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Development of Functionalized Organic Ionic Liquids for Sustainable CO_2 Absorption and Recycling in Industrial Systems

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Abstract: Increasing levels of atmospheric CO_2, primarily derived from fossil fuel combustion and industrial activity, are one of the most pressing challenges facing countries worldwide. This demands innovative strategies for capture and recycling. Conventional mechanisms, including membrane separation, amine scrubbing, and cryogenic processes, are effective, but often suffer from high energy demands, limited scalability, and solvent degradation. Ionic liquids (ILs) have emerged as more beneficial alternatives because of their low volatility, high thermal stability, and structural tunability. However, limitations, including environmental concerns and high viscosity, limit their application. This paper examines the development of functionalized organic ionic liquids (FOILs) as sustainable solvents for CO_2 capture and recycling. It highlights recent advances in structural functionalization strategies and synthesis methods following a literature-based review approach. Case studies provide evidence that amino-functionalized and fluorinated FOILs have superior recyclability, absorption capacity, and stability compared with traditional solvents. Industrial applications in flue gas treatment, natural gas sweetening, and integration with carbon utilization pathways are evaluated, while identifying key challenges like synthesis cost, viscosity, and environmental risks. However, opportunities for pilot-scale validation and green design are also emphasized. FOILs generally represent a next-generation platform for effective industrial CO_2 management, with potential to advance sustainable decarbonization while supporting the transition toward a circular carbon economy.

Keywords: *Functionalized Organic Ionic Liquids (FOILs), Carbon Dioxide Absorption, Industrial Systems, Recycling, Ionic Liquids*.

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I. INTRODUCTION

Global CO_2 emissions are currently at critical levels, with atmospheric concentrations rising from 280 ppm to 413 ppm due to increased dependence on fossil fuels (Anwar et al., 2019). Based on the exponential emissions growth trajectory, there is an urgent need for proactive measures, especially as major emitters such as the United States, China, Russia, India, and Japan contribute significantly to global emissions (Singh et al., 2023). In addition, the pressing issues of accelerated resource exploitation, deforestation, and alarming rates of emission from industrial sectors are evidence that reduction efforts remain insufficient. Bahman et al. (2022) observed that there is limited progress in carbon footprint mitigation across different economic sectors. Therefore, comprehensive solutions comprising capture & storage of carbon, energy efficiency improvements, and renewable energy transitions are required to meet 50-80% emission reductions by 2050 and 100% by 2100 (Kocs, 2017).

Current CO_2 capture techniques, comprising technologies for minimising atmospheric emissions from fossil fuel combustion, exist to foster sustainability. For example, amine scrubbing is recommended as a post-combustion capture method, which involves the use of chemical absorption with solutions such as monoethanolamine (MEA) for selective capturing of CO_2 through the formation of carbamate (Raganati & Ammendola, 2024). In addition to amine scrubbing, alternative capture technologies range from membrane separation to cryogenic processes, physical adsorption using solid sorbents, chemical looping combustion, and physical absorption (Gkotsis, Peleka, & Zouboulis, 2023).

Generally, developing cost-effective alternatives is crucial for widespread commercial implementation of sequestration and carbon capture technologies (Zhang et al., 2024; Knoop et al., 2023). In this context, ionic liquids (ILs) have emerged as promising options. Specifically, these salts remain liquid below 100 degrees Celsius and demonstrate good CO_2 affinity, inherent structural tunability, and non-volatility, which makes them attractive alternatives to traditional solvents (Li et al., 2023). Nonetheless, these materials have certain limitations.

The aim of this review is to discuss the development of functionalized organic ionic liquids (FOILs) for effective and sustainable CO_2 absorption and recycling, especially in industrial applications.

The objectives are:

- To examine the potential of functionalized organic ionic liquids for sustainable CO_2 capture.
- To evaluate the different mechanisms of CO_2 absorption in FOILs in comparison to traditional solvents.
- To examine structural modifications and functionalization techniques for improved efficiency.
- To assess challenges and opportunities for industrial application of FOILs.

II. IONIC LIQUIDS: BACKGROUND AND MECHANISMS

Organic ionic liquids are salts comprising discrete anions and cations, with melting points below 100 degrees Celsius (Zhou et al., 2023). Common cations are ammonium, imidazolium, pyridinium, thiazolium, phosphonium, and triazolium species, which feature large phosphorous- or nitrogen-bearing structures and alkyl chain substituents (Liu et al., 2022). They are paired with coordinating anions, including triflate, tetrafluoroborate, triflimide, hexafluorophosphate, and dicyanamide. One of the key advantages of ionic liquids is their tunability characteristic, where anion and cation combinations are altered and specific properties are designed for some applications (Philippi & Welton, 2021). More than 1 million simple ionic liquids are theoretically possible, and mixtures help to expand possibilities further. According to Al-Bodour et al. (2025), this structural diversity fosters effective selection of desired properties for some applications, although the huge number of combinations complicate experimental investigation, which necessitates molecular-based knowledge for advanced utilization.

Organic ionic liquids demonstrate chemical and physical mechanisms for CO_2 absorption, showing unique thermodynamics signatures that distinguish the processes. Gunawardene et al. (2022) observed that physical absorption occurs when CO_2 occupies the space between ions (due to weak interactions). Chemical absorption involves the formation of bonds between CO_2 and ionic liquid components, which classifies 18 room-temperature liquids according to enthalpy and Gibbs functions, where 10 shows physical absorption and 8 shows chemical absorption with AB and AB2 complexes (Romaos, Vergadou, & Economou, 2022; Li et al., 2023). These absorption types are distinguished and predicted with computational approaches, as chemical absorption corresponds to reaction Gibbs free energies within the range of -30 to 16 kJ/mol. Wylie et al. (2022) argued that task-specific ionic liquids with functional groups promote absorption capacity through chemical bonding, which epoxidized imidazolium ILs demonstrating, enabling physical and chemical absorption of CO_2.

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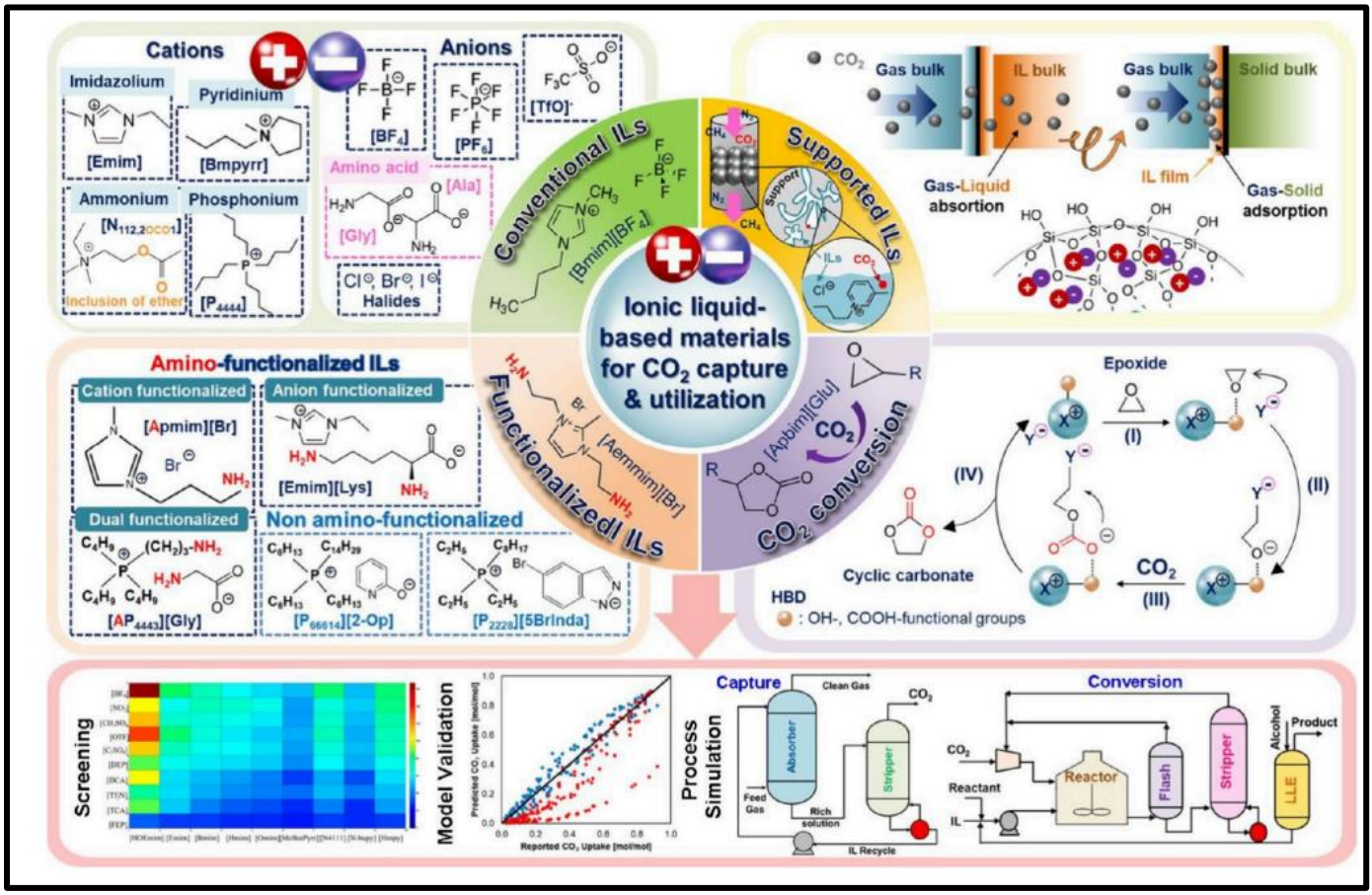

Fig 1: Ionic Liquid-Based Materials for CO2 Capture and Utilization [*Numpilai, Pham, & Witoon, 2024]*

Further, unctional groups are essential for enhancing CO_2 solubility via different mechanisms. Zhang et al. (2020) found that fluorinated chains have superior CO_2-philicity because of favorable interaction structures where CO_2 molecules interact at the tail ends of the surfactant. This leads to better solubility versus oxidative groups despite weaker binding strategies. Amine functionalization improves the capacity to absorb CO_2, as ionic liquids contain primary, hydroxyl groups, and tertiary amine showing nearly threefold increase in volumetric gas and chemical enhancement versus non-functionalized counterparts (Dongare et al., 2024). In the role of polyamines with multiple basic nitrogen groups, especially those with a higher secondary to primary functional groups ratio like TEPA, demonstrate higher absorption rates of CO_2 and capacities versus tertiary amines (Hafizi et al., 2020). However, the reactivity of amines with CO_2 varies in different functional classes, alkanolamines, alkylamines, and fluorinated alkylamines, with distinct trends in carbamate and bicarbonate formation (Said et al., 2020).

Ionic liquids have low volatility properties to get rid of solvent loss during operation. Their tunable structure also allows for optimized CO_2 solubility and selectivity via modification of cations, anions, and functional groups (Li et al., 2023; Zhang et al., 2022). According to Shukla et al. (2019), organic ionic liquids have high CO_2 uptake capacity and can be supported or functionalized on porous materials, including metal-organic frameworks, for improved performance. Numpilai et al. (2024) added that beyond capture, they are also versatile for converting CO_2 into value-added chemicals like cyclic carbonates, which ultimately supports carbon utilization strategies. Ionic liquids, thus, represent a promising alternative to conventional solvents in multiple applications. These are composed of ions and offer unique properties such as high thermal stability, negligible vapor pressure, and high viscosity compared to conventional organic solvents (Hammed, 2023).

Furthermore, ionic liquids behave as polar solvents and can generate biphasic systems for liquid-liquid extraction applications (Basaiahgari & Gardas, 2021), although they exhibit different surface interactions in comparison to molecular liquids, as cation size affects their solvating ability on silica surfaces. Essentially, they present complex kinetic and thermodynamic considerations that distinguish them from traditional molecular solvents (Yu et al., 2022). Solvent effects on synthesis kinetics of ILs are evidenced by varying orders of magnitude based on the solvent used, which requires some descriptors in the quantification of the relationships (Koutsoukos et al., 2022). Likewise, the solvation mechanisms in ionic liquids differ from molecular liquids, which makes traditional classification mechanisms inadequate, complicating

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the kinetic data interpretation (Nordness & Brennecke, 2020). The thermodynamic properties of ILs can also be calculated using quantum statistical thermodynamics, which enables estimation of boiling points, vapor pressures, and enthalpies of vaporization.

III. DESIGN AND DEVELOPMENT OF FUNCTIONALIZED ORGANIC IONIC LIQUIDS

Functionalized organic ionic liquids (FOILs) are designed on the basis of the principle of integrating some functional groups into the ionic framework to promote selectivity, affinity, and recyclability in the capture of CO_2 (Li et al., 2023). Functionalization strategies include anionic or cation moieties modification while incorporating neutral functional groups that can help in reversing interactions with CO_2. Cations can be tailored with pyridinium, imidazolium, and phosphonium bases, while functional groups such as hydroxyl, ether chains, or amino are grafted to enhance chemisorption (Wang et al., 2025).

Some prominent examples are amino-functionalized ionic liquids, with reversible reactions to CO_2 to form bicarbonates or carbamates, providing superior absorption capacity versus non-functionalized counterparts (Dongare et al., 2024; Knoop et al., 2023). Task-specific ionic liquids are another unique class, with reactive functional groups like polyamines or azoles attached to improve CO_2 selectivity and minimize viscosity penalties. In recent years, deep eutectic solvents (DESs), being a subclass of ILs produced by mixing bond acceptors and donors, have gained interest as a result of lower synthetic cost, reduced toxicity versus conventional ILs, and improved biodegradability (Qader & Prasad, 2022).

Moreover, recent synthetic strategies for developing FOILs focus on greener approaches including solvent-free reactions, microwave-assisted synthesis, and application of bio-based precursors to minimize environmental footprint (Usman & Cheng, 2024). Similarly, computational modelling has been crucial in guiding design, with quantum mechanical simulations predicting the interaction sites and Gibbs free energy changes and facilitating more rational functionalization.

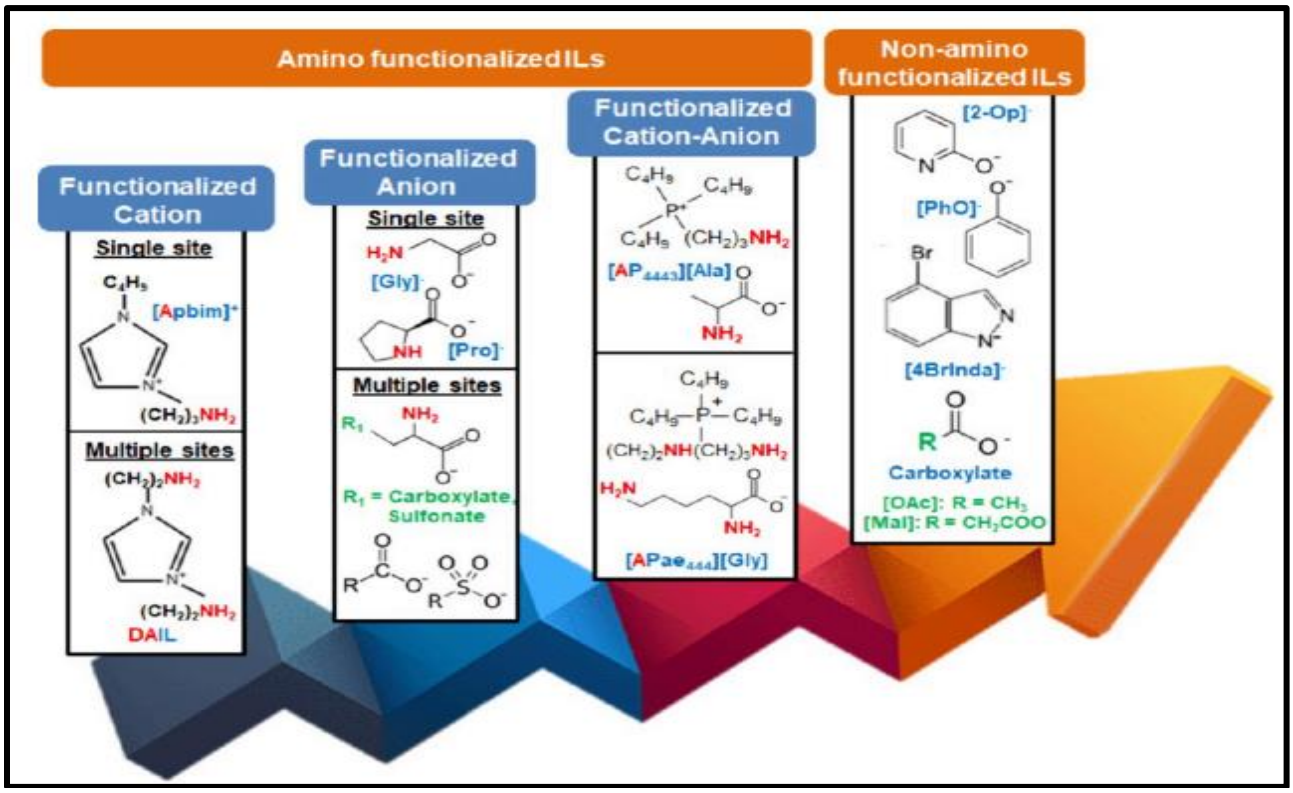

Fig 2: Examples of Functionalized Ionic Liquids

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IV. INDUSTRIAL APPLICATIONS AND CASE STUDIES

Different case studies emphasize the superior performance of FOILs in CO_2 absorption. In Mesbah et al.'s (2019) study, amino-imidazolium ILs showed capacities up to 1.2-1.5 mol CO_2/mol IL with stable regeneration of more than 20 cycles. Polyamine-modified ILs show enhanced recyclability as a result of stable hydrogen bonding networks, and fluorinated ILs demonstrate higher stability under flue gas conditions.

However, the relationships between structure and property indicate certain trade-offs. First, increasing chain length or functional density enhances CO_2 affinity but increases viscosity simultaneously, hindering mass transfer (Li et al., 2022; Ayanleye et al., 2024). Second, hydrophobicity is essential for reducing water uptake in flue gas environments, which thus maintains stability in repeated absorption-desorption cycles. Third, thermal stability is essential as FOILs must have the ability to withstand temperatures of 100-120 degrees Celsius for industrial regeneration without degradation (Galko & Sajdak, 2022; Zhou et al., 2023).

FOILs design generally shows a balance between maximization of CO_2 uptake, maintaining manageable stability, and viscosity. Therefore, continued integration of green synthesis, computational tools, and experimental validation will propel the next generation of FOILs for managing industrial CO_2 (Ali et al., 2023). Moreover, functionalized ionic liquids are being examined for deployment in large-scale CO_2 management systems. In flue gas treatment, these ionic liquids can capture CO_2 from coal-fired power plants with lower energy penalties and higher selectivity than conventional amine scrubbing (Sanni et al., 2022). For instance, amino-functionalized imidazolium ILs have been pilot tested in some absorbers, showing comparable efficiency to MEA, but improved thermal stability and minimal solvent degradation (Alguacil & Robla, 2024). However, although amine scrubbing provides fast absorption rates, excellent regeneration capabilities, and high CO_2 selectivity, it suffers from major drawbacks, including high regeneration energy costs, solvent degradation, equipment corrosion, and environmental risks (Meng et al., 2022)

In natural gas sweetening, functionalized ionic liquids can help to remove H2S and CO_2 from raw gas streams (Gonfa & Ullah, 2024). In comparison to traditional physical solvents like Rectisol or Selexol, these ionic liquids offer resistance and tunability to volatile losses (Li et al., 2023). Moreover, fluorinated ILs have shown strong CO_2 solubility, especially under high-pressure gas conditions, and thus improve separation efficiency.

Meanwhile, beyond capture capability, organic ionic liquids are important to circular carbon economy initiatives. Captured CO_2 can undergo catalytic conversion into value-added products like cyclic carbonates, polymers, and methanol (Chen & Mu, 2019). Also, task-specific ionic liquids have been successfully used as reaction media and CO_2 absorbents, hence coupling conversion and capture processes into an integrated system (Qu et al., 2022). This double role highlights their advantage over traditional solvents, which require different process stages.

Simulation studies and techno-economic assessments prove that organic ionic liquids could cut regeneration energy requirements by up to 25-30% versus MEA-based systems and extend solvent lifecycles significantly (Cuellar-Franca et al., 2021). However, there are limitations on real-world demonstrations. For example, pilot plant trials in Asia and Europe are testing these liquids under industrial flue gas conditions, indicating reliable absorption rates and long-term stability (Li et al., 2023; Greer, Jacquemin, & Hardacre, 2020). Compared to existing technologies, functionalized organic ionic liquids provide greater structural tunability, potential integration with downstream utilization of CO_2, and improved recyclability (Lebedeva, Kultin, & Kustov, 2023). Yet, synthesis costs, scalability, and viscosity management are barriers, but if addressed, FOILs could become a key material in capturing industrial CO_2 and recycling frameworks.

V. CHALLENGES AND LIMITATIONS

Although FOILs have great potential and wide applicability, they face environmental, technical, and economic challenges that limit their large-scale deployment. One of the most key barriers is high viscosity, hindering mass transfer and reducing absorption rates (Jafarizadeh et al., 2024; Numpilai, Pham, & Witoon, 2024). Moreover, functionalization improves selectivity, but viscosity is worsened by excessive substitution, resulting in the need to weigh off kinetics versus absorption capacity (Wylie et al., 2022). Regeneration efficiency is also critical, since some FOILs need high temperatures for desorption, which offsets energy gains.

Environmentally, biodegradability and toxicity are common concerns. Although marketed as green solvents because of low volatility, many ionic liquids have shown ecotoxic effects, especially aromatic and fluorinated species, accumulating in aquatic environments (Goncalves et al., 2021). Due to the lack of comprehensive life-cycle assessments, full evaluation of environmental risks also remains difficult.

In addition, there are significant economic implications. FOILs synthesis is cost-intensive in comparison to conventional solvents, particularly when fluorinated anions or complex functional groups are involved (Blaga, Tucaliuc, & Kloetzer, 2022). With limited scalability, industrial adoption is yet constrained by uncertainty in compatibility and long-term stability with existing infrastructure.

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There are also research gaps, especially as most studies are confined to laboratory settings, with limited full-scale or pilot demonstrations. Again, there is insufficient data on long-term recyclability under impurity and mixed gas conditions. Therefore, addressing these gaps is crucial in the transition of FOILs from laboratory materials with potential to industrially viable solutions.

VI. FUTURE RECOMMENDATIONS

The future development of functionalized organic ionic liquids should focus on green design principles (sustainability-based) that minimize environmental risks and enhance performance. Ionic liquids synthesized from renewable feedstocks, including carbohydrates, amino acids, and choline, provide promising alternatives, integrating high CO_2 affinity with biodegradability (Miao, Atkin, & Warr, 2022). Also, hybrid systems including IL-nanoparticle composites can reduce viscosity, improve absorption kinetics, and improve thermal conductivity.

Regarding the policy and industrial aspects, adoption strategies must include carbon capture and utilization incentives, international collaboration to share learnings from pilot-scale, and public-private partnerships (Nagireddi, Agarwal, & Vedapuri, 2023). Integrating FOIL-based systems with renewable energy and carbon utilization platforms could consolidate their role in the circular carbon economy.

Therefore, future research should prioritize long-term pilot demonstrations in realistic conditions, techno-economic modelling, and comparative life-cycle assessments. FOILs can evolve from laboratory materials into essential industrial components for sustainable CO_2 management with supportive policy frameworks and targeted innovation.

VII. CONCLUSION

Functionalized organic ionic liquids (FOILs) hold great promise in driving sustainable CO_2 absorption and recycling, providing high selectivity, tunability, and integration with carbon utilization pathways. This paper has shown that functionalization through fluorinated and amino groups enhance CO_2 uptake, and recent advances in computational modelling and synthesis methods support advanced optimization. The competitive edge of these materials over traditional solvents is evidenced in industrial applications ranging from natural gas sweetening to flue gas treatment, although challenges of synthesis costs, viscosity, and environmental impacts persist. It is crucial to address the limitations by employing hybrid systems, green chemistry, and pilot-scale techniques. In conclusion, FOILs have huge potential in industrial decarbonization methods in transitioning to a low-carbon future.

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