A Survey of Carbon Capture Using Amine Solvents: Emissions, Degradation, and Environmental Impact

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Abstract

Carbon capture technologies are pivotal in mitigating climate change by reducing atmospheric CO2 concentrations, predominantly from fossil fuel combustion. This survey paper provides a comprehensive examination of these technologies, focusing on post-combustion capture using amine solvents. The paper outlines the significance of carbon capture in climate mitigation, emphasizing its integration with renewable energy systems. It explores various technologies, including absorption, adsorption, and membrane separation, while highlighting the challenges of amine emissions and degradation products. These emissions can form harmful compounds, impacting human health and ecosystems, necessitating advanced analytical methods for monitoring. The survey reviews these methods, evaluating their benefits and limitations, and discusses strategies to mitigate emissions, such as advanced solvent formulations and process optimization. The integration of renewable energy with capture systems is also examined, showcasing its potential to enhance sustainability. The paper concludes by summarizing key findings and identifying future research directions, emphasizing the need for continued innovation in carbon capture technologies to achieve deep decarbonization and stabilize atmospheric CO2 levels.

1 Introduction

1.1 Significance of Carbon Capture in Climate Mitigation

Carbon capture technologies are essential for mitigating climate change by reducing atmospheric carbon dioxide concentrations, primarily resulting from fossil fuel combustion. These technologies are vital for meeting the ambitious targets of international agreements like the Paris Agreement, which seeks substantial reductions in global CO2 emissions [1]. The power sector, in particular, necessitates feasible strategies for phasing out fossil fuels and expanding low-carbon energy sources, with carbon capture playing a crucial role [2].

Integrating carbon capture and storage (CCS) with renewable energy sources emerges as a promising pathway to achieving carbon neutrality by 2050. For example, in Japan, a combination of CCS and renewable technologies is projected to facilitate a CO2 reduction of up to 67% by 2050, showcasing significant environmental and economic advantages [3]. This synergy underscores the complementary role of carbon capture in enhancing the effectiveness of renewable energy systems in emission reductions.

Advanced carbon capture technologies, such as CCSNet, offer efficient alternatives to traditional methods, addressing the high energy demands and inefficiencies of current thermochemical approaches [4]. These innovations are critical for overcoming barriers to widespread adoption and optimizing carbon capture system performance.

Moreover, the Inflation Reduction Act (IRA) in the United States, in conjunction with CCS technologies, is anticipated to significantly influence the electrification of transportation, contributing to the

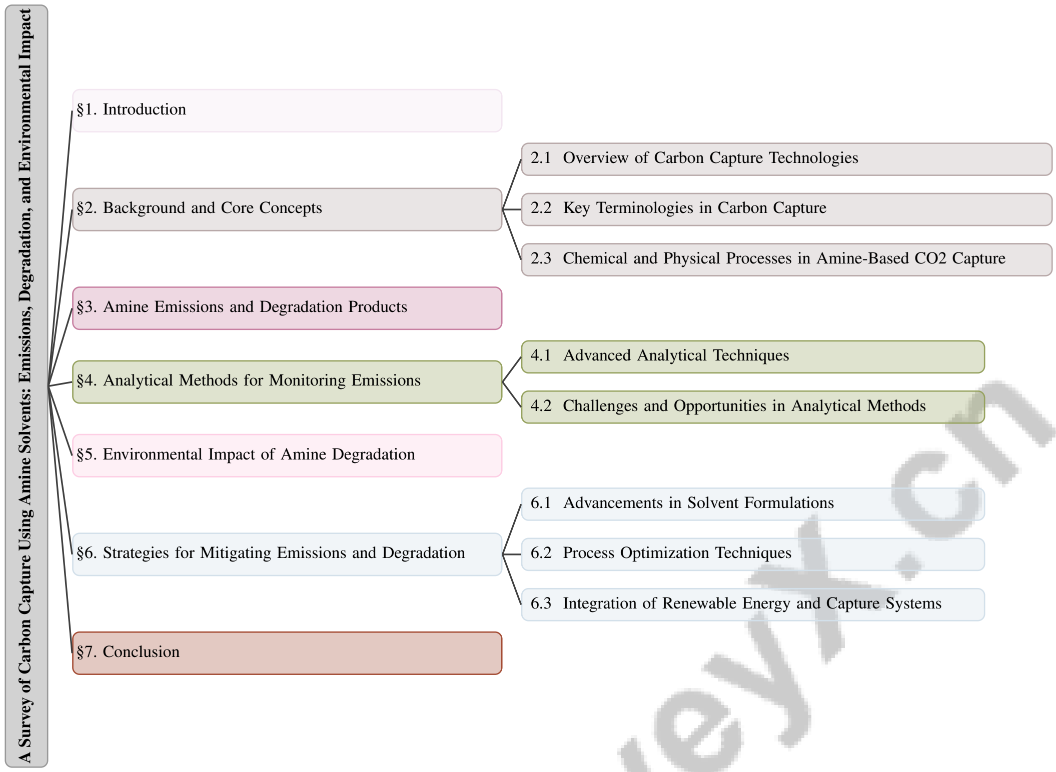


Figure 1: chapter structure

net-zero emissions target by 2050 [5]. This legislative support emphasizes the significance of carbon capture in national strategies aimed at emissions reduction across various sectors.

1.2 Structure of the Survey

This survey presents a comprehensive examination of carbon capture technologies, focusing on post-combustion capture using amine solvents. It begins with an introduction to the significance of carbon capture in climate mitigation, emphasizing its role in reducing global CO2 emissions and its integration with renewable energy systems [5]. Following this, core concepts and background information on various carbon capture technologies, including absorption, adsorption, membrane processes, biological capture, and cryogenic separation, are outlined [6].

The survey then delves into amine emissions and degradation products, assessing their environmental and health impacts, and reviews advanced analytical methods for monitoring these emissions, discussing the benefits and limitations of current techniques. It scrutinizes the environmental impact of amine degradation and explores regulatory frameworks alongside implementation challenges [7].

Strategies for mitigating emissions and degradation are examined, highlighting advancements in solvent formulations, process optimization, and the integration of renewable energy with capture systems [8]. The survey concludes with a summary of key findings and a discussion on future directions and research needs, emphasizing emerging technologies and innovations in carbon capture [9]. This structured approach ensures a thorough exploration of the topic, enhancing understanding of the challenges and opportunities in carbon capture and storage [10].The following sections are organized as shown in Figure 1.

2 Background and Core Concepts

2.1 Overview of Carbon Capture Technologies

Carbon capture technologies are instrumental in reducing CO2 emissions across various industrial sectors. These technologies are classified into post-combustion, pre-combustion, and oxy-fuel combustion methods, each offering distinct pathways for CO2 capture and storage [11]. Post-combustion capture (PCC), commonly implemented in power plants, involves extracting CO2 from flue gases using chemical solvents like amines. Despite its efficacy, PCC faces challenges such as solvent degradation and high energy demand [12]. Pre-combustion capture, on the other hand, removes CO2 before combustion through gasification, converting fossil fuels into syngas, which facilitates CO2 extraction prior to combustion [13].

Oxy-fuel combustion offers an alternative by burning fuel in pure oxygen, resulting in a flue gas mainly composed of CO2 and water vapor, simplifying the capture process [11]. This method enhances efficiency by producing a concentrated CO2 stream.

Advances in materials science have led to the development of innovative adsorbent materials and membrane technologies, significantly improving carbon capture efficiency. Metal-organic frameworks (MOFs) are particularly promising for CO2 capture from flue gases, especially in humid environments typical of natural gas power plants [14]. Characterized by high surface areas and customizable pore structures, MOFs optimize CO2 adsorption [15]. The integration of artificial intelligence and machine learning further enhances the performance and cost-effectiveness of these materials [4].

Direct Air Capture (DAC) technologies, which extract CO2 directly from the atmosphere, represent an emerging research area. While scalability and cost challenges persist, new sorbent materials and innovative process designs are being explored [16]. The valorization of captured CO2 into valuable products, such as through electrocatalysis within MOFs, exemplifies the potential for transforming CO2 into usable commodities, supporting a circular carbon economy [2]. Additionally, quantum computing applications in designing next-generation sorbing materials highlight innovative approaches being pursued to enhance carbon capture technologies [17].

The interplay of chemical, physical, and biological innovations in carbon capture technologies is crucial for reducing global CO2 emissions and mitigating climate change [1]. The Generalized Potential-Solution Method (GPSM) proposed by [18] enhances understanding of fluid dynamics in these technologies, providing insights into their operational mechanisms. Linear optimization models, such as those proposed by [3], evaluate the contributions of renewable energy and carbon capture and storage (CCS) in maximizing CO2 reductions while considering economic factors. This comprehensive understanding is essential for optimizing the integration of carbon capture technologies with renewable energy systems, as highlighted by the framework introduced by [5], which examines the combined effects of policy and technology on transportation electrification.

2.2 Key Terminologies in Carbon Capture

Understanding key terminologies in carbon capture is essential for navigating this complex field. 'Amine emissions' refer to the release of amine solvents, predominantly used in post-combustion carbon capture (PCCC) processes to absorb CO2 from flue gases. These emissions can lead to 'degradation products', chemical by-products resulting from amine solvent breakdown, posing significant environmental and health risks [19]. The environmental impact of these emissions necessitates robust monitoring and mitigation strategies.

The term 'carbon emissions' encompasses the release of carbon dioxide (CO2) into the atmosphere, a primary driver of climate change. Carbon capture technologies aim to mitigate these emissions by employing various methods to capture and store CO2, thereby reducing its atmospheric concentration. 'Direct Air Capture' (DAC) refers to technologies that extract CO2 directly from the atmosphere, offering a complementary approach to traditional capture methods [15].

In materials science, 'hydrolysis reactions' occur when CO2 dissolves in water, forming intermediates such as the pyrocarbonate anion, which are critical in CO2 capture mechanisms. Optimizing adsorbent materials for carbon capture, including their regeneration temperatures and CO2 adsorption capacities, remains a significant focus in ongoing research. The efficient design of MOFs with high CO2 adsorption capacities, while ensuring the synthesizability of the linkers used in their construction, is a key area of study [15].

Additionally, terminologies such as 'fluid flow', 'steady-state solutions', and 'junction potentials' are essential for understanding the underlying processes in carbon capture systems [18]. These terms relate to fluid dynamics within capture systems, impacting the efficiency and effectiveness of CO2 sequestration. Collectively, these terminologies provide a foundational understanding of the processes and challenges associated with carbon capture and ongoing efforts to optimize these technologies for environmental sustainability.

2.3 Chemical and Physical Processes in Amine-Based CO2 Capture

Amine-based CO2 capture is a pivotal component of post-combustion carbon capture systems, primarily utilizing amine solvents such as monoethanolamine (MEA) to facilitate CO2 absorption from flue gases. The chemical process begins with the reaction of CO2 with the amine group, forming carbamate intermediates through a nucleophilic attack mechanism. This reaction produces a zwitterionic intermediate, which rearranges to yield a stable carbamate structure [19]. The efficiency of this reaction is influenced by several thermodynamic parameters, including molar heat capacity at constant pressure, affecting the overall energy dynamics of the system.

Physical processes in amine-based CO2 capture involve complex interactions between CO2, amine solvents, and impurities such as water vapor in flue gas. These interactions can lead to solvent degradation, producing by-products that may diminish CO2 absorption capacity, necessitating effective monitoring and mitigation strategies [4]. Advanced computational models, including those developed in CCSNet, utilize convolutional neural networks (CNNs) to predict changes in CO2 saturation and pressure, providing insights into the dynamic behaviors of these systems under operational conditions.

Recent advancements in materials science have introduced MOFs as potential enhancers of CO2 capture efficiency. The GHP-MOFassemble framework, a high-performance generative AI tool, facilitates the design of MOFs with superior CO2 adsorption capacities, optimizing material properties for enhanced capture performance [15]. Such innovations highlight the potential for integrating AI-driven design with traditional amine-based systems to improve overall capture efficiency.

The interplay between chemical reactions and physical system dynamics is critical for optimizing industrial applications of amine-based CO2 capture. Linear programming frameworks, as demonstrated in evaluating renewable energy and CCS deployment, provide a structured approach to assess the integration of these technologies across various regions [3]. These methodologies underscore the importance of strategic planning in enhancing the effectiveness and sustainability of carbon capture technologies.

The integration of advanced computational modeling, AI-driven material design, and strategic integration approaches presents innovative solutions to address the limitations of amine-based CO2 capture systems. Recent advancements in AI have enabled the automated discovery of polymer membranes tailored for carbon capture, overcoming previous challenges in training data generation and performance validation at the meso-scale. Furthermore, the GHP-MOFassemble framework allows for the rapid design and screening of MOFs with exceptional CO2 adsorption capabilities, demonstrating the potential for significantly enhanced efficiency in carbon capture technologies. Leveraging these cutting-edge methodologies is essential for accelerating the development of more effective materials for CO2 filtration and separation processes [15, 20]. Continued research and development in these areas are crucial for achieving more efficient and sustainable solutions to global CO2 emissions challenges.

The increasing focus on carbon capture technologies necessitates a comprehensive understanding of the various emissions associated with these systems. In this context, it is essential to explore the hierarchical structure of amine emissions and their degradation products. Figure 2 illustrates this structure, categorizing the types and sources of emissions, the chemical reactions leading to degradation, and the associated environmental and health impacts. Furthermore, the figure emphasizes the strategies for mitigation, thereby providing a holistic view of the challenges and solutions in managing amine-related emissions in carbon capture systems. This visual representation not only enhances our understanding but also serves as a critical reference point for future research and policy development in this field.

3 Amine Emissions and Degradation Products

3.1 Types and Sources of Amine Emissions

Amine emissions in post-combustion carbon capture systems primarily result from the volatilization and degradation of amine solvents like monoethanolamine (MEA), used for CO2 absorption from

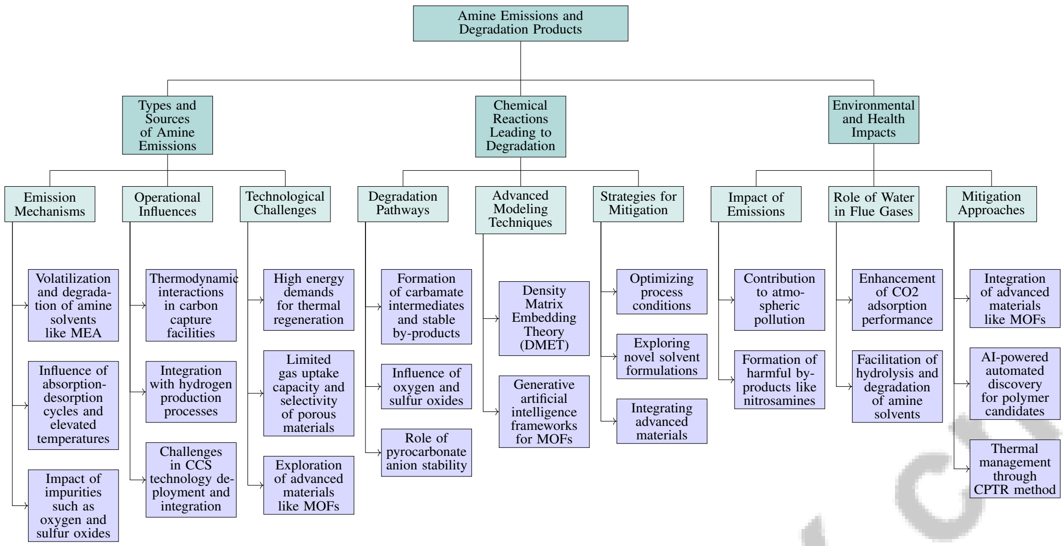


Figure 2: This figure illustrates the hierarchical structure of amine emissions and degradation products in carbon capture systems, categorizing the types and sources of emissions, chemical reactions leading to degradation, and the environmental and health impacts, along with the strategies for mitigation.

flue gases. The high vapor pressure of amines facilitates their release, particularly during absorption-desorption cycles involving elevated temperatures and oxidative conditions. Impurities such as oxygen and sulfur oxides accelerate amine degradation, producing by-products with environmental and health risks. This degradation reduces CO_2 capture efficiency and complicates hazardous substance management, necessitating higher purity in amine solutions for enhanced stability and efficacy [21, 22, 7, 23, 24].

Operational dynamics within carbon capture facilities significantly impact amine emissions, with thermodynamic interactions between CO_2 and oxygen mixtures influencing amine stability and emission profiles. Integrating carbon capture systems with hydrogen production processes, such as those in fuel cell vehicles, introduces additional emission sources due to amine-related by-products [12]. The slow deployment of carbon capture and storage (CCS) technologies and uncertainties in their integration with existing transportation electrification strategies further complicate effective amine emission management [5].

Challenges in addressing amine emissions stem from the inefficiencies and economic constraints of current carbon capture technologies. High energy demands for thermal regeneration processes and the degradation of absorbents hinder large-scale adoption and financial incentives for carbon-neutral practices. Additionally, the limited gas uptake capacity and selectivity of existing porous materials restrict their effectiveness in CO_2 separation [14]. The vast chemical space of potential building blocks for advanced materials, such as metal-organic frameworks (MOFs), presents significant challenges in exhaustively exploring combinations using traditional methods [15].

Innovative approaches, including the functionalization of MOFs with diamines, may enhance CO_2 capture mechanisms by improving sorbent efficiency and potentially reducing amine emissions. However, the development of electrosorbents for CO_2 capture faces constraints due to the availability of effective materials, posing barriers to the advancement of electrosorption as a viable carbon capture method [4]. The complexities of the CO_2-H_2O interface, including interfacial tension and phase behavior under varying pressures, further challenge the optimization of carbon capture processes.

3.2 Chemical Reactions Leading to Degradation

The degradation of amine solvents in post-combustion carbon capture systems is driven by complex chemical reactions that yield degradation products adversely affecting system efficiency and environmental impact. Key to these reactions is the interaction between amines and CO_2, forming carbamate intermediates that can transform into stable by-products like urea derivatives and organic acids, ultimately reducing the CO_2 absorption capacity of the solvent [19].

Impurities such as oxygen and sulfur oxides in flue gases exacerbate degradation, leading to the formation of nitrosamines and other harmful compounds with significant environmental and health risks. The stability of the pyrocarbonate anion is crucial in these pathways, influencing amine solvent breakdown [19]. Additionally, the dynamics of multiphase flow, including dissolution rates, contribute to the chemical reactions within the solvent, further promoting degradation.

Recent advancements in material science, such as Density Matrix Embedding Theory (DMET) combined with variational quantum algorithms, have improved modeling of CO2 interactions in complex materials, providing insights into degradation mechanisms [14]. These advanced techniques enhance understanding of the thermodynamic and kinetic aspects of degradation pathways, particularly under high pressures and near-critical conditions.

The development of novel metal-organic frameworks (MOFs) through generative artificial intelligence frameworks presents potential solutions for mitigating degradation by creating stable environments for CO2 sorption, thus reducing degradation product formation [15]. Addressing degradation challenges requires a comprehensive understanding of underlying chemical reactions and robust strategies to minimize their impact, including optimizing process conditions, exploring novel solvent formulations, and integrating advanced materials. Enhancing the sustainability of carbon capture technologies is essential for reducing environmental impact and improving the efficacy of carbon capture and utilization (CCU) strategies. Recent advancements in carbon capture methods, including novel solvents and electrochemical processes, may significantly lower energy requirements and improve scalability. Integrating CCU pathways with energy, water, and food systems can create valuable commodities from captured CO2, optimizing supply chains and addressing resource competition, which is crucial for achieving global carbon neutrality goals and mitigating climate change effects [7, 3, 2, 25].

3.3 Environmental and Health Impacts

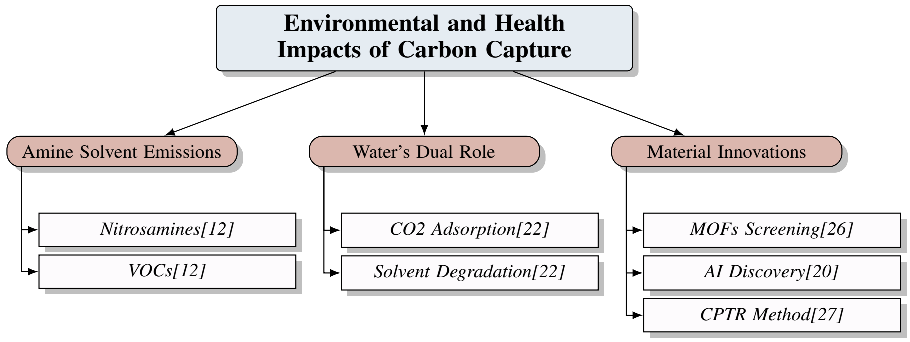
The environmental and health impacts of emissions and degradation products from amine solvents in carbon capture systems are significant due to their potential contributions to atmospheric pollution and human health risks. Amine emissions, primarily from the volatilization and degradation of solvents like MEA, can lead to harmful by-products, including nitrosamines and other volatile organic compounds (VOCs) [12]. These compounds are persistent in the environment and exhibit carcinogenic properties, necessitating stringent monitoring and mitigation strategies.

Water in flue gas streams plays a dual role in the environmental impact of carbon capture systems. While it can enhance CO2 adsorption performance, achieving over 90% capture efficiency from humid flue gases [22], it also facilitates the hydrolysis and degradation of amine solvents, increasing emissions of degradation products that contribute to secondary pollution and health risks for nearby populations.

Figure 3 illustrates the key environmental and health impacts associated with carbon capture systems, focusing on the emissions from amine solvents, the dual role of water in flue gas streams, and material innovations to mitigate these impacts. It highlights the formation of harmful by-products like nitrosamines and VOCs, the enhancement of CO2 adsorption, and the degradation of solvents. Additionally, it showcases the potential of advanced materials like metal-organic frameworks (MOFs), AI-powered discovery methods, and the CPTR method in optimizing carbon capture processes.

Integrating advanced materials, such as metal-organic frameworks (MOFs), offers potential solutions to mitigate these impacts. High-throughput screening of MOFs has shown promise in optimizing gas adsorption properties, paving the way for materials that minimize degradation and emissions [26]. Additionally, AI-powered automated discovery (AIMD) approaches can significantly reduce the time and resources needed to identify polymer candidates tailored for specific applications, potentially enhancing the environmental performance of carbon capture systems [20].

Thermal effects associated with carbon capture processes also influence environmental impact. The Constrained Pressure-Temperature Residual (CPTR) method effectively manages these effects, leading to faster convergence and improved scalability in large-scale simulations [27]. By optimizing process conditions, CPTR contributes to reducing energy consumption and emissions associated with carbon capture, thereby enhancing the overall sustainability of these systems.



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4 Analytical Methods for Monitoring Emissions

4.1 Advanced Analytical Techniques

Advanced analytical techniques are critical for accurately detecting and quantifying amine emissions and their degradation products in carbon capture systems, enhancing the understanding of complex interactions during carbon capture. Innovations in pre-combustion, post-combustion, and oxyfuel methods, alongside advancements in sorbent materials and electrochemical processes, are pivotal for effective carbon capture solutions. Novel solvents with reduced regeneration energy and renewable electricity in electrochemical systems offer significant opportunities for reducing energy demands and improving scalability [7, 2].

Bayesian Active Learning-Driven High-Throughput Experimentation (BAL-HTE) optimizes processes like lithium carbonate production and CO2 capture by refining experimental designs through Bayesian learning, enhancing CO2 capture efficiency by identifying optimal conditions [28]. Incorporating BAL-HTE into carbon capture frameworks aids in optimizing solvent formulations and operational parameters, reducing emissions and degradation products.

The POD-MLP-EKF method combines Proper Orthogonal Decomposition with a multi-layer perceptron neural network and an extended Kalman filter, enabling accurate state estimation for real-time monitoring of amine concentrations and degradation pathways [29]. This capability is vital for timely interventions to optimize capture efficiency.

Markov Chain Monte Carlo (MCMC) simulations enhance analytical capabilities by calibrating computational models, offering insights into model performance and reliability, leading to more accurate amine emissions and degradation predictions [30]. This approach refines predictive models for emission assessments.

The Constrained Pressure-Temperature Residual (CPTR) method effectively manages thermal effects and improves convergence rates in large-scale simulations, optimizing process conditions to minimize energy consumption and emissions, promoting sustainability [27]. Its computational efficiency is critical for real-time process optimization and large-scale deployment.

Deep reinforcement learning (DRL) agents offer advanced capabilities for optimizing energy system scheduling integrated with carbon capture technology, enabling dynamic optimization and enhancing system performance and efficiency [13].

Integrating these advanced techniques significantly improves the accuracy, efficiency, and adaptability of carbon capture processes, addressing traditional methods' limitations. Innovations like electrochemical carbon capture and novel sorbents, including modulated amine blends, reduce energy requirements and enhance CO2 adsorption capacities, facilitating effective monitoring and optimization of carbon capture and utilization technologies. These advancements help the industry tackle high

CO_2 emissions challenges and progress toward net-zero emissions targets [7, 9, 2, 31]. Continued development and integration of these technologies are vital for achieving substantial reductions in amine emissions and degradation products, contributing to carbon capture systems' sustainability.

Figure 4 illustrates the hierarchical structure of advanced analytical techniques in carbon capture, highlighting innovative methods, optimization techniques, and emerging technologies that enhance the efficiency and scalability of carbon capture processes. The first study showcases a carbon-negative approach to lithium extraction, minimizing carbon emissions, while the second tracks atmospheric CO_2 concentrations and global emissions, correlating these trends with temperature anomalies [28, 6]. These examples underscore the importance of advanced analytical techniques in monitoring and mitigating environmental impacts.

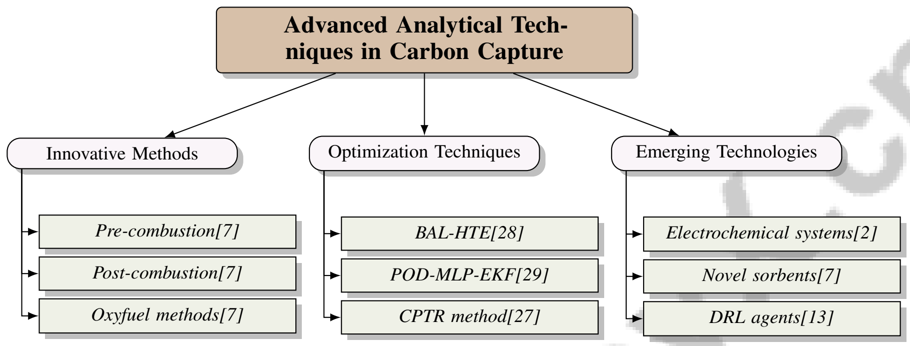

Figure 4: This figure illustrates the hierarchical structure of advanced analytical techniques in carbon capture, highlighting innovative methods, optimization techniques, and emerging technologies that enhance the efficiency and scalability of carbon capture processes.

4.2 Challenges and Opportunities in Analytical Methods

Monitoring amine emissions and degradation products in carbon capture systems presents challenges due to the complexity and variability of chemical processes, mirroring those faced in adopting low-carbon technologies [32]. Accurate detection of low-concentration amine emissions within complex flue gas matrices is a key challenge, as traditional techniques often lack the sensitivity and specificity needed for trace levels of degradation products, which pose environmental and health risks [7, 25, 33, 2, 31]. Impurities in flue gases further complicate accurate measurement, necessitating more robust and selective methods.

Real-time monitoring of dynamic processes is crucial for advancing carbon capture technologies. Emerging electrochemical methods using renewable electricity for CO_2 separation require comprehensive monitoring to optimize performance and efficiency [7, 2, 31]. Variability in operational conditions affects amine solvent stability, leading to inconsistent emission profiles. Current methods often lack real-time insights necessary for timely process adjustments.

Significant opportunities exist for enhancing analytical methods through advanced technologies. Integrating machine learning and AI into emission monitoring systems can improve tracking precision and efficiency. AI frameworks facilitate automated discovery and validation of materials for carbon capture, enhancing emission reduction technologies. AI-driven optimization methods are being developed for processes like lithium carbonate production, contributing to carbon capture efforts. Computer vision techniques analyze subsurface geometry in carbon capture projects, improving decision-making and land management [15, 34, 20, 28]. These technologies enable predictive models for complex interactions within carbon capture systems, allowing precise control and optimization.

High-throughput screening techniques integrated with advanced sensor technologies enhance sensitivity and selectivity, particularly in developing efficient materials for carbon capture and gas separation applications. Automated discovery of polymer membranes utilizes AI-driven methodologies, streamlining material design and validation. Recent advancements in sorbent technologies demonstrate improved performance metrics, such as lower energy requirements and enhanced adsorption capacities [7, 26, 20]. These innovations lead to more reliable and cost-effective monitoring solutions capable of operating under diverse conditions.

Exploring novel materials, such as MOFs, for sensor development presents opportunities for enhancing analytical detection capabilities. Innovative materials can be engineered to improve sensor selectivity and sensitivity, addressing current detection technique shortcomings. Advancements in AI-driven polymer membrane design enable optimized materials for carbon capture, while living porous ceramics exhibit self-regulating gas sensing and carbon capture through bacterial colonization [6, 20, 35].

Despite challenges, significant potential for advancement exists through innovative technologies and approaches. Research emphasizes electrochemical carbon capture processes utilizing renewable electricity to reduce energy requirements and enhance CCS technologies' scalability. Breakthroughs in materials science, like automated polymer membrane discovery, pave the way for more efficient filtration methods. These advancements signal a transformative shift in effectively monitoring and mitigating amine emissions, contributing to more effective climate change strategies [21, 22, 20, 7, 2]. Continued research and development are crucial for overcoming existing limitations and achieving more effective and sustainable carbon capture systems.

5 Environmental Impact of Amine Degradation

The degradation of amine solvents in post-combustion carbon capture (PCCC) systems leads to chemical transformations that significantly impact ecosystems and human health. This understanding is crucial for developing strategies to mitigate adverse effects, particularly in carbon capture and utilization technologies aimed at optimizing CO2 recovery and minimizing resource competition [21, 22, 25, 33, 2]. This section delves into the chemical and environmental impacts of amine solvent degradation, focusing on the by-products, their persistence, and associated risks.

5.1 Chemical and Environmental Impacts of Amine Degradation

Amine degradation in PCCC systems results in by-products like nitrosamines and volatile organic compounds (VOCs), which pose significant environmental and health risks due to their carcinogenic nature and persistence [19]. The presence of oxygen and sulfur oxides in flue gases exacerbates these processes, forming stable, harmful by-products that contribute to atmospheric pollution. Understanding these complex chemical interactions, influenced by CO2 structural behavior at the H2O interface, is essential for assessing the impacts of carbon capture technologies. Advanced methodologies like CCSNet enhance understanding of saturation distributions and pressure buildup in CO2 storage projects, offering insights into degradation pathways and their ecological and health effects [4].

Advanced materials, such as metal-organic frameworks (MOFs), offer promising solutions for mitigating amine degradation's environmental impact. The GHP-MOFassemble framework identifies AI-generated MOFs with high CO2 adsorption capacities, highlighting the potential for discovering high-performance materials for carbon capture [15]. These materials can reduce the environmental footprint by enabling efficient CO2 capture and regeneration, surpassing traditional methods.

Assessing technology mixes, as in Japan, emphasizes the importance of tailored strategies for maximizing environmental and economic outcomes [3]. Policies like the Inflation Reduction Act (IRA) necessitate balancing electrification rates with CCS technology deployment to ensure sustainable environmental impacts [5]. Addressing amine degradation impacts requires a multifaceted approach, including advanced materials development, process optimization, and sustainable technology integration. Initiatives like carbon capture and utilization (CCU) technologies, which convert CO2 into valuable products, and innovative methods such as electrochemical processes, significantly improve CO2 management, supporting global climate goals and optimizing resources within the energy, water, and food nexus [7, 3, 25, 33, 2].

5.2 Regulatory Frameworks and Implementation Challenges

Regulatory frameworks for carbon capture technologies, particularly those using amine solvents, are crucial for safe and effective implementation. However, developing and enforcing these regulations face challenges impeding widespread adoption and optimization. Current regulatory approaches often lack the granularity needed to address the complex technical and environmental issues associated with amine emissions and degradation products, partly due to reliance on high-level assumptions that may not capture real-world intricacies [8].

A primary challenge is the need for comprehensive technical assessments and feasibility analyses to understand the specific conditions influencing carbon capture systems' performance and environmental impact. For instance, modeling fluid plume dispersion in subsurface storage sites is critical for ensuring safe and efficient CO2 sequestration. Future research should refine these models to incorporate variable fluid properties and assess applicability across different aquifer types and conditions [36].

Integrating carbon capture with renewable energy systems introduces regulatory challenges as nations strive for carbon neutrality by 2050. Combining renewable sources like solar and wind with CCS technologies, especially those using renewable electricity for CO2 separation, requires careful oversight to ensure effective deployment and economic viability, essential for achieving significant CO2 emission reductions across sectors [7, 3, 2]. These technologies' dynamic nature demands flexible and adaptive regulatory frameworks capable of accommodating rapid advancements and market changes. Policymakers must balance stringent environmental protections with promoting innovation and economic viability in the carbon capture sector.

Successful regulatory framework implementation for CCU and CCS relies on collaboration among government agencies, industry stakeholders, and research institutions. This collaboration is vital for optimizing resource management and integrating CCU pathways within the energy-water-food nexus, enhancing decision-making, fostering innovative technologies, and promoting cross-sectoral synergies that drive economic and environmental benefits in transitioning to sustainable energy systems [8, 25]. Such collaboration is crucial for developing standardized methodologies for monitoring and reporting emissions and establishing best practices for managing amine degradation products' environmental and health impacts.

6 Strategies for Mitigating Emissions and Degradation

The pressing challenge of climate change has spurred research into innovative strategies for reducing emissions and environmental degradation, with a focus on advanced solvent formulations to enhance carbon capture efficiency. Recent advancements in these formulations are pivotal for improving CO2 capture processes and reducing greenhouse gas emissions. This section explores key innovations and their implications for carbon capture efficiency.

6.1 Advancements in Solvent Formulations

Recent innovations in solvent formulations for carbon capture emphasize efficiency and sustainability. The GHP-MOFassemble framework exemplifies this by expanding the metal-organic framework (MOF) design space, enabling the discovery of MOFs with superior CO2 adsorption capacities [15]. Additionally, bilayer graphtriyne membranes improve selectivity and permeability, enhancing CO2 separation efficiency compared to single-layer configurations [37, 12]. Integrating deep reinforcement learning with automated hyperparameter tuning further optimizes solvent formulations, enhancing system performance.

Electrochemical methods for CO2 capture offer lower energy requirements than traditional thermal processes, especially for concentrated CO2 sources. Comparative analyses highlight the potential for reducing energy consumption in carbon capture technologies [7, 2, 31]. The flexible force field methodology advances computational modeling of thermodynamic properties, crucial for optimizing amine solvent design, leading to better predictions of solvent performance [20, 19].

These solvent formulation advancements are crucial for reducing emissions and improving capture efficiency. By integrating advanced materials, computational techniques, and process optimization strategies, recent developments bolster global efforts to reduce CO2 emissions, supporting the transition to a low-carbon economy and addressing the urgent need for effective carbon management solutions [7, 3].

6.2 Process Optimization Techniques

Process optimization techniques are essential for enhancing carbon capture efficiency and minimizing by-product formation. Advanced computational methods and machine learning algorithms have significantly contributed to these objectives. The Sorbent Materials Foundry (SMF) method exemplifies this approach by rapidly iterating through synthesis and characterization processes, optimizing material properties for Direct Air Capture (DAC) performance [38]. Robust optimization techniques inform process strategies, addressing economic and operational uncertainties in carbon capture systems [32].

Innovative methods, such as Markov State Models with Ab Initio Molecular Dynamics, unveil hidden reaction kinetics, enhancing process optimization by providing insights into molecular interactions [39]. Incorporating operability constraints into design frameworks ensures economic viability and addresses dynamic operational challenges, utilizing real-time optimization techniques like the ACIVP method [40].

Exploring framework flexibility on CO2 dynamics and optimizing inter-crystalline spacing are critical for enhancing capture efficiency [41]. The RZEMPC method integrates robust control strategies, balancing safety and efficiency in carbon capture systems [42]. The Generalized Potential-Solution Method (GPSM) enhances fluid dynamics understanding, contributing to process optimization by improving CO2 capture modeling [18].

Recent developments highlight the importance of integrating process design with techno-economic assessments to tackle operational challenges. Innovative alternatives, such as modulated amine blends and graphene-type materials, demonstrate lower energy requirements and enhanced adsorption capacities, essential for optimizing carbon capture units within low-carbon energy systems [7, 43]. Continued research is vital for achieving sustainable carbon capture solutions.

6.3 Integration of Renewable Energy and Capture Systems

Integrating renewable energy sources with carbon capture systems enhances sustainability and efficiency, addressing the energy demands and inefficiencies of conventional methods. Advanced technologies like reaction swing absorption, utilizing triethylamine for high CO2 absorption rates, support the transition to clean energy and climate change mitigation [7, 9].

Developing MOFs that capture CO2 and catalyze its conversion into carbon monoxide and oxygen significantly enhances system efficiency [44]. The STEP process optimizes renewable energy integration, driving electrochemical reactions for CO2 capture and conversion [45]. Future research should refine the STEP process and explore new integration avenues.

Incorporating renewable energy into magnetohydrodynamic (MHD) generator design offers opportunities to enhance sustainability, aligning energy output with process demands [11]. Further advancements in integrating renewable energy and carbon capture systems can be achieved through developing bicarbonate electrolyzers, enhancing sustainability by improving efficiency and integration [9]. This integration supports CO2 emissions reduction and the transition to a low-carbon economy.

7 Conclusion

7.1 Future Directions and Research Needs

Advancing carbon capture technologies necessitates a focus on enhancing process efficiency and sustainability through the development of novel materials and optimization of existing systems. The exploration of electrochemical processes stands out as a promising avenue, as it offers the potential to significantly boost carbon capture efficiency by introducing innovative materials and catalysts into established frameworks. This approach, coupled with the refinement of algorithms in automated deep reinforcement learning, could unlock new configurations and foster technological advancements.

The integration of renewable energy with carbon capture systems represents a pivotal opportunity to improve overall system efficiency and sustainability. Future research should delve into complex scenarios, such as industrial decarbonization and the implementation of cutting-edge technologies like direct air capture, to assess their impact on CO2 reduction. Expanding the scope of CCSNet to include more intricate scenarios and processes is essential for advancing research in this field.

In the realm of computational modeling, employing homotopic continuation methods could provide new insights into enhancing carbon capture technologies by elucidating steady-state solutions in complex systems. Additionally, increasing public awareness of carbon capture and storage (CCS) technologies, refining deployment strategies, and exploring the interplay between policy initiatives, such as the Inflation Reduction Act, and CCS deployment across diverse regional contexts are critical areas of focus.

The investigation of advanced materials, including redox-active metal-organic frameworks (MOFs), is vital for enhancing CO2 capture and release efficiency. Conducting field tests and exploring alternative functionalities are necessary steps to validate the industrial applicability of these materials. Furthermore, optimizing the synthesis of porous ceramics and incorporating additional functionalities into engineered living materials could pave the way for innovative enhancements in carbon capture processes.

These research directions are integral to driving innovation and achieving significant progress in carbon capture technologies. By capitalizing on emerging technologies and optimizing existing processes, these efforts will contribute to global initiatives aimed at mitigating climate change and facilitating the transition to a low-carbon economy.

AI-generated, for reference only.

References

[1] Minwoo Hyun, Aleh Cherp, Jessica Jewell, Yeong Jae Kim, and Jiyong Eom. Feasibility trade-offs in decarbonisation of power sector with high coal dependence: A case of korea, 2021.

[2] Mohammad Rahimi, Aliza Khurram, T Alan Hatton, and Betar Gallant. Electrochemical carbon capture processes for mitigation of co 2 emissions. *Chemical Society Reviews*, 51(20):8676–8695, 2022.

[3] Dinh Hoa Nguyen, Andrew Chapman, and Takeshi Tsuji. Assessing the optimal contributions of renewables and carbon capture and storage toward carbon neutrality by 2050, 2023.

[4] Gege Wen, Catherine Hay, and Sally M. Benson. Ccsnet: a deep learning modeling suite for co_2 storage, 2021.

[5] Samrat Acharya, Malini Ghosal, Travis Thurber, Ying Zhang, Casey D. Burleyson, and Nathalie Voisin. Impact of the inflation reduction act and carbon capture on transportation electrification for a net-zero western u.s. grid, 2024.

[6] Xiaoxing Wang and Chunshan Song. Carbon capture from flue gas and the atmosphere: a perspective. *Frontiers in Energy Research*, 8:560849, 2020.

[7] Ahmed I Osman, Mahmoud Hefny, MIA Abdel Maksoud, Ahmed M Elgarahy, and David W Rooney. Recent advances in carbon capture storage and utilisation technologies: a review. *Environmental Chemistry Letters*, 19(2):797–849, 2021.

[8] Matteo DAndrea, Mario Garzon Gonzalez, and Russell McKenna. Synergies in offshore energy: a roadmap for the danish sector, 2021.

[9] Kezia Megagita Gerby Langie, Kyungjae Tak, Changsoo Kim, Hee Won Lee, Kwangho Park, Dongjin Kim, Wonsang Jung, Chan Woo Lee, Hyung-Suk Oh, Dong Ki Lee, et al. Toward economical application of carbon capture and utilization technology with near-zero carbon emission. *Nature communications*, 13(1):7482, 2022.

[10] Andrew Chapman, Dinh Hoa Nguyen, Hadi Farabi-As, Kenshi Itaoka, Katsuhiko Hirose, and Yasumasa Fujii. Hydrogen penetration and fuel cell vehicle deployment in the carbon constrained future energy system, 2020.

[11] Osama A. Marzouk. Combined oxy-fuel magnetohydrodynamic power cycle, 2017.

[12] Noelia Faginas-Lago, Yusuf Bramastya Apriliyanto, and Andrea Lombardi. Carbon capture and separation from co2/n2/h2o gaseous mixtures in bilayer graphtriyne: A molecular dynamics study, 2020.

[13] Tobi Michael Alabi, Nathan P. Lawrence, Lin Lu, Zaiyue Yang, and R. Bhushan Gopaluni. Automated deep reinforcement learning for real-time scheduling strategy of multi-energy system integrated with post-carbon and direct-air carbon captured system, 2023.

[14] Gabriel Greene-Diniz, David Zsolt Manrique, Wassil Sennane, Yann Magnin, Elvira Shishenina, Philippe Cordier, Philip Llewellyn, Michal Krompiec, Marko J. Rančić, and David Muñoz Ramo. Modelling carbon capture on metal-organic frameworks with quantum computing, 2023.

[15] Hyun Park, Xiaoli Yan, Ruijie Zhu, E. A. Huerta, Santanu Chaudhuri, Donny Cooper, Ian Foster, and Emad Tajkhorshid. A generative artificial intelligence framework based on a molecular diffusion model for the design of metal-organic frameworks for carbon capture, 2024.

[16] Gopal Ramesh Dahale. Quantum simulations for carbon capture on metal-organic frameworks, 2023.

[17] Kin Tung Michael Ho, Kuan-Cheng Chen, Lily Lee, Felix Burt, Shang Yu, Po-Heng, and Lee. Quantum computing for climate resilience and sustainability challenges, 2024.

[18] Shriram Srinivasan, Nishant Panda, and Kaarthik Sundar. On the existence of steady-state solutions to the equations governing fluid flow in networks, 2024.

[19] William R. Smith, Jan Jirsák, Ivo Nezbeda, and Weikai Qi. Molecular simulation of caloric properties of fluids modelled by force fields with intramolecular contributions: Application to heat capacities, 2017.

[20] Ronaldo Giro, Hsianghan Hsu, Akihiro Kishimoto, Toshiyuki Hama, Rodrigo F. Neumann, Binquan Luan, Seiji Takeda, Lisa Hamada, and Mathias B. Steiner. Ai powered, automated discovery of polymer membranes for carbon capture, 2022.

[21] Geonhui Lee, Yuguang C Li, Ji-Yong Kim, Tao Peng, Dae-Hyun Nam, Armin Sedighian Rasouli, Fengwang Li, Mingchuan Luo, Alexander H Ip, Young-Chang Joo, et al. Electrochemical upgrade of co2 from amine capture solution. *Nature Energy*, 6(1):46–53, 2021.

[22] Rebecca L Siegelman, Phillip J Milner, Alexander C Forse, Jung-Hoon Lee, Kristen A Colwell, Jeffrey B Neaton, Jeffrey A Reimer, Simon C Weston, and Jeffrey R Long. Water enables efficient co2 capture from natural gas flue emissions in an oxidation-resistant diamine-appended metal–organic framework. *Journal of the American Chemical Society*, 141(33):13171–13186, 2019.

[23] Julia H. Yang, Amanda Whai Shin Ooi, Zachary A. H. Goodwin, Yu Xie, Jingxuan Ding, Stefano Falletta, Ah-Hyung Alissa Park, and Boris Kozinsky. Room-temperature decomposition of the ethaline deep eutectic solvent, 2025.

[24] Xuancan Zhu, Tianshu Ge, Fan Yang, Meng Lyu, Chunping Chen, Dermot O'Hare, and Ruzhu Wang. Efficient co 2 capture from ambient air with amine-functionalized mg–al mixed metal oxides. *Journal of Materials Chemistry A*, 8(32):16421–16428, 2020.

[25] Ikhlas Ghiat and Tareq Al-Ansari. A review of carbon capture and utilisation as a co2 abatement opportunity within the ewf nexus. 2021.

[26] Pieremanuele Canepa, Calvin A. Arter, Eliot M. Conwill, Daniel H. Johnson, Brian A. Shoemaker, Karim Z. Soliman, and T. Thonhauser. High-throughput screening of small-molecule adsorption in mof, 2013.

[27] Matthias A. Cremon, Jacques Franc, and Francois P. Hamon. Constrained pressure-temperature residual (cptr) preconditioner performance for large-scale thermal co2 injection simulation, 2024.

[28] S. Shayan Mousavi Masouleh, Corey A. Sanz, Ryan P. Jansonius, Samuel Shi, Maria J. Gendron Romero, Jason E. Hein, and Jason Hattrick-Simpers. Artificial intelligence-enabled optimization of battery-grade lithium carbonate production, 2024.

[29] Siyu Liu, Xunyuan Yin, and Jinfeng Liu. State estimation of a carbon capture process through pod model reduction and neural network approximation, 2023.

[30] Peter W. Marcy and Curtis B. Storlie. Bayesian calibration of computer models with informative failures, 2020.

[31] Muneer Mohammad and Mehrdad Ehsani. A quantitative investigation of co2 sequestration by mineral carbonation, 2015.

[32] Tom Savage, Antonio del Rio Chanona, and Gbemi Oluleye. Robust market potential assessment: Designing optimal policies for low-carbon technology adoption in an increasingly uncertain world, 2023.

[33] Jay Fuhrman, Andres F. Clarens, Haewon McJeon, Pralit Patel, Scott C. Doney, William M. Shobe, and Shreekar Pradhan. The role of negative emissions in meeting china's 2060 carbon neutrality goal, 2021.

[34] Wei Chen, Yunan Li, and Yuan Tian. Carbonnet: How computer vision plays a role in climate change? application: Learning geomechanics from subsurface geometry of ccs to mitigate global warming, 2024.

[35] Alessandro Dutto, Anton Kan, Zoubeir Saraw, Aline Maillard, Daniel Zindel, and André R. Studart. Living porous ceramics for bacteria-regulated gas sensing and carbon capture, 2024.

[36] Benjamin W. A. Hyatt and Yuri Leonenko. Dispersion of a fluid plume during radial injection in an aquifer, 2021.

[37] Joyjit Kundu, Tod Pascal, David Prendergast, and Stephen Whitelam. Selective gas capture via kinetic trapping, 2016.

[38] Austin McDannald, Howie Joress, Brian DeCost, Avery E. Baumann, A. Gilad Kusne, Kamal Choudhary, Taner Yildirim, Daniel W. Siderius, Winnie Wong-Ng, Andrew J. Allen, Christopher M. Stafford, and Diana Ortiz-Montalvo. Reproducible sorbent materials foundry for carbon capture at scale, 2022.

[39] Chu Li, Yuan Yao, and Ding Pan. Unveiling the hidden reaction kinetic network of carbon dioxide in supercritical aqueous solutions, 2024.

[40] Mostafa Goodarzi and Qifeng Li. Real-time optimization for wind-to-h2 driven critical infrastructures: High-fidelity active constraints and integer variables prediction enhanced by feature space expansion, 2023.

[41] I. Dhiman, M. C. Berg, David R. Cole, and Siddharth Gautam. Correlation between structure and dynamics of co_2 confined in mg-mof-74 and the role of inter-crystalline space: A molecular dynamics simulation study, 2022.

[42] Benjamin Decardi-Nelson and Jinfeng Liu. Robust economic mpc of the absorption column in post-combustion carbon capture through zone tracking, 2022.

[43] Steven Sachio, Adam Ward, Ronny Pini, and Maria M. Papathanasiou. Operability-economics trade-offs in adsorption-based co_2 capture process, 2023.

[44] Neel Redkar. Carbnn: A novel active transfer learning neural network to build de novo metal organic frameworks (mofs) for carbon capture, 2023.

[45] Stuart Licht. Step: Efficient carbon capture and solar thermal electrochemical production of ammonia, fuels, cement, carbon nanotubes, metals and bleach, 2019.

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