

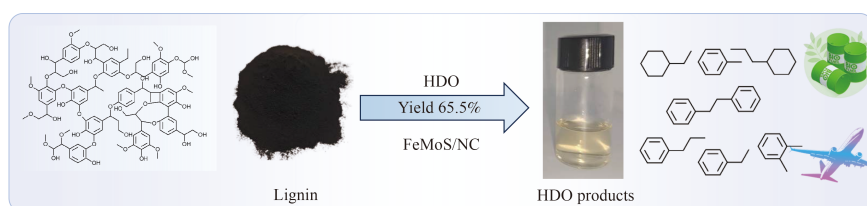
Fe-modified MoS₂/NC catalyst for hydrodeoxygenation of lignin into aviation fuel-range arenes

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Abstract: Lignin contains abundant aromatic ring structures, which can be converted into green sustainable aviation fuel-range arenes through hydrodeoxygenation (HDO).



A series of supported FeMoS/NC catalysts were synthesized by a hydrothermal method. The HDO performance of the catalysts was evaluated using 4-ethylguaiacol as a model compound at 340 °C under 3 MPa H₂. The MoS₂/NC catalyst exhibited a deoxygenation degree of 83.4%, whereas the Fe-modified catalyst (Fe_{0.3}MoS/NC) attained complete deoxygenation (100%) with an arenes selectivity of 78.6%. Beyond the optimal ratio, the deoxygenation degree is inversely proportional to the Fe/Mo molar ratio. The catalysts were characterized by X-ray diffraction (XRD), transmission electron microscopy (TEM), low-temperature nitrogen adsorption (BET method) and X-ray photoelectron spectroscopy (XPS). The characterization results indicated that the introduction of Fe enhanced the uniform dispersion of MoS₂ on the NC support surface. This modification further increased the acidity of the catalyst surface and raised the concentration of sulfur vacancies, thereby promoting the adsorption of oxygen-containing compounds. Furthermore, the HDO performance of the Fe_{0.3}MoS/NC catalyst was evaluated using actual lignin as a feedstock under the conditions of 340 °C, 3 MPa H₂ and 12 h. The results showed a green hydrocarbon yield of 65.5%, of which the C₈–C₁₆ fraction accounted for 54.4% of the total hydrocarbons. Within this fraction, aromatic compounds constituted 63.4%, suggesting its potential use as green aviation fuel-range arenes. This work thus establishes a viable catalytic pathway for efficient conversion of lignin to arenes.

Key words: activated carbon; FeMoS/NC; hydrodeoxygenation; 4-ethylguaiacol; lignin; aromatic hydrocarbon

The transition to green energy has emerged as a globally established consensus. Sustainable Aviation Fuel (SAF) is recognized by the International Air Transport Association as a crucial pathway for achieving carbon neutrality and emission reduction in the aviation sector. To ensure the seal swell characteristics of engine fuel systems, SAF formulations must contain a specific proportion of arenes (8%–25%)^[1–2]. Arenes serve to prevent the hardening and shrinkage of rubber seals while reducing mechanical wear in fuel pumps and nozzles. Lignin, as the only renewable source of naturally occurring aromatic compounds, holds

significant potential for biomass fuel conversion, especially in the production of green hydrocarbons *via* depolymerization and hydrodeoxygenation (HDO)^[3–4]. Under suitable conditions, lignin can undergo HDO in the presence of a catalyst to yield arenes within the aviation fuel range (C₈–C₁₆).

MoS₂-based catalysts are widely employed in HDO reactions due to their favorable catalytic activity^[5]. Typically, introducing promoter metals such as Ni and Co can enhance hydrogen activation and generate abundant sulfur vacancies, which serve as active sites for cleaving the

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C–O bonds in phenolic compounds. Iron (Fe), located in the same group as Ni and Co in the periodic table, is also a transition metal and offers advantages in terms of low cost and wide availability. Studies suggest that Fe species in catalysts can function as oxophilic sites^[6], adsorbing and activating oxygenated compounds to promote C–O bond cleavage. Resasco et al.^[7] proposed that strong interactions between the oxygen atom of hydroxyl groups and oxophilic Fe enhance deoxygenation activity while suppressing aromatic ring hydrogenation, leading to high toluene selectivity during *m*-cresol HDO of over a CuNiFe catalyst.

Activated carbon, as a catalyst support, exhibits excellent resistance to acid and alkali corrosion. Its surface is abundant in oxygen-containing functional groups and possesses a well-developed pore structure, making it a promising material for catalytic applications^[8–10]. Recently, to further improve the catalytic performance of carbon-based supports, numerous studies have introduced nitrogen atoms to modify their structure and properties^[11]. For instance, Tian et al.^[12] incorporated a nitrogen source into a lignin-derived carbon-supported cobalt catalyst and applied it in the HDO of vanillin. Their findings indicated that nitrogen doping not only provided a rich porous architecture but also improved metal dispersion and stability. Moreover, nitrogen atoms can effectively modulate the charge distribution and the electronic structure of adjacent carbon atoms, thereby improving catalytic activity^[13]. In another study, Yang et al.^[14] utilized nitrogen-doped carbon as a support for an iron-based catalyst. The interaction between Fe particles and the doped N sites promoted particle anchoring, enhanced dispersion, increased the number of surface-active sites, and resulted in a favorable arene yield in the HDO of *m*-cresol. In this work, a series of FeMoS/NC catalysts were prepared by loading sulfided FeMo species onto a nitrogen-doped carbon support. The HDO performance of these catalysts was evaluated using both the lignin model compound 4-ethylguaiacol and real lignin as feedstocks. Furthermore, the catalytic mechanism of the Fe-modified MoS₂/NC catalyst was systematically investigated.

1 Experimental

1.1 Materials

Ammonium molybdate tetrahydrate ((NH₄)₆Mo₇O₂₄·4H₂O, AR), ferrous sulfate heptahydrate (FeSO₄·7H₂O, AR) and thiourea (CH₄N₂S, AR) were obtained from Sinopharm Chemical Reagent Co., Ltd. Melamine (C₃H₆N₆, AR), *n*-hexane (C₆H₁₄, AR), 4-ethylguaiacol (C₉H₁₂O₂, AR), absolute ethanol (C₂H₆O, AR), carbon disulfide (CS₂, AR), and acetic acid (C₂H₄O₂, AR) were purchased from Shanghai Aladdin Biochemical Technology Co., Ltd. (China). Activated carbon (AC) supplied by Zhuqing Co., Ltd. (China) was sieved through a 200-mesh screen prior to use. Papermaking black liquor was provided by Shandong Sun Paper Industry Co., Ltd.

1.2 Catalyst preparation

1.2.1 Preparation of different supports

About 2 g of activated carbon (AC), 2 g of melamine, and 18 g of deionized water were stirred continuously at 70 °C for 5 h. The treated activated carbon was dried in an oven and subsequently calcined at 700 °C for 3 h under a N₂ atmosphere to obtain nitrogen-doped activated carbon (NC).

1.2.2 Preparation of FeMoS/NC catalyst

The FeMoS/NC catalyst was synthesized *via* a hydrothermal method. First, the calculated amounts of FeSO₄·7H₂O, (NH₄)₆Mo₇O₂₄·4H₂O, and C₃H₆N₆ were dissolved in 30 mL of deionized water, with the total theoretical loading of active components (calculated as FeS₂ and MoS₂) fixed at 20%. After stirring until complete dissolution, the resulting solution was transferred to a 50 mL autoclave along with the NC support and reacted at 180 °C for 24 h. Upon cooling to room temperature, the solid product was collected by suction filtration, and the filter cake was dried under vacuum at 60 °C for 12 h. For ease of description, the final sample is denoted as Fe_xMoS/NC, where *x* represents the Fe/Mo molar ratio.

The FeMoS/NC(A) catalyst was prepared using an impregnation method. Calculated amounts of FeSO₄·7H₂O, (NH₄)₆Mo₇O₂₄·4H₂O were first dissolved in an appropriate volume of deionized water under stirring. The NC support was then added to the solution and stirred at 70 °C until the water gradually evaporated. The obtained solid was dried under vacuum at 80 °C for 10 h and subsequently calcined in a muffle furnace at 400 °C for 4 h. Pre-sulfidation step was carried out in a high-pressure autoclave, in which 20 g of dodecane, 0.4 g of carbon disulfide (CS₂) and 2 g of the calcined solid were loaded. The reactor atmosphere was purged three times with hydrogen to remove air, after which the system was pressurized with H₂ to 4 MPa and maintained at 340 °C for 8 h. Following reaction, the system was cooled to room temperature, and the solid catalyst was isolated by filtration, yielding the final Fe_xMoS/NC(A) catalyst.

1.3 Catalyst characterization

The crystal structure of the catalysts was characterized by X-ray diffraction (XRD) using a PANalytical X'Pert PRO MPD diffractometer (Netherlands). X-ray photoelectron spectroscopy (XPS) analysis was performed on a Thermo Scientific K-Alpha photoelectron spectrometer. The N₂ adsorption-desorption isotherms of the catalysts were obtained using an Autosorb-6B instrument (Quantachrome Instruments, USA). The TEM images of the catalysts were observed using an FEI Talos F200X field emission electron microscope. The metal element content in the samples was detected using a Thermo Scientific iCAP 6300 ICP-OES

instrument after 50 fold dilution. Raman spectroscopy was performed using a Renishaw in *via* (U.K.) at room temperature with a 532 nm excitation wavelength. The sulfur vacancies and their relative content in the catalysts at room temperature were determined using an electron paramagnetic resonance spectrometer. NH₃-TPD and H₂-TPD were measured using a Quantachrome CHEMBET-3000 fully automated temperature-programmed adsorption instrument.

1.4 Catalytic evaluation

A mixture of 0.2 g of 4-ethylguaiacol, 0.1 g of catalyst, and 30 mL of *n*-hexane was added into a 100 mL high-pressure autoclave. After sealing the reactor, the system was leak-checked under a nitrogen atmosphere. The autoclave was purged 3 times with nitrogen to evacuate air and then pressurized with H₂ to 3 MPa. With mechanical agitation set at 700 r/min, the system was heated to the target temperature and maintained for a predetermined duration. After reaction, the reactor was cooled to room temperature to collect the liquid products. The effects of reaction temperature and catalyst dosage were systematically investigated. The liquid products were analyzed using an Agilent 7890A-5975C gas chromatograph/mass spectrometer (GC-MS), with dodecane employed as the internal standard for quantitative analysis.

The conversion of the reactant, along with the yield, selectivity, and deoxygenation degree of the products, were calculated using the following equations:

$$\text{Conversion(\%)} = (\text{Moles of reactant fed} - \text{Moles of unreacted reactant}) / \text{Moles of reactant fed} \times 100\% \quad (1)$$

$$\text{Selectivity(\%)} = \text{Moles of aspecific product formed} / \text{Total moles of all products formed} \times 100\% \quad (2)$$

$$\text{Deoxygenation degree(\%)} = (1 - \text{Moles of oxygenated products} / \text{Moles of oxygen in feedstock}) \times 100\% \quad (3)$$

$$\text{Product yield(\%)} = \text{Moles of a specific product formed} / \text{Initial moles of substrate} \times 100\% \quad (4)$$

$$\text{Aromatic yield(\%)} = \text{Moles of aromatic hydrocarbons produced} / \text{Initial moles of substrate} \times 100\% \quad (5)$$

1.5 Preparation and Characterization of kraft lignin

Kraft lignin was extracted from papermaking black liquor (40% solids content) by acid precipitation. In a typical

procedure, 50 g of black liquor was stirred while diluted acetic acid was added dropwise until the pH value reached 4. The resulting mixture was centrifuged to collect the precipitate, which was then washed repeatedly with deionized water until the supernatant became neutral. The washed solid was finally dried under vacuum at a low temperature for 24 h to obtain purified kraft lignin.

The structural features of the extracted lignin were analyzed by two-dimensional heteronuclear single quantum coherence nuclear magnetic resonance (2D HSQC NMR) spectra on a 600 MHz Bruker Avance spectrometer. Molecular weight distribution was determined by gel permeation chromatography (GPC) performed on an Agilent 1260 high-performance liquid chromatography (HPLC) system.

1.6 Catalytic hydrodeoxygenation of kraft lignin

About 0.4 g of kraft lignin and 0.4 g of catalyst were mixed with 30 mL of *n*-hexane in a 100 mL high-pressure autoclave. After purging the reactor to remove air, the system was pressurized with hydrogen to 3 MPa. The mixture was then heated to 340 °C under continuous stirring at 700 r/min and maintained for 12 h. Upon completion, the reactor was cooled to room temperature. Ethanol was added to the reaction mixture, followed by ultrasonication for 20 min. The resulting slurry was filtered to collect the liquid filtrate, from which the solvent was evaporated to obtain the HDO products (green hydrocarbons). The chemical composition of the HDO products was analyzed by GC-MS, and their molecular weight distribution was determined by GPC.

$$\text{Yield of Green Hydrocarbons(\%)} = (\text{Mass of green hydrocarbon products} / \text{Mass of lignin feedstock}) \times 100\% \quad (6)$$

$$\text{Selectivity(\%)} = (\text{Moles of an individual product formed} / \text{Total moles of all products formed}) \times 100\% \quad (7)$$

2 Results and discussion

2.1 Catalyst characterization results

The phase composition and crystal structure of the catalysts were analyzed by X-ray diffraction (XRD), as shown in Figure 1. Except for the diffraction peak at $2\theta = 26.5^\circ$, which is attributed to the (002) plane of hexagonal graphite (PDF#01-0646), the nitrogen-doped activated carbon (NC) support exhibited no other distinct diffraction peaks. The amorphous nature of the NC support was essentially preserved after metal loading. In the MoS₂/NC catalyst, weak diffraction peaks at around 32.2° and 57.4° , which are assigned to the (100) and (110) planes of MoS₂

(PDF#27-0421), respectively. The absence of other MoS₂-related diffraction peaks can be ascribed to the uniform dispersion of the MoS₂ phase on the activated carbon support, which limits the crystallization degree^[15], as well as to the predominantly amorphous or low-crystalline state of the MoS₂ phase. Furthermore, TEM images (Figure 3) show that the layered MoS₂ particles consist of only a few stacked layers, which may also contribute to the weak peak intensity. Characteristic diffraction peaks corresponding to FeS₂ (PDF#37-0475) are observed at 25.8°, 33.2°, 37.2°, 38.9° and 52.0°. For the FeS₂/NC catalyst, the peak at 33.2° exhibits relatively high intensity, sharp profile, and good symmetry, and is assigned to the (101) plane of FeS₂. Compared with FeS₂/NC, the diffraction peak at 25.8° in the hydrothermally synthesized Fe_{0.3}MoS/NC shifts toward a higher angle, suggesting that Mo atoms are incorporated into the FeS₂ lattice, leading to a strong metal-metal interaction^[16]. For the Fe_{0.3}MoS/NC(A) catalyst prepared by the impregnation, diffraction peaks at 29.9°, 33.9°, 43.8° and 53.1° can be assigned to FeS (PDF#42-1340). These results indicate that different preparation methods yield distinct active phases. Specifically, the hydrogen pretreatment during sulfidation in the impregnation route facilitates the transformation of FeS₂ into FeS^[6].

As shown in Figure 2(a), the N₂ adsorption-desorption isotherms of the FeMoS/NC catalyst series all exhibit type IV behavior with H4-type hysteresis loops, indicating the presence of a microporous-mesoporous composite structure. Table 1 reveals that the pore size distributions of the catalysts are concentrated mainly in the micropore range of 0.4–0.8 nm and the mesopore range of 3–5 nm. After the post-treatment nitrogen doping, the specific surface area of the activated carbon decreased only slightly from 691.6 to

621.7 m²/g, suggesting that the nitrogen modification did not significantly alter the original pore structure of the activated carbon^[12]. Upon loading Fe and Mo species, the specific surface area of NC further decreased from 691.6 to 410.0 m²/g, likely due to the partial pore blockage or filling by the metal species^[14]. Compared with Fe_{0.3}MoS/NC, the Fe_{0.3}MoS/NC(A) catalyst exhibits a smaller specific surface area, which can be attributed to the larger particle size and lower dispersion of metal sulfides formed *via* the impregnation method. The observed decrease in pore volume accompanied by an increase in average pore diameter suggests that the metal sulfide active components occupy the micropores of the support, leading to the collapse of some micropores and the formation of more mesopores. Notably, Fe_{0.3}MoS/NC shows a larger specific surface area than the monometallic MoS₂/NC and FeS₂/NC catalysts, demonstrating that the bimetallic loading promotes a higher dispersion of the active components, which is beneficial for the adsorption and activation of reactants.

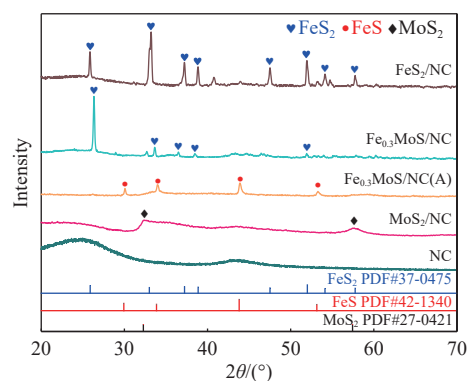
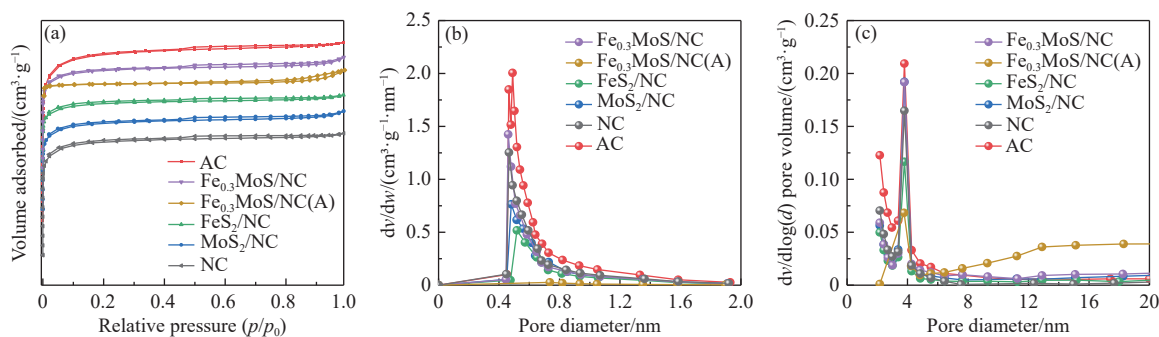


Fig. 1 XRD patterns of FeMoS/NC

Table 1 Pore structure properties of FeMoS/NC catalyst series

Catalyst	Specific surface area/(m ² ·g ⁻¹)	Total pore volume/(cm ³ ·g ⁻¹)	Average pore size/nm
Fe _{0.3} MoS/NC	410.0	0.25	4.5
Fe _{0.3} MoS/NC(A)	170.9	0.12	10.6
MoS ₂ /NC	364.2	0.23	4.2
FeS ₂ /NC	291.7	0.17	3.8
NC	621.7	0.29	3.2
AC	691.6	0.42	3.1



(a): N₂ adsorption/desorption profiles; (b): Microporous pore size distribution; (c): Mesopore size distribution.

Fig. 2 N₂ adsorption/desorption profiles of FeMoS/NC catalyst series

As shown in Figure 3(e), the Fe_{0.3}MoS/NC catalyst exhibits a uniform nanoflower-like morphology^[17–18]. In contrast, significant agglomeration is observed in the monometallic catalysts, indicating that Fe incorporation enhances the dispersion of MoS₂ on the NC and promotes a stronger interaction. High-resolution TEM images (Figure 3(g)) reveal lattice fringes with two distinct interplanar spacings: 0.601 and 0.263 nm, corresponding respectively to the (002) plane of MoS₂ and the (101) plane of FeS₂^[6]. The selected-area electron diffraction (SAED) pattern (Figure 3(h)) shows diffraction rings with four different spacings, which are indexed to the (002) plane of MoS₂ and the (031), (200) and (101) planes of FeS₂. In the MoS₂/NC catalyst, the interplanar spacing of the MoS₂(002) plane is 0.673 nm (Figure 3(d)). Compared with MoS₂/NC, this spacing decreases to 0.601 nm in the Fe_{0.3}MoS/NC catalyst. This reduction is likely attributed to the doping of smaller Fe atoms (117 pm) into the crystal lattice sites typically occupied by larger Mo atoms (130 pm)^[19], which results in slight lattice contraction.

As shown in Figure 4(a), the Fe 2*p* spectrum is deconvoluted into three peaks at 706.9/719.8, 710.6/723.0 and 716.5/728.8 eV, which are attributed to Fe⁰, Fe²⁺, Fe³⁺

species, respectively^[20–21]. Compared with the monometallic FeS₂/NC catalyst, the FeMoS/NC catalyst exhibits new peaks (Fe⁰), indicating the coexistence of both ionic and metallic Fe states, which reflects a strong interaction between the active components and the NC support. Furthermore, the peaks for both Fe²⁺ and Fe³⁺ species shift to lower binding energies compared to those in FeS₂/NC, suggesting electron transfer from Fe to Mo species and further confirming a strong interaction between the two metals^[22].

The Mo 3*d* spectrum (Figure 4(b)) shows deconvoluted peaks at 228.2/231.4, 229.6/232.8 and 232.0/235.2 eV, which are assigned to Mo⁴⁺, Mo⁵⁺ and Mo⁶⁺ species, respectively^[15]. The presence of Mo⁵⁺ and Mo⁶⁺ species may result from incomplete sulfidation during the hydrothermal process or surface oxidation of MoS₂ upon exposure to air. With Fe incorporation, the Mo 3*d* peaks shift towards higher binding energies, indicating the electron transfer from Fe to Mo and a corresponding decrease in the electron density of Mo. The S 2*s* peak (*E*_b(S 2*s*) = 225.6 ± 0.2 eV) adjacent to the Mo 3*d* region further confirms the presence of Mo–S bonds.

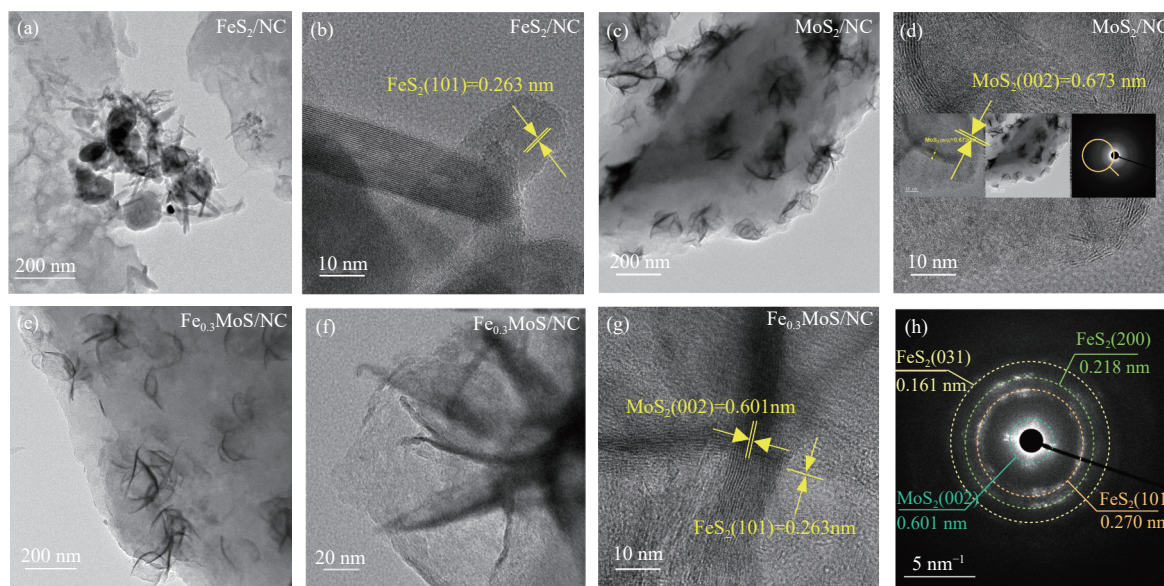
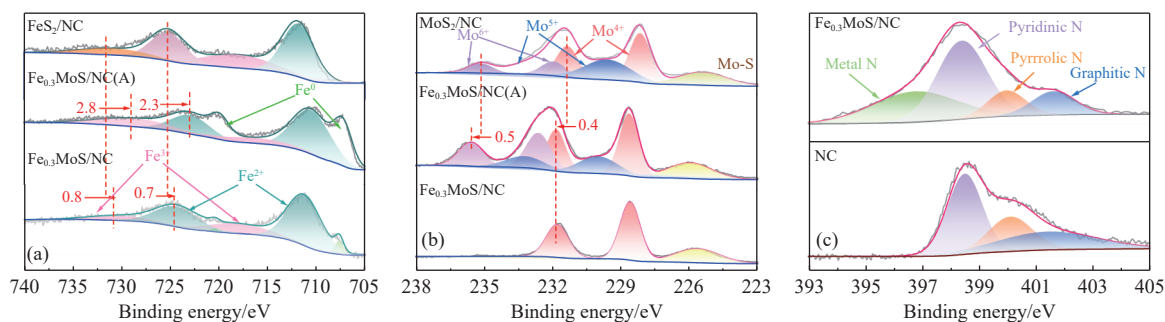


Fig. 3 TEM images of FeS₂/NC (a) and (b), MoS₂/NC (c) and (d), Fe_{0.3}MoS/NC (e)–(g) and SAED images of Fe_{0.3}MoS/NC (h)



(a): Fe 2*p*; (b): Mo 3*d*; (c): N 1*s*.

Fig. 4 XPS spectra of FeMoS/NC catalyst series

Compared with the impregnated catalyst, Fe_{0.3}MoS/NC exhibits a higher relative content of Mo⁴⁺ species and an absence of Fe⁰ signals, suggesting stronger bimetallic interaction in the hydrothermally synthesized catalyst.

The N 1s spectrum of the NC support (Figure 4(c)) can be deconvoluted into three peaks corresponding to graphitic nitrogen (401.4 eV), pyrrolic nitrogen (400.1 eV) and pyridinic nitrogen (398.6 eV)^[23]. The carbon atoms adjacent to graphitic and pyridinic N atoms can provide Lewis acid sites, promoting the binding and removal of oxygen atoms in reactant molecules. In contrast, pyrrolic nitrogen may induce the formation of oxygen-active site on the proximal carbon atoms^[24–25], thereby enhancing the adsorption capacity for oxygenated compounds. Furthermore, the Fe_{0.3}MoS/NC catalyst shows a characteristic peak at around 396.8 eV, which is assigned to Fe–N species and reflects a strong interaction between active metal Fe and NC^[20,26].

Raman spectroscopy was used to assess the graphitization degree and structural disorder of the supports. As shown in Figure 5, the characteristic D band observed around 1341 cm⁻¹ is attributed to disordered carbon or defective graphitic structures, while the G band at 1578 cm⁻¹ is assigned to the in-plane tangential vibration of carbon atoms in hexagonal graphitic carbon^[25]. The intensity ratio of the D band to the G band (I_D/I_G) is inversely related to the graphitization degree^[27]. Compared with the unmodified activated carbon (AC), the NC exhibits a higher I_D/I_G ratio, indicating a lower graphitization level and a higher degree of structural disorder after nitrogen doping, which confirms the successful introduction of additional defects into the carbon matrix^[28]. Following the loading of metal active components, the I_D/I_G ratio decreases slightly, suggesting an increase in graphitization and a corresponding reduction in defect density.

The catalysts were characterized by NH₃-TPD and H₂-TPD, as shown in Figure 6. Both Fe_{0.3}MoS/NC and FeS₂/NC exhibit two NH₃ desorption peaks, corresponding to weak acid sites (100–250 °C) and medium acid sites (250–500 °C). In contrast, MoS₂/NC shows only one NH₃ desorption peak associated with weak acid sites, indicating that Fe incorporation enhances the surface acidity of the catalyst. The H₂-TPD was further used to investigate the interaction between Fe and Mo species. As shown in Figure 6(b), compared with MoS₂/NC, the Fe_{0.3}MoS/NC catalyst exhibits a higher H₂ desorption peak temperature and a larger peak area, suggesting that the Fe-Mo interaction enhances stronger H₂ adsorption and facilitates H₂ dissociation, thereby generating more active hydrogen species.

The concentration of sulfur vacancies in the catalysts was analyzed by electron paramagnetic resonance (EPR) spectroscopy (Figure 7). A distinct EPR signal at $g = 2.003$ confirms the presence of sulfur vacancies^[29]. The intensity of this sulfur-vacancy signal initially increases and then decreases with increasing Fe/Mo molar ratio. Fe_{0.3}MoS/NC shows the strongest EPR signal, indicating the highest concentration of sulfur vacancies, which favors the

exposure of more defective sites.

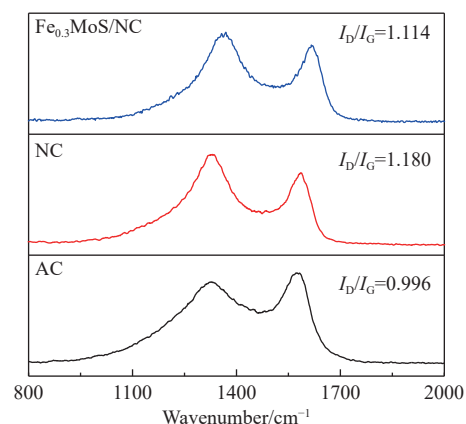


Fig. 5 Raman spectra of Fe_{0.3}MoS/NC catalyst and its support

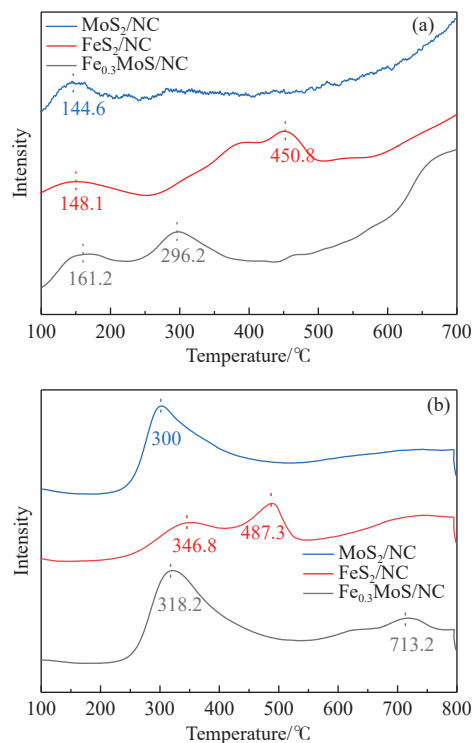


Fig. 6 NH₃-TPD (a) and H₂-TPD (b) profiles of Fe_{0.3}MoS/NC various samples

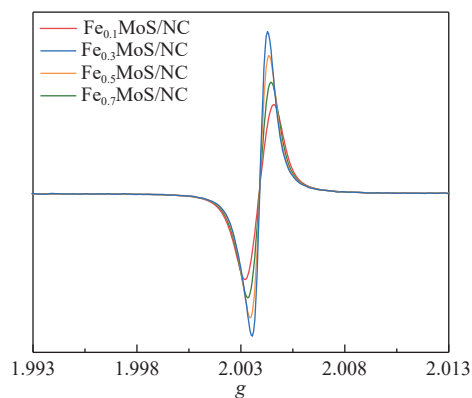


Fig. 7 EPR spectra of FeMoS/NC

Further increase in Fe doping leads to a gradual decrease in the signal intensity, the intensity of the sulfur vacancy peak gradually diminishes, likely due to the lowered dispersion of active components and the consequent reduction in sulfur vacancy formation.

The adsorption behavior of guaiacol on the Fe_{0.3}MoS/NC and MoS₂/NC catalysts was studied using *in situ* FT-IR spectroscopy (Figure 8). For Fe_{0.3}MoS/NC, absorption peaks at 1509, 1263 and 1023 cm⁻¹ are assigned to the $\nu(\text{C}=\text{C})$, $\nu(\text{C}-\text{OH})$ and $\nu(\text{C}-\text{O}-\text{C})$ vibrational modes of guaiacol, respectively. Compared with MoS₂/NC, these peaks show a redshift and higher intensity on Fe_{0.3}MoS/NC, indicating that Fe incorporation enhances the adsorption of the oxygenated compound on the catalyst surface.

The elemental composition of catalysts with different loadings was determined by ICP-OES, as shown in Figure 9. The results indicate that the total loading of Fe, Mo and S elements remains approximately 20% and the Fe/Mo molar ratio is maintained at around 0.3.

2.2 Evaluation of the hydrodeoxygenation performance of 4-ethylguaiacol over the catalysts

4-ethylguaiacol, a representative lignin-derived phenol, was selected as a model compound for lignin oil. It contains C_{ar}-OH and C_{ar}-OCH₃ bonds with bond energies of 414 and 356 kJ/mol, respectively^[30–31]. The catalytic activities of various catalysts were evaluated *via* the hydrodeoxygenation of 4-ethylguaiacol at 340 °C under 3 MPa H₂ for 5 h. As shown in Table 2, the hydrogenation products of 4-ethylguaiacol include hydrocarbons and phenols. The absence of ethers in the products can be attributed to the relatively low bond energy of the methoxy group, which leads to its rapid cleavage under the elevated reaction temperature.

As shown in Table 2, 4-ethylguaiacol did not undergo complete conversion at 340 °C in the absence of a catalyst. When the NC was used as the catalyst, 4-ethylguaiacol was completely converted, indicating that NC possesses certain catalytic activity. After loading 20% Mo species, complete conversion of 4-ethylguaiacol was maintained, and the deoxygenation degree increased to 83.4% compared to NC.

The yields of ethylbenzene and 4-ethylphenol were relatively high at 41.5% and 26.9%, respectively, while ethylcyclohexane was obtained in only 10.2% yield, suggesting that the MoS₂ active centers exhibit significant deoxygenation activity but relatively low hydrogenation activity^[32]. In contrast, the monometallic FeS₂/NC catalyst achieved a deoxygenation degree of only 61.9%, indicating lower catalytic activity than MoS₂/NC. For the impregnation-prepared Fe_{0.3}MoS/NC(A) catalyst, the introduction of Fe increased the deoxygenation degree to 74%, implying that the coexistence of Fe and Mo species effectively promotes the HDO reactivity. The improvement likely arises from sulfur vacancies generated by sulfur loss in FeS₂, which facilitate hydrogen activation and increase the number of active sites^[6]. However, the larger particle size and lower dispersion of the active components in the impregnated catalyst limit the number of accessible sites. Remarkably, the hydrothermally synthesized Fe_{0.3}MoS/NC catalyst achieved both complete conversion and 100% deoxygenation of 4-ethylguaiacol. The total yield of arenes (including ethylbenzene, 1-ethyl-2-methylbenzene and 1-ethyl-3-methylbenzene) reached 78.6%, demonstrating excellent catalytic performance. To examine the role of bimetallic interaction, a physical mixture of 50 mg FeS₂/NC and 50 mg MoS₂/NC catalysts was tested. The resulting deoxygenation degree was lower than that obtained with 100 mg of the integrated Fe_{0.3}MoS/NC catalyst, highlighting the importance of intimate Fe-Mo interaction. Furthermore, compared with Fe_{0.3}MoS/NC, the Fe_{0.3}MoS/AC catalyst (supported on activated carbon) failed to achieve complete deoxygenation and showed lower arene selectivity (73.4%). This confirms that nitrogen doping promotes the binding and removal of oxygen atoms from reactant molecules. Additionally, the nitrogen-containing groups modify the electronic structure of the FeMoS catalyst, thereby enhancing its overall HDO performance.

Figure 10 illustrates the influence of the Fe/Mo molar ratio on the conversion of 4-ethylguaiacol and the corresponding product yields. Initially, as the Fe/Mo molar ratio increases, the yield of phenolic compounds decreases, while the hydrodeoxygenation degree increases. At a Fe/Mo molar ratio of 0.3, 4-ethylguaiacol undergoes complete deoxygenation with the highest arene yield.

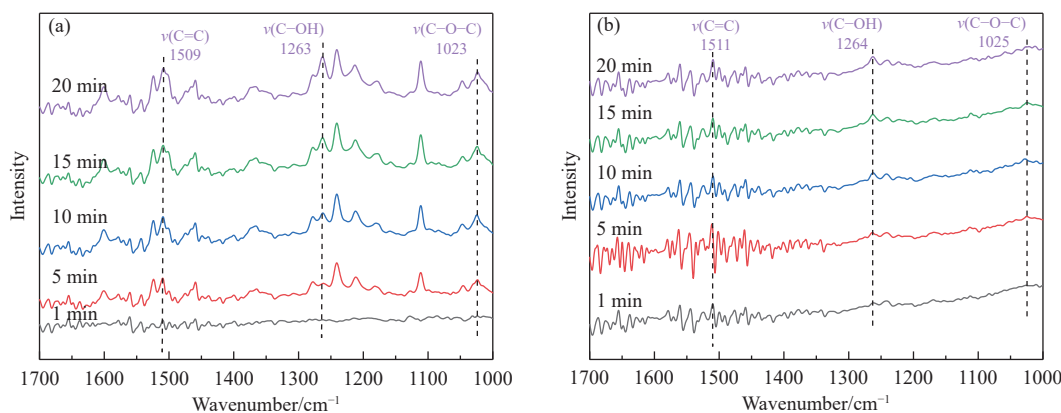


Fig. 8 *In situ* FT-IR spectra of guaiacol adsorption on Fe_{0.3}MoS/NC (a) and MoS₂/NC (b)

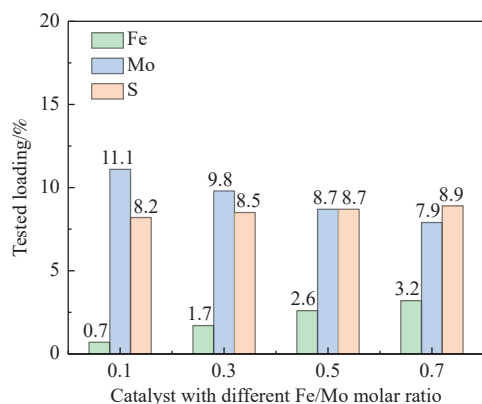


Fig. 9 Elemental distribution maps of catalysts with varying Fe/Mo molar ratios

However, further increase in the Fe/Mo ratio, accompanied by higher Fe loading and lower Mo loading, leads to a significant decline in the deoxygenation degree. When the Fe/Mo molar ratio reaches 0.7, the deoxygenation degree drops to 68.0%, which can likely be attributed to the deposition of excess FeS₂ species at high Fe/Mo ratios. These excess species may cover the original active centers on MoS₂ and consequently hinder the adsorption of C–O bonds and the subsequent deoxygenation reaction^[6].

The effect of catalyst dosage on the reaction is shown in Figure 11(a). When the dosage was 40 mg, the deoxygenation degree was 80.2%. Increasing the dosage to 100 mg raised the deoxygenation degree to 100%, whereas a further increase to 120 mg resulted in only a marginal improvement in arene yield. Considering both catalytic activity and cost, 100 mg was identified as the optimal catalyst dosage, corresponding to a reactant-to-catalyst mass ratio of 2:1. The influence of reaction temperature on the

HDO of 4-ethylguaiaicol was also investigated (Figure 11(b)). At a low temperature of 260 °C, the conversion of 4-ethylguaiaicol was only 20.7%. Complete conversion was achieved at 300 °C, accompanied by a deoxygenation degree of 60.4%. The deoxygenation degree increased progressively as the temperature was further raised. At 340 °C, no oxygenated compounds were detected, indicating complete deoxygenation. These results demonstrate that the Fe_{0.3}MoS/NC catalyst efficiently cleaves the C_{aryl}–OH and C_{aryl}–OCH₃ bonds in 4-ethylguaiaicol. When the temperature was increased from 340 to 360 °C, the arene yield decreased slightly, while the yields of ethylcyclohexane and ethylcyclohexene increased, suggesting that minor aromatic ring hydrogenation occurred. To maximize the yield of aviation fuel-range arenes, the optimal reaction temperature for the HDO of 4-ethylguaiaicol was determined to be 340 °C.

Based on the aforementioned reaction results, a plausible reaction pathway for the hydrodeoxygenation of 4-ethylguaiaicol over the FeMoS/NC catalyst is proposed, as illustrated in Figure 12. The bold lines represent the predominant reaction pathways. HDO of 4-ethylguaiaicol primarily proceeds *via* a direct deoxygenation pathway. The initial step involves demethoxylation of 4-ethylguaiaicol to form 4-ethylphenol. Concurrently, a minor pathway entails the cleavage of the C_(sp²)O–CH₃ bond of the methoxy group, leading to the formation of 4-ethylcatechol, which subsequently undergoes dehydration to also yield 4-ethylphenol. The primary intermediate, 4-ethylphenol, then undergoes direct dehydroxylation to produce ethylbenzene. As the reaction proceeds, a small fraction of ethylbenzene may be hydrogenated to ethylcyclohexene and ethylcyclohexane.

Table 2 Hydrogenolysis of 4-ethylguaiaicol over different catalysts

4-ethylguaiaicol			Ethylcyclohexane A	4-ethylcyclohex-1-ene B	Ethylbenzene C	1-ethyl-2/3-methylbenzene D	4-ethylphenol E	4-ethyl-2/3-methylphenol F
Catalyst	Conversion ^a /%	Deoxygenation /%	Product yield/%					
			A	B	C	D	E	F
No catalyst	91.7	48.4	0.2	1.1	3.0	0.7	65.5	21.2
NC	100.0	58.5	4.5	3.2	4.7	4.5	58.0	25.1
MoS ₂ /NC	100.0	83.4	10.2	3.5	41.5	11.5	26.9	6.4
FeS ₂ /NC	100.0	61.9	5.0	4.8	13.4	0.7	66.7	9.5
Fe _{0.3} MoS/NC(A)	100.0	74.0	6.5	3.5	37.4	0.6	49.4	2.6
MoS ₂ /NC+FeS ₂ /NC	100.0	71.8	8.3	5.2	29.2	0.9	53.4	3.0
Fe _{0.3} MoS/NC	100.0	100.0	17.3	4.1	63.6	15.0	–	–
Fe _{0.3} MoS/AC	100.0	96.0	13.5	5.2	57.3	16.1	6.6	1.4

^a: Reaction conditions: $m_{\text{sub}}/m_{\text{cat}} = 2$, IHP 3 MPa, 5 h, 340 °C, 40 mL *n*-hexane.

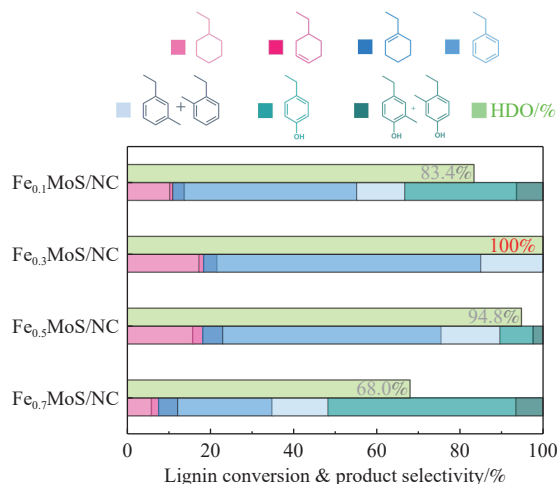


Fig. 10 Influence of Fe/Mo ratio on 4-ethylguaiaicol conversion and product selectivity

Furthermore, the methyl cation (CH_3^+) generated from the cleavage of the $\text{C}_{(\text{sp}^2)}\text{O}-\text{CH}_3$ bond can undergo methylation with 4-ethylphenol, producing 4-ethyl-2-methylphenol and 4-ethyl-3-methylphenol^[33], which

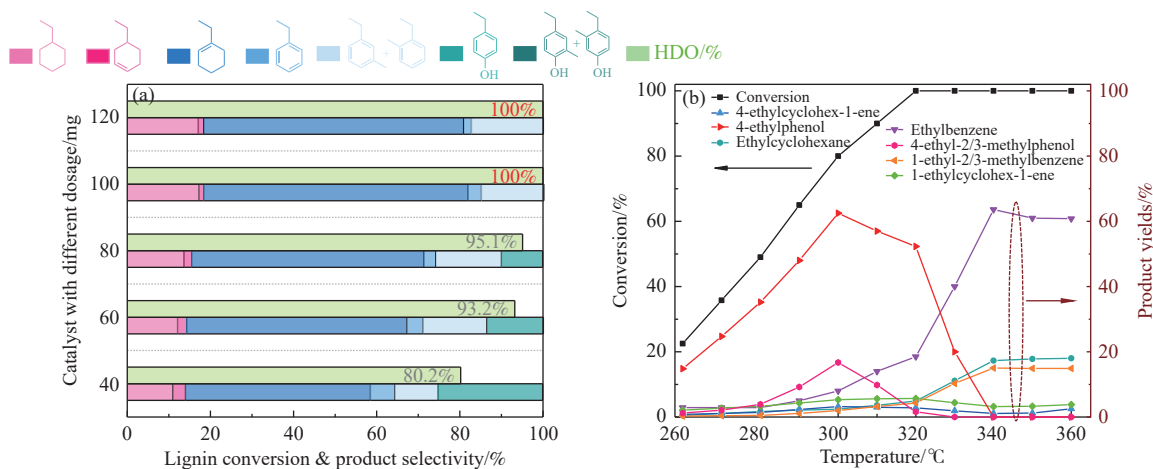


Fig. 11 Effects of (a) catalyst dosage and (b) reaction temperature on 4-ethylguaiaicol conversion over Fe_{0.3}MoS/NC catalyst

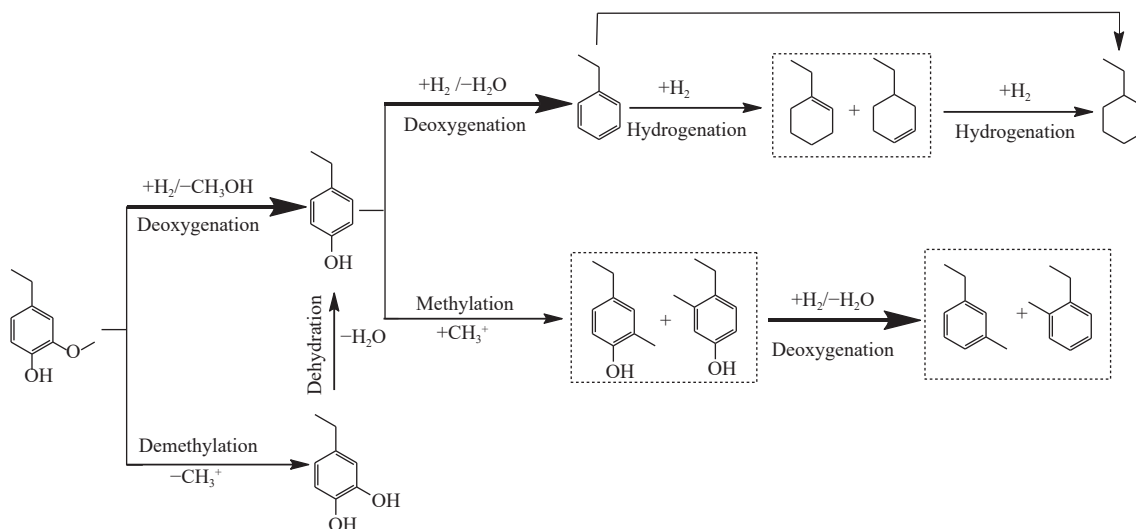
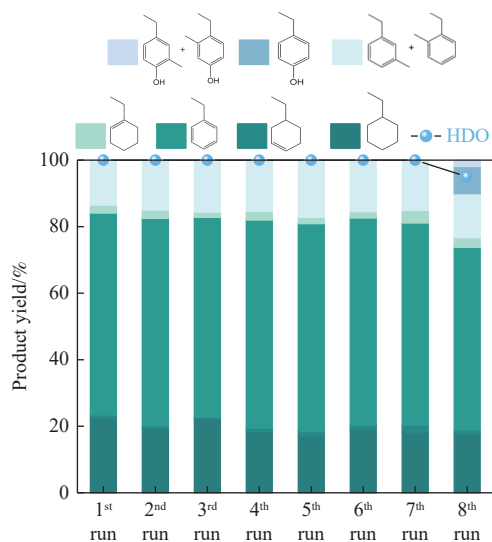


Fig. 12 Proposed mechanism for the hydrogenolysis of 4-ethylguaiaicol over 4-ethylguaiaicol

subsequently undergo dehydroxylation to form 1-ethyl-2-methylbenzene and 1-ethyl-3-methylbenzene, respectively.

A stability test for the Fe_{0.3}MoS/NC catalyst was conducted at 340 °C under 3 MPa H₂ (Figure 13). After the eighth run, the deoxygenation degree decreased by only 5%, while high arene selectivity was maintained, indicating excellent catalyst stability. GC-MS analysis further confirmed that no 4-ethylguaiaicol was detected in the products after the eighth run, corroborating the sustained high activity of the catalyst.

To further investigate the cause of the activity decline in the Fe_{0.3}MoS/NC catalyst after the eighth run, thermogravimetric analysis (TGA) and Fourier transform infrared (FT-IR) spectroscopy were conducted on both the fresh catalyst and the spent catalyst (Figure 14). As shown in Figure 14(a), the spent catalyst adsorbed approximately 6.6% of organic species compared with the fresh catalyst. In the FT-IR spectrum of the catalyst (Figure 14(b)), the absorption peak at 1586 cm^{−1} is attributed to the stretching vibration of C=C bonds, while the peaks at 1099 and 614 cm^{−1} correspond to the stretching vibrations of C–O–C and C–H bonds, respectively.

Fig. 13 Reusability test results of Fe_{0.3}MoS/NC

Compared with the fresh catalyst, the spent catalyst shows significantly enhanced intensities at 1099 and 614 cm⁻¹, indicating the formation of carbonaceous deposits on the catalyst surface after repeated use, which is responsible for

the partial deactivation of the catalyst.

2.3 Evaluation of Hydrodeoxygenation Performance of Real Lignin over the Catalysts

The chemical structure of the kraft lignin was analyzed by 2D HSQC NMR. As shown in Figure 15, in the side-chain region ($\delta_C/\delta_H = 50\text{--}90/3.0\text{--}5.0$), the cross-signals correspond to the β -O-4 (A), β -5 (B) and β - β (C) linkages. In the aromatic region ($\delta_C/\delta_H = 100\text{--}125/6.0\text{--}8.0$), the cross-signals are assigned to syringyl (S), guaiacyl (G) and *p*-hydroxyphenyl (H) units. Simultaneously, a signal from methoxy groups is observed at $\delta_C/\delta_H = 55/3.6$. The characteristic peaks were volume-integrated using MestReNova software. The results indicate that this kraft lignin consists predominantly of guaiacyl units (68%), along with a portion of syringyl units (32%), and contains almost no *p*-hydroxyphenyl units.

To further validate the HDO performance of the FeMoS/NC catalyst, the HDO of lignin was conducted over the Fe_{0.3}MoS/NC catalyst at 340 °C under 3 MPa H₂ for 12 h, and obtaining a green hydrocarbon yield of 65.5%.

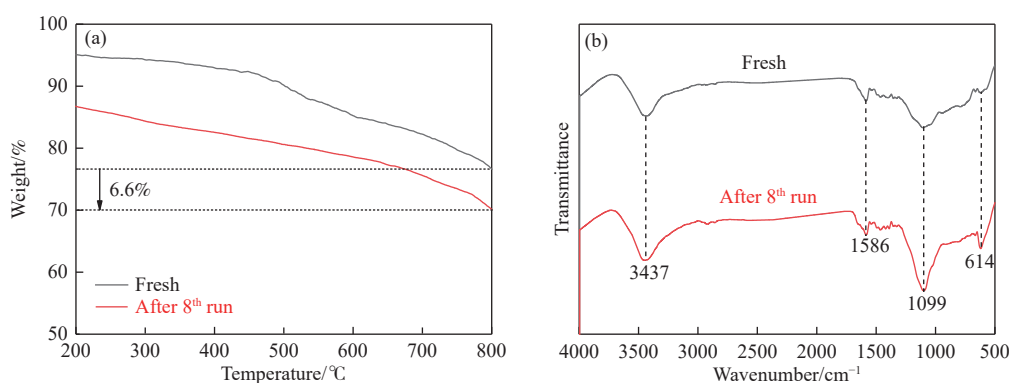
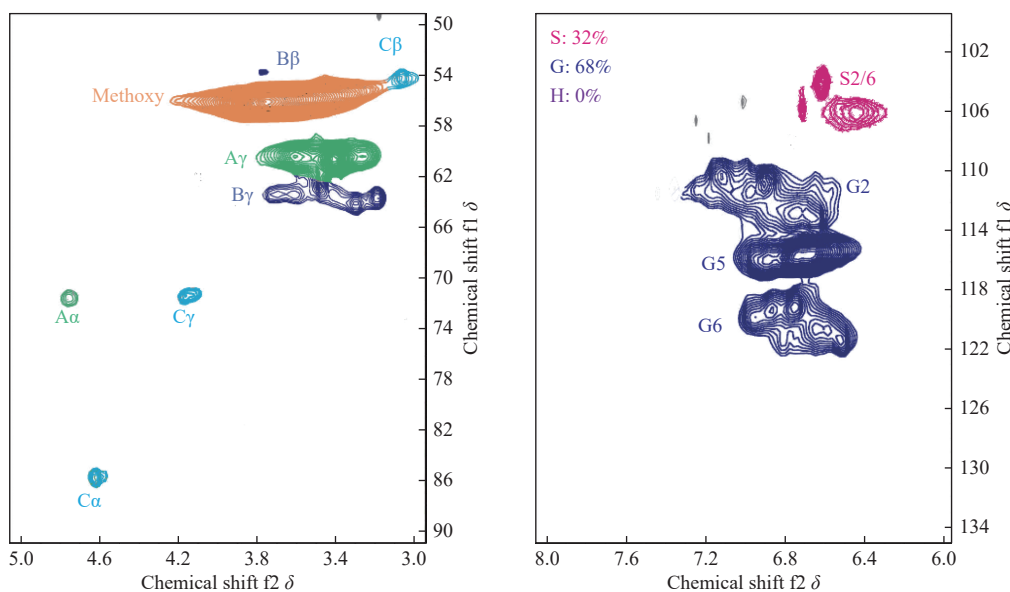
Fig. 14 TG curves (a) and FT-IR spectra (b) of the fresh and recycled Fe_{0.3}MoS/NC catalyst

Fig. 15 2D HSQC NMR spectra of lignin

As shown in Figure 16, the HDO products consist mainly of arenes and cycloalkanes, including cyclohexane, benzene, methylcyclohexane (MCH), toluene, ethylcyclohexane (ECH), ethylbenzene, o-xylene, propylcyclohexane (PCH), propylbenzene, hexahydroindane (HI), indane, 1-methylindane (MI), tetralin (TN), 5-methyltetralin (MTN), 1,2-dicyclohexylethane (DCE), and 1,2-diphenylethane (DPE). The C₈–C₁₆ fraction accounts for 54.4% of the total products, with arenes exhibiting a selectivity of 63.4%

within this fraction. Table 3 presents the molecular weight distribution of the lignin before and after the HDO reaction. After the reaction, the weight-average molecular weight (M_w) decreased significantly from 3496 to 169 g/mol, demonstrating the effective depolymerization of lignin into low molecular weight compounds during the HDO process. These results confirm that the Fe_{0.3}MoS/NC catalyst possesses significant HDO activity and can selectively convert lignin into arenes within the carbon range suitable for SAF.

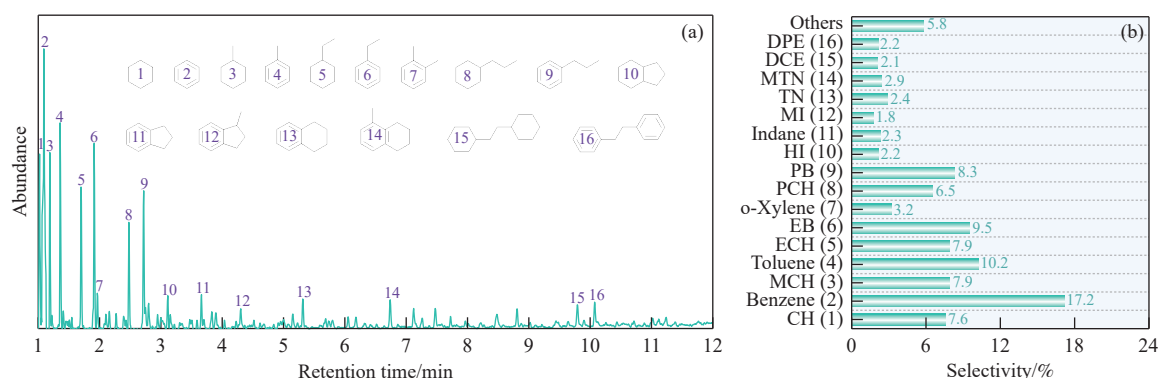


Fig. 16 GC-MS result (a) and product selectivities (b) of identified compounds in hydrodeoxygenation products

Table 3 Molecular weight distribution of lignin and its hydrodeoxygenation products

Sample	$M_w/(g \cdot mol^{-1})$	$M_n/(g \cdot mol^{-1})$	Polydispersity index (PDI)
lignin	3496	1480	2.3
Products	169	157	1.1

3 Conclusion

In this work, a series of nitrogen-doped FeMoS/NC bimetallic catalysts were prepared *via* a hydrothermal method. Using 4-ethylguaiacol as a model compound, the influence of Fe on the HDO performance of MoS₂-based catalysts was systematically investigated. The experimental results demonstrate that appropriate Fe incorporation effectively promotes electron transfer and enhances the interaction between metals. The addition of Fe increases the concentration of sulfur vacancies, improves the dispersion of MoS₂ on the NC and generates more surface active sites. Among the catalysts with varying Fe content, the Fe_{0.3}MoS/NC catalyst with an optimal Fe/Mo molar ratio of 0.3 exhibited the best HDO performance, achieving complete conversion of 4-ethylguaiacol at 340 °C under 3 MPa H₂ for 5 h, along with 100% deoxygenation and 78.6% arene selectivity. The HDO reaction pathway of 4-ethylguaiacol over Fe_{0.3}MoS/NC primarily proceeds *via* a direct deoxygenation route. The HDO performance was further evaluated using real lignin as the feedstock. After 12 h of reaction, a green hydrocarbon yield of 65.5% was obtained. The C₈–C₁₆ fraction accounted for 54.4% of the total products, with an aromatic selectivity of 63.4% within this fraction. These results confirm that the Fe_{0.3}MoS/NC

catalyst can selectively convert lignin into green arenes suitable for SAF applications.

Declaration of Competing Interest

The authors declare no conflict of interest.

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Fe 修饰的 MoS₂/NC 催化剂用于木质素加氢脱氧制绿色芳烃航煤组分

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摘要: 木质素包含丰富的芳环结构, 对其加氢脱氧可制备绿色可持续航空燃料的芳烃组分。采用水热法合成了一系列负载型 FeMoS/NC 催化剂, 并采用 4-乙基愈创木酚作为模型化合物, 在反应温度 340 °C、氢气压力 3 MPa 的条件下进行了性能评价。结果表明, MoS₂/NC 催化剂的脱氧率为 83.4%, 而 Fe 修饰的 MoS₂/NC 催化剂(Fe_{0.3}MoS/NC)加氢脱氧率达到 100%, 芳烃选择性为 78.6%。增加 Fe/Mo 物质的量比, 脱氧率降低。通过 XRD、TEM、低温 N₂ 吸附-脱附、XPS 等手段对催化剂进行表征, 结果表明, Fe 的引入促进了 MoS₂ 在 NC 载体表面的均匀分散, 增强了催化剂表面的酸性, 增加了硫空位的浓度, 促进了催化剂对含氧化合物的吸附。采用真实木质素为原料, 在反应温度 340 °C、氢气压力 3 MPa、反应 12 h 的条件下, 对 Fe_{0.3}MoS/NC 催化剂的加氢性能进行了性能评价, 结果表明, 绿色烃收率为 65.5%, 碳数分布为 C₈-C₁₆ 的组分含量为 54.4%, 其中, 芳烃选择性为 63.4%, 可作为绿色芳烃航煤组分, 该研究可为木质素直接加氢脱氧制绿色芳烃航煤组分提供参考。

关键词: 活性炭; FeMoS/NC; 加氢脱氧; 4-乙基愈创木酚; 木质素; 芳烃

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