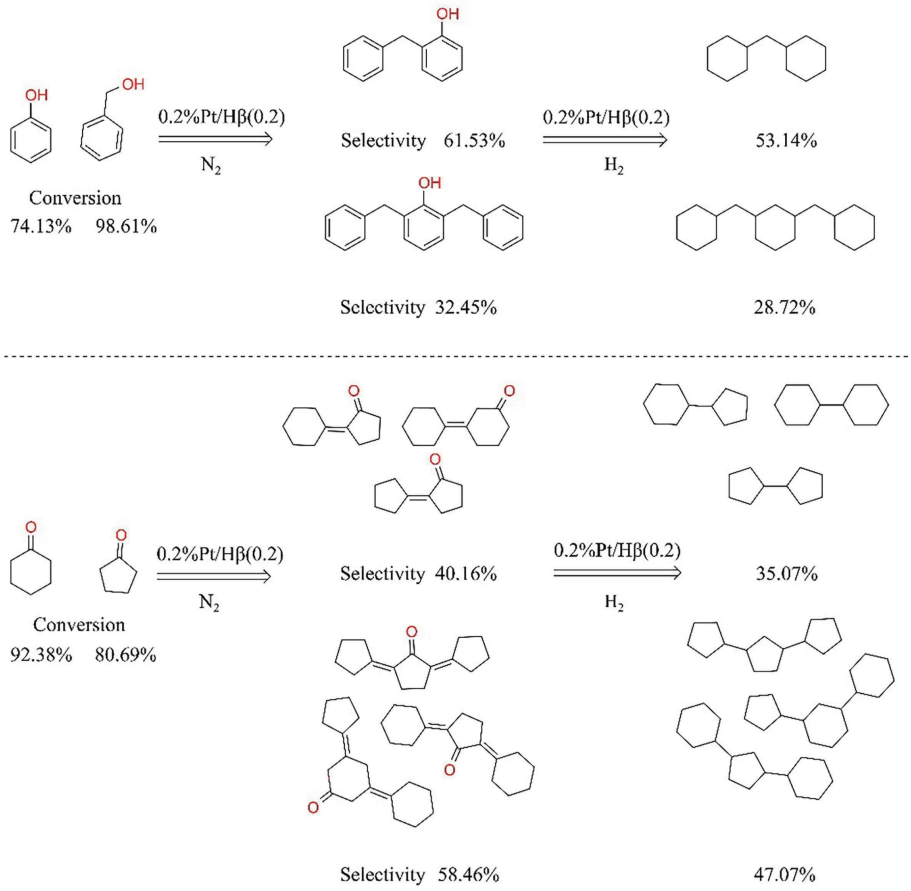


Fig. 17 Synthesis of polycyclic alkanes over a bifunctional Pt/Hβ catalyst: reaction of phenol with benzyl alcohol and reaction of cyclohexanone with cyclopentanone[107]
(with permission from Elsevier)

Furthermore, through intramolecular cyclization strategies, lignin derivatives can be converted into high-energy-density fuels predominantly composed of fused-ring alkanes. Bai et al.[108] demonstrated that alkylation between phenol and benzyl acetate catalyzed by montmorillonite (MMT) yields C_{13}-oxygenated compounds (diphenylmethane derivatives), wherein the Lewis acid sites of MMT effectively facilitated the formation of benzyl cations. Following hydrodeoxygenation catalyzed by 5% Pd/C, this intermediate was primarily transformed into a mixture dominated by perhydrofluorene and dicyclohexylmethane, exhibiting a density of 0.956 g/cm^3 and a volumetric heating value of 38.9 MJ/L. Notably, this intramolecular cyclization mechanism demonstrates broad applicability, as various diphenylmethane derivatives can be selectively converted into perhydrofluorene-type high-density fuel components with high efficiency under pure Pd/C catalysis.

By regulating catalyst types, diphenylmethane derivatives can be selectively and directionally converted into various high-energy-density fuels with high selectivity. When employing zeolite-Pd/C dual catalyst, the primary product was dicyclohexylmethane; whereas utilizing Pd/C catalyst enabled the synthesis of perhydrofluorene with 96% selectivity, as illustrated in Figure 18. Although the synthesized perhydrofluorene exhibited a density of 0.96 g/mL and a volumetric heating value of 40.1 MJ/L, its kinematic viscosity (1752 mm^2/s at 20 °C) and freezing point (−15 °C) limited its direct application as a hydrocarbon fuel. After blending with JP-10 at a 1∶1 mass ratio, the mixed hydrocarbon fuel achieved a freezing point below −75 °C while maintaining a high density of 0.95 g/mL, and its kinematic viscosity at 20 °C was reduced to 17.4 mm^2/s[109].

In analogous reactions, the product composition can be optimized by modulating catalyst types, yielding a blended fuel comprising 68.6% perhydrofluorene and 31.4% dicyclohexylmethane. This mixture demonstrated a density of 0.93 g/mL and a freezing point of −40 °C, indicating promising application prospects[110].

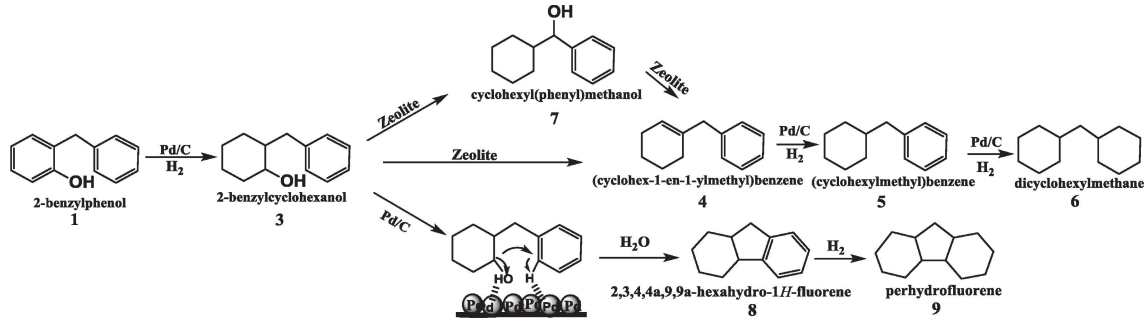


Fig. 18 Reaction pathways for the conversion of 2-benzylphenol into dicyclohexylmethane and perhydrofluorene[109] (with permission from Elsevier)

5 Summary and outlook

In recent years, biomass-derived hydrocarbon fuels have drawn increasing attention owing to their high energy density and sustainability, particularly in the aerospace industry. This review provides a comprehensive survey of the advances in synthesizing hydrocarbon fuels from biomass-based sources—such as lipids, terpenoids, cellulose/hemicellulose, and lignin. It compares reaction conditions and product performance across different synthesis pathways and discusses key aspects including the development of efficient catalysts, the optimization of process design, and the application of computational chemistry.

Despite considerable progress in the research on biomass-derived hydrocarbon fuels, their large-scale industrial deployment still confronts numerous challenges. To address future development needs, efforts in this field should focus on breakthroughs in the following key directions: (1) Innovation in catalyst systems. Developing highly efficient and stable multifunctional catalysts is crucial. By creating synergistic active sites that facilitate tandem catalytic reactions—such as hydrogenation and deoxygenation—such catalysts enable precise control over product distribution and significantly enhance yield. This strategy not only improves the economic viability of biomass-based fuel production but also reinforces its sustainable competitive advantage. (2) Process optimization and intensification in synthesis. The focus lies on developing novel, efficient, and cost-effective synthetic strategies, exploring direct conversion pathways for biomass feedstocks to reduce intermediate steps and improve atom economy. Biphasic tandem methodologies retain the advantages of catalyst/product separation, enabling multi-step reaction coupling within "one-pot" processes; meanwhile, dual-bed flow reactor systems achieve reaction-separation integration, allowing flexible regulation of reaction conditions and significantly reducing energy consumption associated with separation. (3) Computational chemistry-guided fuel molecule design. Integrating computational chemistry with machine learning to establish molecular structure–property relationships will offer theoretical guidance for designing novel fuel molecules. This approach promises to substantially accelerate the development of high-performance biomass-derived hydrocarbon fuels.

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Declaration of Competing Interest

The authors declare no conflict of interest.

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生物质基碳氢燃料的化学合成研究进展

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摘　要：生物质基碳氢燃料作为传统化石燃料的替代品之一，因其可再生性和环境友好特性，在能源领域备受关注。本工作综述了近年来生物质基碳氢燃料化学合成的研究进展，分别梳理了以油脂、萜类、纤维素/半纤维素和木质素等为原料的转化路径，针对不同原料可通过环化、缩合、催化加氢等反应制备出具有不同结构特征的产物。在整个合成过程中，高效催化剂的开发、生产工艺的优化以及基于计算化学的分子设计起到了关键性作用。展望了未来生物质碳氢燃料合成研究的发展方向。

关键词：生物质；碳氢燃料；催化剂开发；工艺优化；分子设计；计算化学

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