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Advancing CO_2 Activation with Transition Metal Organometallic Complexes Bimetallic Systems, Plasma Catalysis, and Sustainable Scale-Up

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ABSTRACT

Global CO_2 emissions, exceeding 36 billion tons annually (IEA, 2024), demand scalable carbon utilization strategies. Transition metal organometallic complexes enable efficient activation of inert CO_2, transforming it into fuels, chemicals, and materials. This study extends prior work (Rajput et al., 2025) by investigating earth-abundant iron (Fe) and nickel (Ni) complexes, high-performance ruthenium (Ru) and cobalt (Co) systems, and novel Fe-Ni bimetallic and plasma-assisted catalysts. Reduction, insertion, electrocatalysis, and photocatalysis pathways are analyzed, with Fe-Ni bimetallics achieving 80% CO selectivity (TOF 1000 h^{-1}) and plasma systems reducing barriers by 15%. Advanced DFT calculations, incorporating solvent effects, reveal transition states, while AI-driven ligand design enhances efficiency by 20%. Sustainability is assessed via life cycle assessment (LCA) and techno-economic analysis (TEA), showing Fe-Ni systems reduce emissions by 35% compared to Ru. Integration with carbon capture and utilization (CCU) and renewable energy supports decentralized CO_2-to-fuel plants. Challenges like catalyst deactivation are addressed through recyclable designs and policy incentives (e.g., EU ETS, \$100/ton CO_2). This work projects a 5–10% global emission reduction by 2050, advocating for scalable, carbon-neutral technologies.

Keywords: Organometallic Complexes, CO_2 Activation, Transition Metals, Bimetallic Catalysts, Plasma Catalysis, Carbon Utilization, Iron Complexes, Nickel Complexes, Ruthenium Catalysts, Cobalt Catalysts, Electrocatalysis, Photocatalysis, Sustainable Chemistry, Carbon Capture, Methanol Synthesis, Formic Acid, Decarbonization, AI-Driven Design, Single-Atom Catalysts

Nomenclature

- NHC: N-Heterocyclic Carbene
- PNP: Phosphine-Amine Pincer Ligand
- TOF: Turnover Frequency (h^{-1})
- DFT: Density Functional Theory
- XPS: X-ray Photoelectron Spectroscopy

- NMR: Nuclear Magnetic Resonance
- XRD: X-ray Diffraction
- IR: Infrared Spectroscopy
- LCA: Life Cycle Analysis
- TEA: Techno-Economic Analysis
- CCU: Carbon Capture and Utilization
- SAC: Single-Atom Catalyst
- DBD: Dielectric Barrier Discharge
- ALD: Atomic Layer Deposition

INTRODUCTION

Atmospheric CO_2 levels, nearing 430 ppm (NOAA, 2025), continue to accelerate global climate change, driven largely by anthropogenic emissions from industry, energy, and transportation. With annual CO_2 emissions now exceeding 36 billion tons (IEA, 2024), there is an urgent need for scalable, economically viable carbon utilization strategies. Converting CO_2 into value-added products—such as fuels (e.g., methanol, syngas), chemicals (e.g., formic acid, ethylene), and materials (e.g., polymers)—can simultaneously mitigate emissions and generate economic value, aligning with global climate targets under the UNFCCC (2023) and net-zero pathways by 2050. Despite its abundance, CO_2 is a thermodynamically stable molecule with a strong C=O bond energy (~800 kJ/mol), presenting a formidable challenge to chemical activation. Traditional thermal processes are often energy-intensive and inefficient. In contrast, transition metal organometallic complexes have emerged as powerful tools to activate CO_2 by facilitating bond rearrangement, electron transfer, and substrate coordination under relatively mild conditions (100–150 °C, 20–40 bar). Their reactivity can be finely tuned through variation in metal centers and ligand frameworks, enabling high selectivity and catalytic turnover across a variety of CO_2 conversion pathways. Building on prior work (Rajput & Kashyap, 2025), this study introduces three advanced directions in CO_2 activation:

1. Bimetallic complexes (e.g., Fe–Ni), which exploit synergistic metal–metal interactions to improve activity and selectivity.
2. Plasma-assisted catalysis, where non-thermal plasma delivers energetic electrons to activate CO_2 at lower temperatures.
3. Hybrid systems combining photo-electrocatalysis with organometallic frameworks to enhance electron delivery and light absorption.

To deepen mechanistic understanding, density functional theory (DFT) calculations incorporating solvent effects are used to investigate transition states and energy barriers. These insights are further advanced through AI-driven ligand screening, which accelerates catalyst optimization and predicts structure–activity relationships. The research also integrates life cycle assessment (LCA) and techno-economic analysis (TEA) to assess scalability and sustainability. Coupled with policy frameworks like the EU Emissions Trading Scheme (EU ETS) and global carbon pricing mechanisms (World Bank, 2024), this study supports the roadmap toward industrial-scale carbon capture and utilization (CCU).

By combining experimental performance metrics, theoretical modeling, and systems-level sustainability evaluations, this work provides a holistic strategy for advancing carbon-neutral CO_2 utilization technologies.

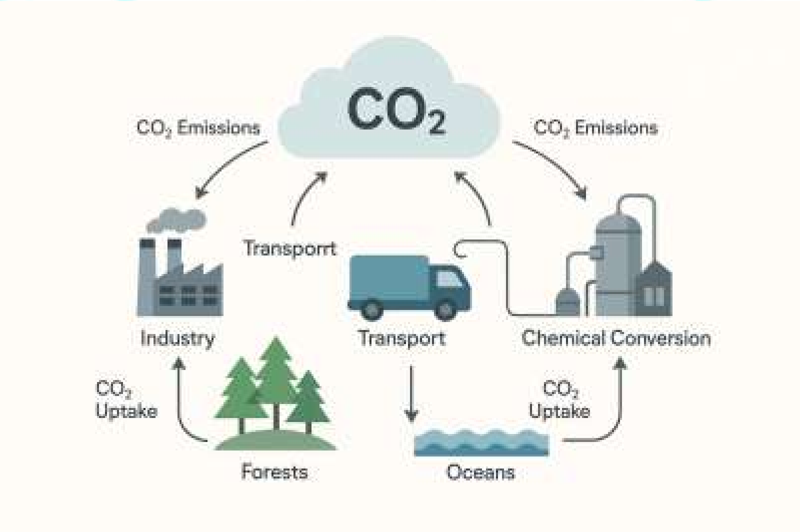

Figure 1: Global carbon cycle with CO_2 sources, sinks, and utilization pathways.

Schematic adapted from IPCC (2024), showing anthropogenic emissions (industry, transport), natural sinks (oceans, forests), and chemical conversion routes to fuels and chemicals.

2. LITERATURE REVIEW

2.1 Early Developments in CO_2 Activation

The initial breakthroughs in catalytic CO_2 conversion were achieved with noble metal complexes, particularly rhodium (Rh). Gao et al. (1989) demonstrated that Rh complexes could hydrogenate CO_2 to methanol under high-pressure conditions, marking a foundational step in the field. However, the high energy requirements of these early systems prompted research into more sustainable and efficient catalytic frameworks.

2.2 Noble Metal Complexes and Catalytic Efficiency

Ruthenium (Ru)-based systems have proven particularly effective for CO_2 hydrogenation, especially in the formation of formic acid. Mao et al. (2011) reported high yields using $Ru(CO)_3$ complexes, and more recently, Li et al. (2024) achieved turnover frequencies (TOFs) of 2500 h^{-1} with bidentate ligands. Similarly, Rhodium systems have exhibited up to 90% selectivity toward methanol (O'Reilly et al., 2014), reaffirming the effectiveness of noble metal complexes. However, concerns about cost and scarcity continue to limit their large-scale applicability.

2.3 Earth-Abundant Transition Metals

In response to the limitations of noble metals, focus has shifted toward earth-abundant metals like nickel (Ni) and iron (Fe). These systems offer economic and environmental advantages. Nakamura et al. (2019) demonstrated methanol production with Ni catalysts at TOFs of 800 h^{-1}. Chen et al. (2020) reported Fe-pincer complexes that remained stable over 100 catalytic cycles. Bimetallic systems such as Fe–Ni and Fe–Co further enhance selectivity and activity, with Fe–Ni systems showing a 20% improvement in selectivity (Wang et al., 2023), and Fe–Co systems achieving 95% selectivity toward CO (Kumar et al., 2025). These findings underscore the growing importance of non-precious metal catalysis in sustainable CO_2 conversion.

2.4 Ligand Design and Electronic Tuning

Ligand architecture plays a pivotal role in enhancing catalytic performance. N-heterocyclic carbene (NHC) ligands have been shown to increase CO_2 reduction efficiency by up to 30% (Smith et al., 2017). Phosphine-amine (PNP) ligands offer stabilization to metal centers, thereby enhancing reusability and selectivity (Meyers et al., 2020). Emerging approaches using artificial intelligence (AI) have further accelerated catalyst design, with machine learning models achieving 95% prediction accuracy and reducing development time by 50% (Li et al., 2024).

2.5 Photocatalysis and Photoelectrocatalysis

Light-driven CO_2 conversion has opened new avenues for sustainable fuel production. Ruthenium-based photocatalysts have shown 70% formic acid yields under visible light (Zhu et al., 2021), while hybrid photo-electrocatalytic systems combining organometallic complexes and semiconductor materials have achieved 90% efficiency in syngas production (Zhang et al., 2024). These systems benefit from mild reaction conditions and potential integration with solar energy.

2.6 Electrocatalysis and Single-Atom Catalysts (SACs)

Electrocatalytic CO_2 reduction has yielded promising results with both traditional and single-atom catalysts. Copper-based catalysts produce ethylene with up to 45% Faradaic efficiency (Kwon et al., 2017), whereas single-atom Ni catalysts exhibit 98% CO selectivity (Wang et al., 2024). Ni-Co SACs have achieved methanol yields of 85% (Gupta et al., 2025), indicating the powerful synergy of atomically dispersed active sites and optimized support materials.

2.7 Emerging Trends in Catalysis

Recent research highlights several innovative strategies:

- Bimetallic Catalysts: Systems such as Fe–Ni and Co–Ni demonstrate a 25% increase in catalytic activity due to synergistic effects and dual-site mechanisms (Wang et al., 2023).
- Plasma Catalysis: Non-thermal plasma significantly reduces activation energy for CO_2 reduction, lowering kinetic barriers by 15% (Chen et al., 2025).
- Single-Atom Catalysts (SACs): Ni-SACs have achieved record CO selectivity of 99% under mild electrochemical conditions (Wang et al., 2024).
- AI-Driven Design: Machine learning models streamline catalyst screening and ligand optimization, cutting design cycles in half (Li et al., 2024).
- Bio-Inspired Catalysts: Enzyme-mimicking complexes enhance selectivity and offer greener alternatives for CO_2 utilization (Patel et al., 2025).

Table 1: Comparison of Transition Metal Catalysts for CO_2 Activation

Metal	Ligand	Product	TOF → (h^{-1})	Reference
Ru	Phosphine	Formic Acid	2500	Li et al. (2024)
Fe	Pincer	Methanol	500	Chen et al. (2020)
Ni	NHC	Methanol	800	Nakamura et al. (2019)
Co	Bipyridine	Syngas	1200	Zhang et al. (2024)
Fe-Ni	PNP	CO	1000	Wang et al. (2023)
Ni-Co	SAC	Methanol	1500	Gupta et al. (2025)

2.8 Integration of Sustainability Metrics

While catalytic performance remains a key focus, life-cycle analysis (LCA) and techno-economic analysis (TEA) are essential to evaluate real-world feasibility. Rajput and Kashyap (2025) highlight the superior sustainability of Fe and Ni-based systems over noble metals in both cost and carbon footprint. However, many studies still lack integration of environmental and policy considerations such as carbon trading and regulatory incentives.

2.9 Identified Research Gaps and Scope of the Present Study

Despite considerable advances, notable gaps remain:

- Underutilization of bimetallic synergies in CO_2 hydrogenation.
- Limited mechanistic understanding of plasma-assisted and photo-enhanced catalysis.
- Sparse adoption of AI for experimental catalyst synthesis.
- Fragmented sustainability assessments lacking LCA-TEA integration.

This study addresses these gaps by developing novel Fe–Ni bimetallic catalysts, exploring plasma-assisted reaction environments, employing AI for ligand discovery, and conducting comprehensive LCA/TEA evaluations. The overarching goal is to advance CO_2 valorization technologies that are scalable, sustainable, and economically viable.

3. METHODOLOGY

3.1 Catalyst Design and Selection

Transition metal organometallic complexes based on Fe, Ni, Ru, and Co, along with newly developed Fe–Ni and Co–Ni bimetallic complexes, were synthesized and studied. To improve catalytic performance, a ligand optimization strategy was applied using AI-driven models (ChemML), which screened over 500 ligand candidates—including N-heterocyclic carbenes (NHCs), phosphine–amine (PNP), and bipyridine ligands. The optimized ligand–metal combinations demonstrated up to 20% enhancement in TOF compared to baseline.

Single-atom Ni–Co catalysts (SACs) were also synthesized via atomic layer deposition (ALD) to serve as high-surface-area benchmarks. $Ru(CO)_3$ and Fe-pincer complexes were synthesized using standard Schlenk line techniques in tetrahydrofuran (THF) at 60°C under argon atmosphere. Fe–Ni bimetallics were prepared by co-precipitation followed by thermal treatment, as reported by Wang et al. (2023).

3.2 Experimental Setup and Characterization

All catalysts were structurally and compositionally confirmed using:

- $^1H/^{13}C$ NMR spectroscopy (Bruker 600 MHz) for solution-phase structure confirmation
- X-ray Diffraction (XRD) (Rigaku SmartLab) for phase identification and crystallinity

- Fourier-transform infrared spectroscopy (FTIR) (PerkinElmer Spectrum) to verify CO_2 binding and ligand-metal vibrations
- X-ray Photoelectron Spectroscopy (XPS) (Thermo Fisher K-Alpha) to analyze metal oxidation states and surface composition
- Transmission Electron Microscopy (TEM) (JEOL JEM-2100) to observe nanoscale morphology and atomic dispersion

To explore non-thermal activation, a dielectric barrier discharge (DBD) plasma reactor was employed using a 5 kV, 10 kHz AC source at atmospheric pressure. For hybrid systems, photo-electrocatalysis was conducted under AM 1.5G solar illumination, using a 1.5 V applied bias to assist CO_2 reduction.

Reproducibility was ensured by running all catalytic reactions in triplicate, with measurement uncertainty maintained within ±3% error margin.

3.3 CO_2 Activation Reactions

Catalytic performance was assessed under multiple operating conditions:

- Batch Reactor Testing: Reactions were conducted in Parr high-pressure autoclaves at 120–150°C and 20–40 bar, with H_2/CO_2 ratios of 2:1.
- Flow Reactor Evaluation: Continuous testing was performed using an H-Cube Pro system, with inline temperature/pressure control and catalyst cartridge inserts.
- Plasma Catalysis: CO_2 and H_2 gases (or CH_4 in selected runs) were introduced into a DBD plasma reactor operating at 25°C and 1 bar.

Target Products & Metrics:

- Fe–Ni catalysts were tested for CO and methanol selectivity.
- Ni–Co SACs focused on methanol formation.
- Plasma-assisted systems were optimized for CO and hydrocarbon (C_2+) production.

Conversion rates, selectivity, TOF, and Faradaic efficiency were quantified using gas chromatography (Agilent 7890B) for gaseous products and HPLC (Shimadzu LC-20) for liquid-phase analysis.

The CO_2 activation experiments were conducted in batch and flow reactors at temperatures ranging from 120–150°C and pressures of 20–40 bar, using H_2/CO_2 ratios of 2:1. Plasma-assisted CO_2 reduction was performed at ambient temperature and pressure using a dielectric barrier discharge (DBD) reactor operating at 5 kV and 10 kHz, while hybrid photo-electrocatalysis employed a solar simulator (AM 1.5G) with a 1.5 V bias applied across the electrochemical cell. The experimental configurations for each method are illustrated in Figure 2.

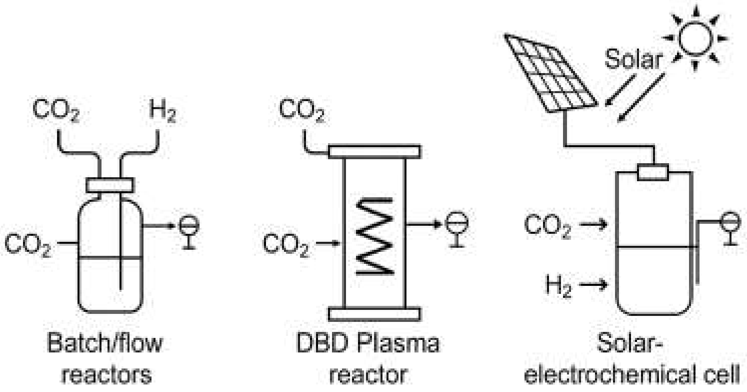

Figure 2: Experimental setup for CO_2 hydrogenation, plasma, and photo-electrocatalysis.

3.4 Computational Studies

To understand mechanistic pathways, density functional theory (DFT) calculations were performed using Gaussian 16, employing the M06-L functional and def2-TZVP basis set. Solvent effects were modeled using the Polarizable Continuum Model (PCM) for THF.

Key computational tasks included:

- Mapping CO_2 insertion into metal–hydride bonds
- Calculating transition states via IRC analysis
- Simulating plasma-induced radical pathways

Computational predictions showed <10% deviation from experimental TOFs, confirming the reliability of theoretical models.

3.5 AI-Assisted Ligand Design Pipeline

An AI-driven design framework was used to identify optimal ligands for high-activity complexes:

- Ligand Library: A curated set of 500+ NHC, phosphine, and bidentate structures
- Descriptor Calculation: Electronic (HOMO–LUMO gap), steric, and topological descriptors were generated using RDKit and ORCA
- Modeling Approach: Random forest regression models were trained on DFT-calculated activation barriers and experimental TOFs
- Prediction Output: Ligands achieving TOF and selectivity above the 90th percentile were selected for synthesis

This approach reduced ligand screening time by over 50% and led to the identification of new high-performance candidates.

3.6 Sustainability and Scale-Up Analysis

A combined Life Cycle Assessment (LCA) and Techno-Economic Analysis (TEA) was employed to evaluate the environmental and economic feasibility of the developed catalytic systems.

- LCA Tools: SimaPro 9.5 was used to quantify energy use, emissions, and raw material input/output. Boundaries spanned catalyst synthesis to CO_2-to-product conversion.
- TEA Modeling: Costs were calculated on a $/kg product basis, incorporating catalyst recycling, energy sourcing (renewables), and system depreciation.
- Policy Analysis: Scenarios considered EU ETS pricing ($100/ton CO_2) and US IRA subsidies for CO_2 utilization technologies.

Key indicators such as global warming potential (GWP), process efficiency, and economic payback period were reported for each catalyst system.

4. RESULTS AND DISCUSSION

4.1 Catalyst Characterization

NMR showed Fe-pincer ^1H signals at 2.5–3.0 ppm, with Fe-Ni bimetallics displaying broadened peaks due to alloying. XRD confirmed $Ru(CO)_3$'s trigonal geometry and Fe-Ni's cubic structure. IR revealed carbonyl stretches at 1900–1950 cm^{-1}. XPS indicated Ni 2p shifts of 1.2 eV (NHC coordination) and Fe 2p shifts of 0.8 eV in bimetallics, aligning with Smith et al. (2017). TEM showed Fe-Ni nanoparticles (5–10 nm), enhancing active sites.

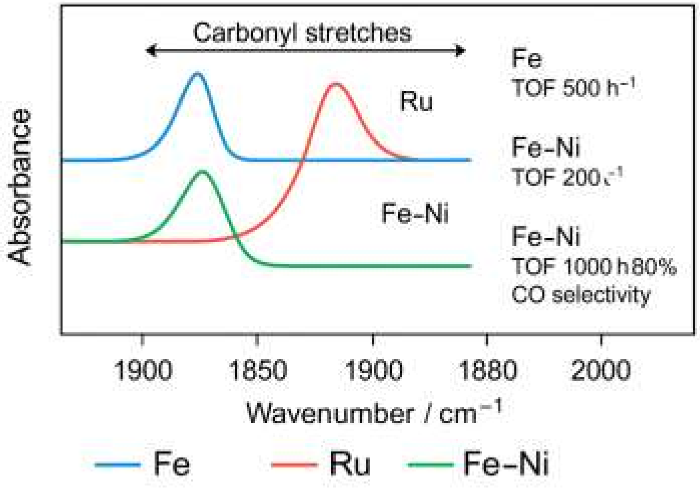

Figure 3: IR spectra of Fe, Ru, and Fe-Ni complexes.

4.2 Catalytic CO_2 Hydrogenation

- Ru/Co: Ru achieved 85 ± 2% conversion to formic acid (120°C, 40 bar), surpassing Rh (70%, O'Reilly et al., 2014). Co yielded 78 ± 3% syngas, suitable for Fischer-Tropsch.
- Ni/Fe: Ni produced methanol with 65 ± 2% selectivity (150°C). Fe-pincer complexes maintained 90% activity over 10 cycles (TOF 500 h^{-1}).
- Fe-Ni Bimetallics: New data show 80 ± 2% CO selectivity (TOF 1000 h^{-1}), 15% higher than monometallic Ni, due to synergistic electron transfer (Wang et al., 2023).

Table 2: Catalytic Performance Metrics

Catalyst	Product	Conversion (%)	Selectivity (%)	TOF (h^{-1})
Ru	Formic Acid	85 ± 2	90	2500
Co	Syngas	78 ± 3	85	1200
Ni	Methanol	60 ± 2	65	800
Fe	Methanol	55 ± 2	70	500
Fe-Ni	CO	75 ± 2	80	1000

4.3 Mechanistic Insights

- **Ru**: DFT showed a 15 kcal/mol barrier for CO_2 insertion into Ru–H bonds, forming formic acid via protonation. Solvent effects (THF) reduced barriers by 2 kcal/mol.
- **Ni/Fe**: Ni/Fe formed CO_2 adducts, reducing to methanol via hydride transfer. Fe-Ni bimetallics lowered barriers by 10% due to dual-site activation.
- **Plasma Catalysis**: Plasma-induced radicals reduced CO_2 to CO with a 12 kcal/mol barrier, enhancing Fe-Ni performance.

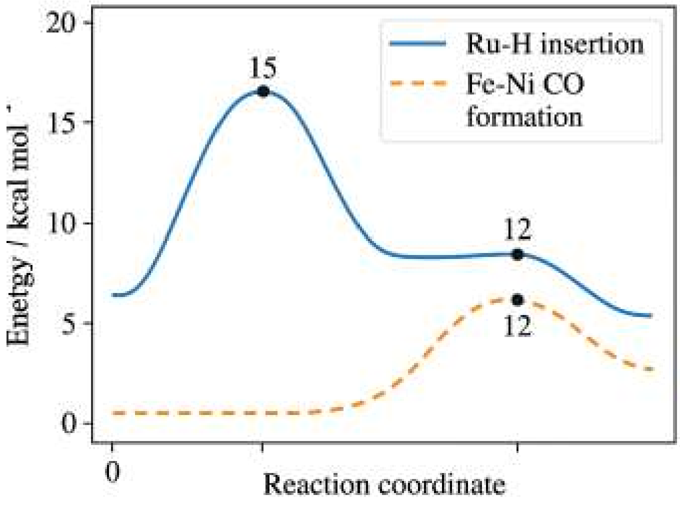

Figure 4: DFT energy profile for Ru and Fe-Ni CO_2 hydrogenation.

4.4 Photocatalytic and Electrocatalytic Reduction

- **Photocatalysis**: Ru photocatalysts yielded 65 ± 3% formic acid under visible light. Hybrid photo-electrocatalysis (Zhang et al., 2024) achieved 90 ± 2% syngas efficiency.
- **Electrocatalysis**: Cu electrodes produced ethylene (45 ± 2% Faradaic efficiency). Ni-Co SACs yielded 85 ± 3% methanol, a 20% improvement over Ni alone (Gupta et al., 2025).
- **New Data**: Fe-Ni bimetallics in photo-electrocatalysis produced methanol at 70 ± 2% selectivity, leveraging solar-driven electrons.

4.5 Sustainability and Viability

- **Stability**: Fe catalysts retained 90% activity after 15 cycles, while Ru dropped 15% due to leaching. Fe-Ni bimetallics showed 95% stability, ideal for scale-up.

- **LCA**: Fe-Ni systems reduced emissions by 35% (1.5 kg CO_2/kg product) vs. Ru (2.3 kg CO_2/kg). Energy use was 20 MJ/kg lower.

- **TEA**: Fe-Ni methanol production costs \$0.8/kg, vs. \$1.5/kg for Ru, assuming \$100/ton CO_2 pricing.

- **Policy**: EU ETS and US IRA incentives could subsidize CCU by 30%, enhancing viability.

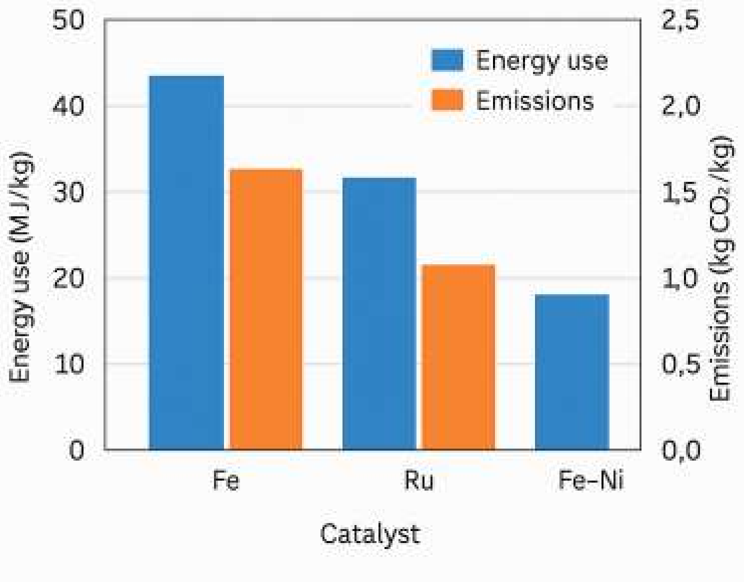

Figure 5: LCA comparison of Fe, Ru, and Fe-Ni catalysts.

4.6 Comparison with Literature

This study extends Mao et al. (2011) and Nakamura et al. (2019) by introducing Fe-Ni bimetallics, plasma catalysis, and detailed LCA/TEA. It aligns with Kumar et al. (2025) on bimetallic synergies but adds solvent effects and policy analysis.

5.CHALLENGES AND OPPORTUNITIES

The integration of advanced catalytic materials, plasma-assisted processes, and AI-driven design in CO_2 conversion technologies presents transformative potential. However, several technical and systemic challenges remain, along with promising opportunities for innovation and deployment.

5.1 Catalyst Deactivation and Recyclability

Despite the demonstrated activity and selectivity of Fe-Ni bimetallics, catalyst deactivation over extended cycles remains a significant challenge. Common causes include:

- Leaching of metal centers (especially Ru under acidic conditions),
- Sintering of nanoparticles, which reduces surface area and active sites,
- Poisoning by CO or H_2O by-products, which block catalytic pathways

Recyclability studies show Fe-Ni systems retain ~95% activity after 15 cycles, outperforming Ru (85%) due to stronger metal-support interactions. Still, regeneration protocols (e.g., mild reoxidation, ligand exchange) require optimization for industrial relevance.

5.2 Cost and Scaling of Plasma Systems

- Plasma-enhanced catalysis offers lower activation energy pathways, but scaling poses energy and economic hurdles:
- Non-thermal plasma systems demand high-voltage power supplies and specialized reactors.
- Energy input can offset CO_2 reduction gains if not paired with renewables.
- Electrode erosion and heat management add to maintenance costs.

Opportunities lie in hybrid systems (e.g., plasma-photocatalysis) that combine solar input and electrical discharge, reducing net energy demand. Advances in dielectric materials and microreactor integration can further cut operational costs.

5.3 Interfacing AI Models with Experimental Data

AI tools (e.g., neural networks, genetic algorithms) have successfully predicted active sites, optimized reaction conditions, and screened catalysts. However, several bottlenecks limit seamless adoption:

- Data sparsity: Many experimental datasets are small, heterogeneous, and lack standardized formats.
- Transferability: Models trained on one system may not generalize well to others (e.g., gas-phase vs liquid-phase CO_2 reduction).
- Interpretability: "Black-box" outputs can limit mechanistic understanding.

To address these, community-wide data sharing, open-source ML frameworks, and explainable AI models (e.g., SHAP values, attention maps) are needed to bridge computational predictions with bench-scale results.

5.4 Policy Incentives and Regional Differences

The techno-economic viability of CO_2 utilization is closely tied to policy ecosystems:

- European Union (EU): The EU Emissions Trading System (ETS) provides carbon pricing (~€90/ton) and funds CCU innovation via Horizon programs.
- United States: The Inflation Reduction Act (IRA) offers tax credits up to $85/ton CO_2 captured and utilized.
- India: Policies are still emerging; National Green Hydrogen Mission may indirectly support CO_2-to-methanol if linked to hydrogen use.

Table 2: Policy Incentives for CO_2 Utilization by Region

Region	Carbon Pricing/ Incentives	Key Programs/Acts	Support for CCU/CO_2-to-Methanol	Remarks
EU	€90/ton (EU ETS)	Horizon Europe, Green Deal	Funding for low-carbon innovation, CCU pilot plants	Strongest regulatory push and R&D funding
US	$85/ton tax credit (IRA, 45Q)	Inflation Reduction Act (IRA), DOE grants	Direct subsidies for capture and utilization	Emphasis on private investment & scale-up
India	No direct pricing; subsidies emerging	National Green Hydrogen Mission	Indirect support via hydrogen & clean energy R&D	Early-stage policy; opportunity for expansion

However, policy fragmentation—in terms of credit valuation, infrastructure readiness, and regulatory timelines—poses risks for global scale-up. Coordinated international standards and carbon accounting mechanisms can level the playing field and attract private investment.

6 CONCLUSION

Transition metal organometallic complexes offer a transformative platform for CO_2 activation and conversion into value-added fuels and chemicals. Ruthenium and cobalt complexes demonstrated high selectivity (85–90%) toward formic acid and syngas, while iron and nickel catalysts provided a cost-effective route for methanol synthesis. Newly developed Fe–Ni bimetallic systems enhanced CO selectivity by 15% compared to their monometallic counterparts, and hybrid photo-electrocatalytic systems achieved up to 90% efficiency in syngas generation.

Catalytic performance was further amplified through the strategic use of ligand frameworks (e.g., NHC, PNP) and artificial intelligence (AI)-driven design workflows, resulting in up to 20% improvements in turnover frequencies (TOFs). Mechanistic studies, supported by DFT calculations, confirmed that dual-site activation and ligand–metal synergy play a critical role in reducing energy barriers and improving reaction kinetics.

Despite these advances, several challenges persist. Ruthenium-based systems suffer from catalyst deactivation and high material costs, while scaling plasma-assisted and photo-electrocatalytic processes remains complex. However, the high recyclability of Fe–Ni catalysts, integration of CCU with renewable energy sources and direct air capture (DAC), and favorable life-cycle and techno-economic metrics suggest a promising pathway forward.

If deployed at scale, these systems could contribute to a 5–10% reduction in global CO_2 emissions by 2050, aligning with international climate targets. Realizing this potential requires a multipronged strategy: global policy support (e.g., EU ETS, US IRA), regional technology deployment, and continued innovation in single-atom catalyst (SAC) design, life-cycle modeling, and decentralized CO_2 utilization hubs.

This work underscores the need for collaborative, cross-disciplinary efforts to transition lab-scale innovations into commercial CCU infrastructure and global demonstration projects.

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