
Solar Thermochemistry and Chemical Looping: A Survey

www.surveyx.cn

Abstract

Solar thermochemistry and chemical looping represent significant advancements in renewable energy technologies, utilizing concentrated solar energy to drive chemical reactions for converting biomass into syngas or other fuels. This survey explores the integration of solar thermochemistry with chemical looping systems, emphasizing the role of oxygen carriers in facilitating oxidation-reduction cycles. The paper highlights the importance of transition metal oxides (TMOs) and compositionally complex perovskite oxides (CCPOs) in optimizing these processes. Key challenges include high reduction temperatures and the need for efficient materials to enhance conversion rates and selectivity. Innovations in materials, such as tungsten carbide for solar absorbers and manganese-iron mixed oxides for oxygen carriers, are discussed for their potential to improve reactor design and energy storage integration. The survey also examines the role of biomass gasification in renewable energy, focusing on the conversion of biomass into syngas using solar energy. Despite challenges like low conversion efficiency and poor syngas quality, advancements in catalyst design and reactor technologies offer promising solutions. The integration of chemical looping with solar processes provides a pathway for clean energy production, with potential for CO₂ capture and storage. Future research directions include optimizing material compositions, exploring strain effects on TMOs, and conducting pilot-scale tests to validate these technologies in real-world applications. These advancements underscore the potential of solar thermochemistry and chemical looping to contribute to sustainable energy production and carbon emission reduction.

1 Introduction

1.1 Overview of Solar Thermochemistry and Chemical Looping

Solar thermochemistry and chemical looping are critical innovations in renewable energy, providing sustainable pathways for fuel production and energy storage. Solar thermochemical hydrogen generation (STCH) utilizes concentrated solar energy for eco-friendly hydrogen production, essential for achieving carbon neutrality through high-temperature reactions that require selective sunlight absorption in solar absorbers [1, 2]. Transition metal oxides (TMOs) play a vital role in these applications, offering unique oxidation energetics and electronic structures crucial for effective energy conversion [3]. The emergence of materials acceleration platforms (MAPs) is set to enhance heterogeneous CO₂ photo(thermal)catalysis, improving the efficiency and scalability of solar-driven processes [4].

Chemical looping, particularly via calcium and metal oxide redox cycles, underpins high-temperature thermochemical energy storage systems, enabling the continuous conversion of solar energy into storable chemical energy [5]. Additionally, advancements in band gap control of transition metal perovskite chalcogenides (TMPCs) aim to address the limitations of traditional photovoltaic materials, thereby enhancing solar energy conversion efficiency [6]. Collectively, solar thermochemistry and

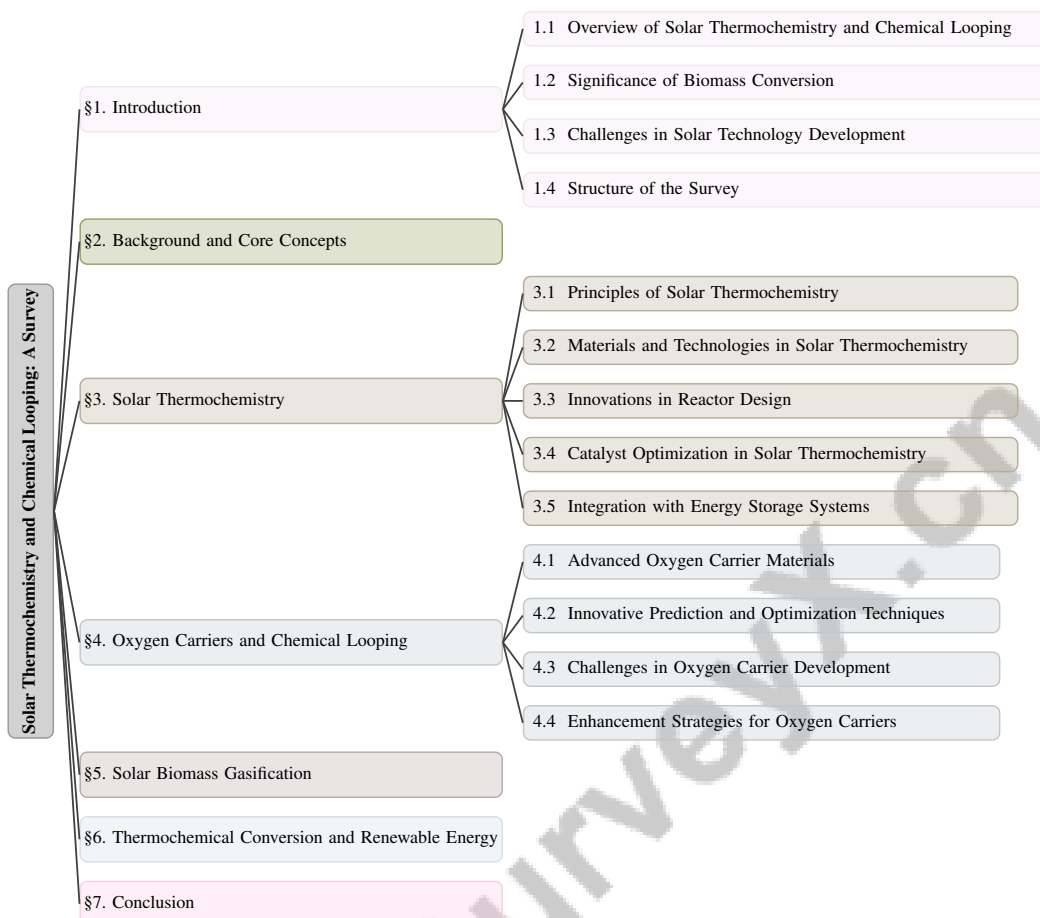


Figure 1: chapter structure

chemical looping not only facilitate sustainable energy production but also drive progress in material science and reactor design, leading to deeper discussions in subsequent sections.

1.2 Significance of Biomass Conversion

Biomass conversion into renewable energy via solar technologies is crucial for tackling the global energy crisis and climate change. As a renewable resource, biomass provides a sustainable alternative to fossil fuels, with solar-driven processes capable of converting it into syngas or other fuels, thereby significantly reducing carbon emissions. Recent advancements in solar thermochemical technologies exhibit high selectivity and efficiency in CO₂ conversion to fuels, closing the anthropogenic carbon cycle and supporting sustainable transportation fuel production [7, 4, 8, 9]. Integrating biomass-derived methane enhances syngas production while minimizing environmental impact, promoting a sustainable energy future.

The potential of bioenergy with carbon capture and storage (BECCS) is particularly significant for achieving negative CO₂ emissions and mitigating climate change [7]. However, challenges such as low mass conversion rates, poor selectivity, and low energy efficiency currently impede the industrial implementation of solar technologies for biomass conversion [9]. Addressing these challenges requires advancements in material design and reactor technologies, particularly in optimizing the band gap of perovskite oxides, which often exceed 3 eV, limiting their effectiveness for visible light absorption [6]. Moreover, integrating chemical looping combustion (CLC) with solar processes presents a promising avenue for clean energy production, as these systems inherently facilitate CO₂ capture, reducing costs [10].

Incorporating calcium looping (CaL) and CLC with concentrated solar power (CSP) systems enhances thermochemical energy storage, improving the efficiency and sustainability of biomass conversion

processes [5]. These advancements underscore the critical role of biomass conversion in transitioning to a sustainable energy future, leveraging solar technologies for efficient and eco-friendly renewable fuel production.

1.3 Challenges in Solar Technology Development

The development and implementation of solar technologies encounter significant challenges that hinder their widespread adoption. A primary obstacle is the high reduction temperature required for ceria, which complicates reactor design and limits hydrogen yield [1]. This is exacerbated by the ineffective conversion of gaseous fuels to CO₂ and H₂O in current methods, resulting in high emissions and inadequate CO₂ capture efficiency [10].

Additionally, the application of density functional theory with generalized gradient approximation (DFT-GGA) in evaluating TMOs presents challenges, as it often overestimates oxidation enthalpies and misrepresents electronic behavior, leading to incorrect ground-state configurations [3]. This highlights the necessity for more accurate computational methods to predict material properties in solar technologies.

Optimizing catalysts and understanding mechanistic pathways are critical for scaling industrial applications. While MAPs aim to address these issues, considerable work remains to optimize existing catalysts and develop scalable solutions [4]. Furthermore, the lack of experimental data on the spectral reflectance of materials like tungsten carbide (WC) limits the understanding of their optical properties and effectiveness as solar selective absorbers [2].

Energy efficiency and selectivity benchmarks also present challenges, as current benchmarks have limitations that new processes must overcome, such as achieving 100

Finally, integrating biofuels into existing chemical looping systems poses technical difficulties, necessitating efficient CO₂ capture methods and economic viability compared to traditional fossil fuel systems [7]. These challenges emphasize the need for ongoing research and innovation to advance solar technology development and implementation.

1.4 Structure of the Survey

This survey is meticulously organized to provide a comprehensive examination of solar thermochemistry and chemical looping, focusing on their applications in renewable energy production. The introductory section presents an overview of these technologies, discussing their significance in biomass conversion and highlighting challenges in solar technology development. Subsequent sections delve into background and core concepts, exploring principles and processes underlying solar thermochemistry, oxygen carriers, chemical looping, and biomass gasification.

The discussion transitions to solar thermochemistry, detailing advancements in reactor design, innovative materials, and technologies that enhance solar-driven process efficiency. It addresses strategies for optimizing catalysts and integrating these systems with energy storage solutions, essential for maximizing renewable energy effectiveness and enabling large-scale industrial applications. Recent research has shown high selectivity and conversion rates in solar thermochemical reactions, indicating significant potential for sustainable fuel production and carbon cycle closure [3, 5, 4, 9]. Following this, the role of oxygen carriers in chemical looping systems is examined, focusing on advanced materials, prediction and optimization techniques, and enhancement strategies.

The survey provides a thorough analysis of solar biomass gasification, elaborating on the conversion process that transforms biomass into syngas through solar energy utilization. It evaluates potential benefits such as reduced greenhouse gas emissions and sustainable energy production, alongside challenges in achieving efficient and scalable implementation within current technological advancements and industrial practices [7, 10, 11, 9, 4]. A broader context is provided through an exploration of thermochemical conversion technologies in renewable energy, emphasizing their contributions to sustainable energy production and potential impacts on carbon emission reduction.

The conclusion synthesizes the main insights presented throughout the paper, highlighting the transformative potential of solar thermochemistry and chemical looping technologies in enhancing renewable energy systems. It emphasizes the importance of these methods in addressing challenges such as carbon emissions and energy storage while proposing specific avenues for future research

aimed at optimizing efficiency, scalability, and integration with existing solar infrastructure. This forward-looking perspective underscores the necessity of developing pilot plants to validate and advance these promising technologies in real-world applications [5, 9]. The following sections are organized as shown in Figure 1.

2 Background and Core Concepts

2.1 Fundamentals of Solar Thermochemistry

Solar thermochemistry harnesses concentrated solar energy to drive chemical reactions, efficiently converting solar to chemical energy, pivotal for sustainable energy systems like solar thermochemical hydrogen generation (STCH) which produces hydrogen without greenhouse emissions [1]. Advances in compositionally complex perovskite oxides (CCPOs), such as $(\text{La}_{0.8}\text{Sr}_{0.2})(\text{Mn}_{(1-x)/3}\text{Fe}_{(1-x)/3}\text{Co}_x\text{Al}_{(1-x)/3})\text{O}_3$, optimize material properties for enhanced solar energy absorption and conversion [1].

Accurate electronic structure and oxidation energetics predictions for transition metal oxides (TMOs) are crucial for energy conversion improvements. The SCAN+U method refines these predictions by correcting self-interaction errors typical in conventional density functional theory (DFT), yielding a more accurate depiction of TMOs' electronic properties [3]. Significant strides in CO_2 photo(thermal)catalysis have led to the identification of key descriptors for catalyst optimization, achieving 100

Innovations in optical measurement systems, such as those quantifying the spectral reflectance of materials like tungsten carbide (WC), provide insights into solar selective absorbers' optical properties, informing solar thermochemical system design [2]. Integrating calcium looping (CaL) and chemical looping combustion (CLC) technologies within solar thermochemical systems enhances energy storage and minimizes carbon emissions [5]. Transition metal perovskite chalcogenides (TMPCs) offer tunable band gaps, expanding material options for solar thermochemical applications [6].

Recent innovations underscore solar thermochemistry's potential to advance renewable energy technologies. Efficient CO_2 splitting into carbon monoxide and oxygen paves the way for sustainable transportation fuel production, addressing the anthropogenic carbon cycle closure challenge. These developments, through advanced materials and modular reactor designs optimizing heat and mass transport, promise large-scale industrial applications, contributing significantly to a sustainable energy future [5, 4, 1, 9].

2.2 Oxygen Carriers and Chemical Looping

Oxygen carriers are crucial in chemical looping systems, enabling efficient combustion and gasification by transferring oxygen between fuel and air reactors. These systems are integral to chemical looping combustion (CLC) and chemical looping partial oxidation (CLPO), which are advanced technologies for energy conversion and CO_2 capture. Manganese-iron mixed oxides enhance combustion efficiency and CO_2 capture from coal combustion [10]. The performance of natural ores, including iron-, manganese-, copper-, and calcium-based ores, is explored as cost-effective alternatives to synthetic materials [12].

Natural ores' efficiency in CLC processes is critical, requiring competitiveness with synthetic alternatives in terms of reactivity, oxygen carrying capacity, and recyclability. Highly stable oxygen carriers are necessary for chemical looping water splitting systems, with doped Fe_2O_3 foams showing improved redox performance and sintering resistance [13]. In CLPO, engineering oxygen carriers for high reactivity and selectivity remains a challenge, as demonstrated by nanoscale iron oxide carriers achieving near 100

Understanding strain effects on perovskite materials' oxygen migration barriers is crucial for optimizing oxygen transport, impacting oxygen carriers' performance [14]. Integrating CaL with CLC technologies offers a novel framework for high-temperature thermochemical energy storage, enhancing renewable energy systems' efficiency [5]. A comprehensive framework categorizing chemical looping technologies by biofuel type and processes advances understanding and application

in sustainable energy production [7]. These advancements highlight oxygen carriers' critical role in chemical looping, offering pathways for efficient energy conversion and carbon capture.

2.3 Biomass Gasification and Renewable Energy

Biomass gasification is vital for converting biomass into renewable energy, offering a sustainable alternative to fossil fuels. This thermochemical conversion produces syngas—a versatile fuel of hydrogen, carbon monoxide, and methane—serving as an intermediate for electricity generation, liquid fuel production, and chemical synthesis. Its significance in renewable energy is amplified by advancements in solar thermochemical and chemical looping systems, enhancing syngas production efficiency and sustainability while reducing carbon emissions [8, 9].

Integrating solar energy into biomass gasification processes boosts efficiency and sustainability. Solar biomass gasification uses concentrated solar power for the high thermal energy needed for gasification, reducing fossil fuel reliance and carbon emissions. This approach supports sustainable fuel production, aligning with efforts to close the anthropogenic carbon cycle and mitigate climate change. Incorporating advanced solar technologies and materials, such as reticulated porous structures and CCPOs, enhances conversion rates and stability, paving the way for scalable industrial applications [5, 2, 1, 9, 4].

Advancements in gasification technologies are crucial for overcoming biomass conversion challenges, particularly low conversion efficiency and suboptimal syngas quality, which hinder effective biomass utilization as a renewable energy source. Enhanced methodologies, including chemical looping and solar thermochemical processes, show promise in improving conversion rates and syngas characteristics, facilitating sustainable biomass-to-energy pathways [7, 10, 9, 4, 8]. Innovations in reactor design and material development are essential for optimizing gasification, improving syngas yield and purity. Incorporating chemical looping techniques into biomass gasification enhances process efficiency and facilitates CO₂ capture, contributing to greenhouse gas emissions reduction.

Advanced materials, particularly transition metal oxides, significantly enhance selectivity and reactivity in gasification systems. Copper-doped iron-based carriers can increase methane conversion rates by up to 470

In recent years, solar thermochemistry has emerged as a pivotal area of research aimed at enhancing sustainable energy conversion. The hierarchical structure of this field can be effectively illustrated through Figure 2, which encompasses its fundamental principles, materials and technologies. This figure delineates the various innovations in reactor design, catalyst optimization, and the integration with energy storage systems. Each section of the figure highlights key components, methods, and applications that contribute significantly to the advancement of solar thermochemical processes. By examining these interconnected elements, we gain a comprehensive understanding of how solar thermochemistry can play a crucial role in the transition towards renewable energy solutions.

3 Solar Thermochemistry

3.1 Principles of Solar Thermochemistry

Solar thermochemistry utilizes concentrated solar energy to drive high-temperature chemical reactions, transforming solar energy into chemical forms that can be stored. The efficiency of these processes hinges on thermodynamic and kinetic factors, particularly the interplay between enthalpy and entropy during reduction and the kinetics of oxygen surface exchange, which are pivotal for enhancing hydrogen production in solar thermochemical hydrogen generation (STCH) systems [1].

As illustrated in Figure 3, the hierarchical structure of solar thermochemistry principles highlights the key efficiency factors, advanced materials, and applications. The efficiency factors, encompassing both thermodynamic and kinetic aspects, are essential for hydrogen production. Manipulating the electronic structures of transition metal oxides (TMOs) is fundamental to these reactions. The SCAN+U method offers improved accuracy over conventional density functional theory (DFT) by capturing complex electronic interactions within TMOs, crucial for optimizing their thermochemical properties in solar-driven reactions [3].

Advanced materials like tungsten carbide (WC) are integrated into solar thermochemical systems, supported by ab initio calculations that highlight their potential in solar energy absorption due to low-

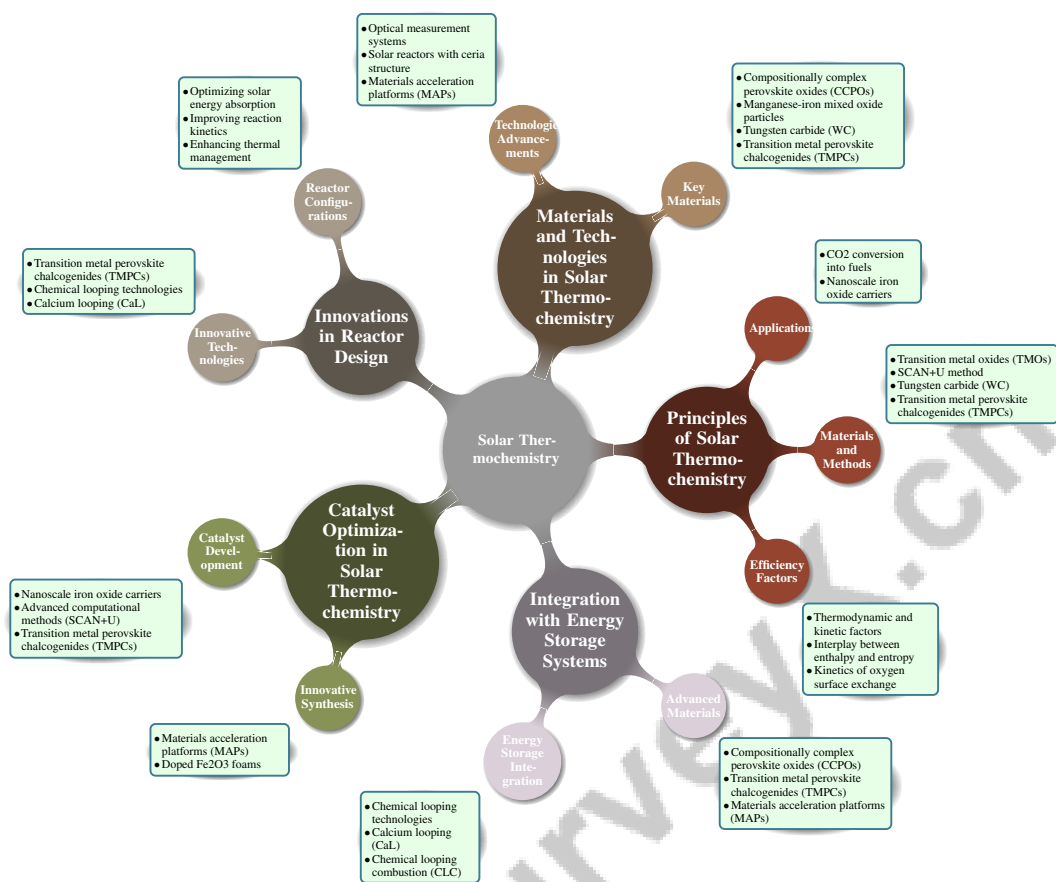


Figure 2: This figure illustrates the hierarchical structure of solar thermochemistry, encompassing its principles, materials and technologies, innovations in reactor design, catalyst optimization, and integration with energy storage systems. Each section highlights key components, methods, and applications that contribute to the advancement of solar thermochemical processes for sustainable energy conversion.

energy plasma excitation [2]. Transition metal perovskite chalcogenides (TMPCs), synthesized via the Catalytic Synthesis Procedure (CSP), enhance reactivity, with iodine optimizing solar thermochemical conversion processes [6].

Applications of solar thermochemistry focus on CO₂ conversion, hydrogen production, and methane oxidation, showcasing its transformative potential in addressing anthropogenic carbon cycle challenges without relying on water resources. This emphasizes the need for solar technologies that efficiently utilize CO₂ [9]. Nanoscale iron oxide carriers exemplify advancements in catalyst design, promoting Fe–O bond cleavage and enhancing CO formation, thereby improving solar thermochemical process efficiency [11]. These principles and innovations position solar thermochemistry as a transformative force in renewable energy technologies, paving the way for efficient and sustainable energy conversion.

3.2 Materials and Technologies in Solar Thermochemistry

Advancements in solar thermochemical applications are driven by the development of robust materials and innovative technologies for efficient solar-to-chemical energy conversion. Compositionally complex perovskite oxides (CCPOs) are pivotal, exhibiting enhanced structural stability during redox cycling and achieving high hydrogen yields without phase transformation, crucial for sustained STCH system performance [1].

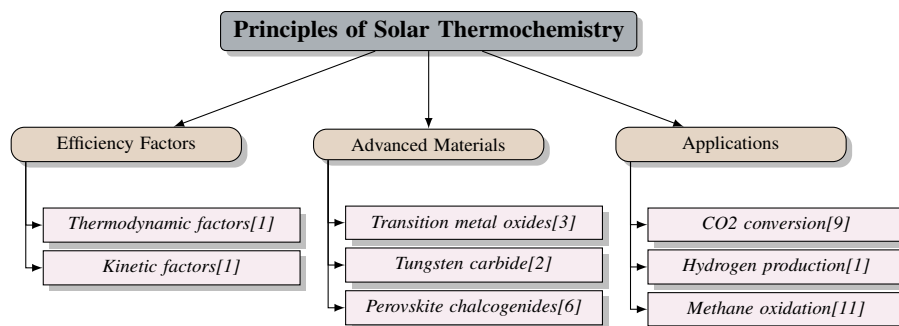


Figure 3: This figure illustrates the hierarchical structure of solar thermochemistry principles, highlighting the key efficiency factors, advanced materials, and applications. The efficiency factors include thermodynamic and kinetic aspects essential for hydrogen production. Advanced materials such as transition metal oxides, tungsten carbide, and perovskite chalcogenides play a crucial role in solar-driven reactions. Applications focus on CO₂ conversion, hydrogen production, and methane oxidation, showcasing the transformative potential of solar thermochemistry.

Manganese-iron mixed oxide particles, used as oxygen carriers in chemical looping combustion (CLC) processes, exemplify strategies to improve energy conversion efficiency, facilitating coal combustion and effective CO₂ capture [10].

The optical properties of materials are equally significant. An optical measurement system, comprising a light source, optical chopper, parabolic mirror, and spectrophotometer, precisely captures the reflectance spectrum of tungsten carbide (WC), providing insights into its effectiveness as a solar selective absorber and aiding in optimizing solar thermochemical reactors [2].

Transition metal perovskite chalcogenides (TMPCs) are promising due to their excellent optical properties and tunable band gaps, enhancing their applicability in photovoltaics and optoelectronics, thereby improving solar energy conversion efficiency [6].

Recent studies underscore transformative advancements in materials and technologies, particularly in converting CO₂ into sustainable fuels. A novel solar reactor utilizing a ceria structure has achieved impressive metrics, including 100

3.3 Innovations in Reactor Design

Innovations in reactor design for solar thermochemical processes are crucial for enhancing renewable energy systems' efficiency and scalability. Advanced reactor configurations aim to optimize solar energy absorption, reaction kinetics, and thermal management, thus improving the overall performance of solar-driven chemical reactions. Materials acceleration platforms (MAPs) facilitate the rapid discovery and optimization of materials for heterogeneous CO₂ photo(thermal)catalysis, enabling systematic exploration of material properties and reaction conditions that lead to efficient solar energy conversion [4].

Incorporating innovative materials, such as transition metal perovskite chalcogenides (TMPCs), into reactor designs addresses traditional photovoltaic materials' limitations. TMPCs, with tunable band gaps and enhanced optical properties, facilitate efficient light absorption and conversion, boosting reactor efficiency [6].

Advanced optical measurement systems that capture the spectral reflectance of materials like tungsten carbide (WC) provide critical insights into reactor components' optical properties, essential for optimizing solar selective absorbers and maximizing efficiency in solar thermochemical processes [2].

Exploring reactor designs incorporating chemical looping technologies, such as calcium looping (CaL), represents significant innovation. These systems enhance thermochemical energy storage capabilities through reversible redox reactions, enabling efficient energy conversion and storage while minimizing carbon emissions. Integrating CaL with chemical looping combustion (CLC) technologies supports developing high-temperature thermochemical energy storage solutions, contributing to sustainable energy systems [5].

Recent advancements in reactor design underscore solar thermochemistry's transformative potential in renewable energy technologies, particularly in the efficient solar-driven thermochemical splitting of CO₂ into carbon monoxide and oxygen. This innovative approach achieves remarkable selectivity and energy efficiency, addressing critical challenges in carbon cycle closure and sustainable fuel production, paving the way for large-scale industrial applications integrated with existing solar infrastructure [5, 1, 9, 3, 4]. By leveraging cutting-edge materials and technologies, researchers advance more efficient and scalable solar-driven processes, offering new pathways for sustainable energy production.

3.4 Catalyst Optimization in Solar Thermochemistry

Catalyst optimization is crucial for enhancing solar thermochemical reactions' efficiency and selectivity. Effective catalysts are essential for facilitating high-temperature reactions driven by concentrated solar energy, thereby improving solar thermochemical system performance. Nanoscale iron oxide carriers significantly promote Fe–O bond cleavage due to low-coordination lattice oxygen atoms on nanoparticle surfaces, optimizing the solar thermochemical conversion process by enhancing CO formation [11].

Advanced computational methods, such as the SCAN+U approach, accurately predict the electronic structures and oxidation energetics of TMOs used as catalysts. This method mitigates self-interaction errors common in conventional DFT calculations, providing a reliable description of TMOs' electronic properties, essential for optimizing their thermochemical properties and catalytic performance in solar-driven reactions [3].

Exploring transition metal perovskite chalcogenides (TMPCs) offers new avenues for catalyst optimization. These materials exhibit tunable band gaps and excellent optical properties, making them promising candidates for solar thermochemical applications. Adjusting the band gap of TMPCs enhances light absorption and conversion, improving catalytic process efficiency [6].

Materials acceleration platforms (MAPs) support catalyst optimization by enabling rapid discovery and refinement of materials for heterogeneous CO₂ photo(thermal)catalysis. These platforms utilize automation and artificial intelligence to systematically investigate material properties and optimize reaction conditions, facilitating the design of highly efficient catalysts for thermochemical CO₂ splitting into CO and O₂. This process achieves near 100

Innovations in catalyst synthesis and fabrication, such as doped Fe₂O₃ foams produced through freeze-casting, exhibit improved redox performance and resistance to sintering. These advancements are crucial for maintaining catalyst stability and activity over extended operational periods, ensuring the long-term viability of solar thermochemical processes [13].

Strategies for optimizing catalysts in solar thermochemistry highlight this technology's transformative potential in renewable energy. By enabling efficient and sustainable energy conversion, these advancements pave the way for developing advanced catalytic materials capable of converting CO₂ into valuable fuels, addressing key carbon management challenges, and contributing to sustainable transportation fuel production globally. Recent studies demonstrate significant improvements in selectivity and efficiency, with solar-driven thermochemical processes achieving 100

3.5 Integration with Energy Storage Systems

Integrating solar thermochemistry with energy storage systems is essential for enhancing renewable energy efficiency and reliability. Solar thermochemical processes inherently allow for energy storage by converting solar energy into chemical energy, which can be stored and released on demand. This capability mitigates the intermittent nature of solar energy, providing stable energy supplies and enhancing grid reliability while facilitating the integration of renewable sources into the energy mix. Advancements in technologies such as chemical looping and thermochemical processes further improve the efficiency and sustainability of energy systems [5, 6, 9].

A promising approach to achieving this integration is through chemical looping technologies, such as calcium looping (CaL) and chemical looping combustion (CLC). These systems enable high-temperature thermochemical energy storage by utilizing reversible redox reactions to store solar energy in chemical bonds, which can be released through controlled oxidation reactions, facilitating continuous electricity or hydrogen fuel generation [5].

Advanced materials, particularly CCPOs and TMPCs, are vital for enhancing the integration of solar thermochemical processes with energy storage systems. CCPOs, such as $(\text{La}_{0.8}\text{Sr}_{0.2})(\text{Mn}_{0.2}\text{Fe}_{0.2}\text{Co}_{0.4}\text{Al}_{0.2})\text{O}_3$ -, demonstrate remarkable stability and efficiency in solar thermochemical hydrogen generation, achieving significant hydrogen yields through optimized redox properties and high cycle stability. Meanwhile, TMPCs exhibit tunable band gaps and high absorption coefficients, making them suitable for solar energy conversion applications. Combining these advanced materials improves the thermodynamic and kinetic performance of solar thermochemical systems and facilitates innovative energy storage solutions, contributing to a more sustainable energy landscape [5, 1, 3, 6, 4]. These materials exhibit excellent thermal stability and redox properties, enabling efficient energy conversion and storage during solar thermochemical cycles.

Moreover, developing materials acceleration platforms (MAPs) supports the rapid discovery and optimization of materials for energy storage applications. These platforms facilitate the systematic exploration of material properties and reaction conditions, leading to the design of systems that effectively integrate solar thermochemistry with energy storage technologies [4].

Integrating solar thermochemistry with energy storage systems also benefits from innovations in reactor design that enhance solar energy absorption and conversion efficiency. Advanced optical measurement systems provide valuable insights into the optical properties of materials used in solar reactors, aiding in optimizing solar selective absorbers and improving overall solar thermochemical process performance [2].

These advancements collectively underscore the potential of integrating solar thermochemistry with energy storage systems to revolutionize renewable energy technologies. By utilizing advanced materials and innovative technologies, researchers significantly enhance the efficiency and scalability of solar-driven processes, such as the solar thermochemical splitting of CO_2 into carbon monoxide and oxygen with remarkable selectivity and energy efficiency. This progress addresses challenges of low conversion rates and selectivity in current methods while opening new avenues for sustainable transportation fuel production, promoting a closed anthropogenic carbon cycle and eco-friendly energy solutions on a global scale [4, 9].

4 Oxygen Carriers and Chemical Looping

4.1 Advanced Oxygen Carrier Materials

Method Name	Material Composition	Performance Enhancement	Technological Integration
Cu-Fe ₂ O ₃ [8]	Iron-based Oxides	Copper Doping	Advanced Fabrication Techniques
SCAN+U[3]	Ce-, Mn-, Fe-oxides	Improved Accuracy Predictions	-
DMEPS[14]	Labo3 Perovskites	Strain Engineering	Density Functional Theory
DF2F[13]	Doped Fe ₂ O ₃	Redox Performance	Freeze-casting Process
Fe ₂ O ₃ @SBA-15[11]	Iron Oxide Nanoparticles	Nanoscale Iron Oxide	Advanced Fabrication Techniques

Table 1: Summary of recent advancements in the design and integration of oxygen carrier materials for chemical looping applications. The table highlights various methods, material compositions, performance enhancements, and technological integrations employed to improve reactivity, stability, and efficiency in energy conversion processes.

The advancement of oxygen carrier materials is essential for improving the efficiency of chemical looping systems, as these materials facilitate oxygen transfer between reactors, enabling effective combustion and gasification. Recent developments have focused on refining nanoscaled iron-based oxygen carriers for heterogeneous CO_2 photo(thermal)catalysis and methane partial oxidation, enhancing their reactivity, stability, and mechanical properties to achieve near 100% CO selectivity while minimizing CO_2 co-production. The integration of automation and artificial intelligence in material design accelerates the discovery of sustainable solutions for solar chemical and fuel generation, addressing climate change challenges [4, 11]. Table 1 presents a comprehensive overview of innovative methods and material compositions that have been developed to enhance the performance and integration of oxygen carrier materials in chemical looping systems.

Innovations such as manganese-iron mixed oxides with optimized molar ratios have improved both reactivity and mechanical strength, overcoming limitations of earlier materials [10]. Additionally, incorporating small amounts of copper into iron-based carriers has been shown to enhance methane

conversion rates, demonstrating the potential for material composition tailoring without compromising performance [8].

The SCAN+U method has significantly advanced the design of oxygen carriers by accurately predicting the oxidation energetics and electronic structures of transition metal oxides (TMOs), enabling the development of materials optimized for solar thermochemical applications [3]. Understanding strain effects on oxygen migration barriers in perovskites has also provided insights into enhancing oxygen mobility, crucial for efficient chemical looping processes [14].

Innovative fabrication techniques, such as producing doped Fe_2O_3 foams with interconnected pore structures, have demonstrated improved stability and redox performance, reducing sintering issues common in high-temperature applications and extending the operational lifespan of oxygen carriers [13]. Moreover, utilizing nanoscale iron oxide carriers embedded in mesoporous silica allows for lower reaction temperatures and enhanced CO production, offering a more efficient pathway for chemical looping compared to traditional methods [11].

The development of advanced oxygen carrier materials is crucial for enhancing chemical looping systems, facilitating efficient energy conversion and carbon capture. Innovations in material design, particularly through materials acceleration platforms (MAPs) in heterogeneous CO_2 photo(thermal)catalysis and solar thermochemical processes, highlight the potential for improved CO_2 conversion into sustainable fuels, contributing to the goals of renewable energy production and addressing climate change challenges [5, 4, 9].

4.2 Innovative Prediction and Optimization Techniques

Predicting and optimizing oxygen carrier performance in chemical looping systems is vital for enhancing efficiency and scalability. Advanced computational methods, such as the SCAN+U approach, provide accurate predictions of the electronic structures and oxidation energetics of transition metal oxides (TMOs), addressing self-interaction errors common in conventional density functional theory (DFT) calculations and enabling the design of optimized oxygen carriers [3].

Research on strain effects on oxygen migration barriers in perovskites has revealed how applied strain can enhance oxygen mobility, essential for developing materials with improved transport capabilities in chemical looping processes [14]. Materials acceleration platforms (MAPs) facilitate rapid discovery and optimization of materials by systematically exploring properties and reaction conditions, leading to the design of oxygen carriers that enhance oxidation-reduction cycles and overall system efficiency [4].

Furthermore, advanced fabrication techniques, such as producing doped Fe_2O_3 foams with interconnected pore structures, have shown improved redox performance and stability, addressing sintering challenges and extending the operational lifespan of oxygen carriers [13]. The innovative prediction and optimization techniques for iron-based oxygen carriers are essential for achieving near 100% CO selectivity during methane partial oxidation at lower operating temperatures, thereby reducing energy consumption and CO_2 co-production [12, 11, 8]. By leveraging cutting-edge computational methods and fabrication techniques, researchers are paving the way for more efficient and scalable chemical looping processes, contributing to sustainable and eco-friendly energy production.

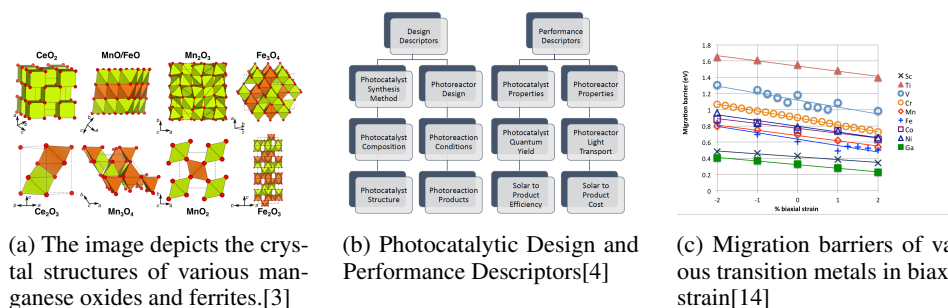


Figure 4: Examples of Innovative Prediction and Optimization Techniques

As illustrated in Figure 4, understanding the intricacies of oxygen carriers and chemical looping processes is essential for advancing sustainable energy solutions. The provided examples of innovative prediction and optimization techniques enhance the efficiency of these processes. The crystal structures of various manganese oxides and ferrites are fundamental for understanding oxygen carrier behavior. The hierarchical structure of photocatalytic design and performance descriptors emphasizes the systematic approach required for optimizing photocatalytic systems, highlighting the importance of design and performance metrics. Additionally, the scatter plot of migration barriers for transition metals under biaxial strain underscores the critical role of strain engineering in optimizing material properties for chemical looping applications. Collectively, these visualizations and descriptors serve as a comprehensive guide to the innovative techniques employed in oxygen carrier prediction and optimization, paving the way for more efficient and sustainable chemical processes [3, 4, 14].

4.3 Challenges in Oxygen Carrier Development

Developing effective oxygen carriers for chemical looping systems presents several challenges that hinder their application and efficiency. A primary concern is the mechanical strength and reactivity of these carriers, which are vital for achieving high combustion efficiencies and CO₂ capture rates. While manganese-iron mixed oxides have shown improvements in these areas, optimizing these properties remains a significant challenge [10].

Stability and reactivity of natural ores used as oxygen carriers in chemical looping combustion (CLC) systems present another critical issue. These ores, including iron-based and calcium-based types, often demonstrate performance variability under different operational conditions, limiting their long-term effectiveness [12]. Balancing reactivity and cost poses substantial hurdles; noble metal dopants can enhance reactivity but introduce significant expenses and potential carbon deposition issues, complicating cost-effectiveness [8].

The impact of strain on oxygen migration barriers in perovskite materials is another area where existing methods fall short. Current approaches inadequately quantify these effects, hindering advancements in designing materials with efficient oxygen transport capabilities [14]. Additionally, sintering of materials used in oxygen carriers leads to reduced pore size and increased densification, hampering efficiency, particularly in hydrogen production, by diminishing the reactive surface area [13].

Achieving high CO selectivity while minimizing CO₂ generation remains a formidable challenge in syngas production, as the chemical stability of CO₂ complicates its reduction, making it difficult to attain desired selectivity and efficiency in chemical looping applications [11].

Addressing these challenges requires ongoing research and innovation in material design, advanced fabrication techniques, and sophisticated computational modeling. Efforts should focus on creating highly efficient oxygen carriers, such as nanoscaled iron-based carriers with near 100% CO selectivity in methane partial oxidation, and exploring novel approaches like solar-driven thermochemical CO₂ splitting, which has shown impressive selectivity and energy efficiency. Utilizing materials acceleration platforms (MAPs) that integrate automation and artificial intelligence can significantly expedite the discovery and optimization of these materials, supporting the transition to sustainable energy solutions [9, 4, 11].

4.4 Enhancement Strategies for Oxygen Carriers

Enhancing the performance of oxygen carriers in chemical looping systems is crucial for advancing sustainable energy technologies. Utilizing natural ores as oxygen carriers offers significant cost advantages due to minimal processing requirements, making them a sustainable option for chemical looping combustion (CLC). However, their limitations, including lower fuel conversion efficiencies, necessitate further optimization [12].

The development of cost-effective, high-performance oxygen carriers can be achieved through the use of non-noble metals, which reduce material costs and enhance catalytic performance at lower operational temperatures, improving overall chemical looping efficiency [8]. This strategy is particularly beneficial in overcoming economic barriers to deploying chemical looping technologies on an industrial scale.

Advanced fabrication techniques, such as incorporating dopants into oxygen carrier materials, present another viable enhancement strategy. Research indicates that optimizing doping levels and exploring additional dopants can significantly improve performance and stability, addressing common issues like sintering and degradation, thereby extending the operational lifespan of carriers [13].

Recent studies on oxygen carriers emphasize the critical need for ongoing research and innovation, including the use of nanoscaled iron-based carriers and natural ores, to achieve near 100% CO selectivity in methane partial oxidation. Exploring cost-effective alternatives that enhance carbon capture efficiency and reduce energy consumption in chemical looping processes is essential [12, 11]. By leveraging natural ores, non-noble metals, and advanced doping techniques, researchers can pave the way for more efficient and cost-effective chemical looping systems, contributing to the broader goals of sustainable and renewable energy production.

5 Solar Biomass Gasification

5.1 Principles of Solar Biomass Gasification

Solar biomass gasification leverages concentrated solar energy to convert biomass into syngas, composed mainly of hydrogen, carbon monoxide, and methane. This process is rooted in thermochemical principles, utilizing solar energy as the thermal source for endothermic reactions. Recent advancements, such as thermochemical CO₂ splitting into carbon monoxide and oxygen, underscore the potential of solar-driven technologies. Solar reactors with reticulated porous ceria structures demonstrate high selectivity and efficiency in syngas production, promoting sustainable fuel generation and aiding the closure of the anthropogenic carbon cycle [4, 9].

The gasification process involves the controlled partial oxidation of biomass within a reactor, regulated by the precise supply of oxygen or steam. This not only facilitates syngas production but also enhances the efficiency of subsequent chemical reactions for sustainable fuels and chemicals. Optimizing reactor conditions, such as temperature and pressure, is crucial for maximizing syngas yield and minimizing byproducts, contributing to cleaner energy solutions [10, 11, 9]. Concentrated solar energy serves as the primary heat source, enabling reactions at elevated temperatures (700°C to 1000°C), essential for decomposing complex organic structures into simpler gaseous components.

Improving the efficiency of solar biomass gasification depends on optimizing reactor materials and design. Tungsten carbide (WC) emerges as a promising solar selective absorber due to its spectral reflectance, which effectively captures and converts solar energy, enhancing thermal efficiency [2]. Additionally, catalysts play a crucial role in boosting conversion efficiency and selectivity. For instance, doping iron oxide (Fe₂O₃) with 1

The principles of solar biomass gasification illustrate the integration of solar energy with advanced materials and catalytic strategies to achieve efficient and sustainable biomass conversion into renewable fuels. This innovative process significantly reduces carbon emissions by transforming CO₂ into valuable fuels through solar-driven thermochemical methods. It aligns with global sustainable energy objectives, providing an efficient and scalable alternative to fossil fuels and facilitating the transition to renewable energy sources [7, 4, 9].

6 Thermochemical Conversion and Renewable Energy

6.1 Role of Thermochemical Conversion in Sustainable Energy

Thermochemical conversion processes are essential for transforming renewable resources into usable fuels, contributing significantly to sustainable energy advancement. Techniques like solar thermochemical CO₂ splitting and chemical looping not only enhance fuel production efficiency but also play a crucial role in reducing carbon emissions, aligning with renewable energy objectives [9]. Solar thermochemical CO₂ splitting is particularly effective in producing sustainable fuels while minimizing water dependency, thereby closing the anthropogenic carbon cycle.

Chemical looping technologies, enhanced by biofuels, are pivotal for achieving negative CO₂ emissions, offering substantial climate change mitigation potential [7]. The use of manganese-iron mixed oxides in chemical looping combustion systems has shown high combustion efficiencies and effective CO₂ capture, presenting a promising option for coal utilization [10]. These advancements highlight

chemical looping's role in enhancing energy system sustainability through efficient carbon capture and storage.

Natural ores as oxygen carriers in chemical looping systems offer a cost-effective and sustainable alternative, despite generally lower performance compared to synthetic options. They have demonstrated potential in syngas and coal combustion [12]. Iron-based oxygen carriers, improved through copper doping, have enhanced reactivity and conversion rates, reducing operational temperatures and saving energy [8].

Advanced materials, such as transition metal perovskite chalcogenides (TMPCs), optimize thermochemical conversion processes due to their tunable band gaps and high absorption coefficients, enhancing solar energy applications [6]. Materials acceleration platforms (MAPs) are promising for accelerating discoveries in CO₂ photo(thermal)catalysis, steering the catalytic industry towards sustainability [4]. Notably, Fe₂O₃@SBA-15 in chemical looping methane partial oxidation achieves near 100

6.2 Advancements in Material Design and Performance

Recent advances in material design have significantly improved thermochemical conversion processes' efficiency and sustainability. Enhancing materials for solar thermochemical and chemical looping systems is crucial for optimizing energy conversion and integrating these technologies with renewable sources. This includes developing mixed oxide carriers for increased reactivity and recyclability, and exploring sorbent stabilizers to maintain CO₂ carrying capacity in calcium looping. Integrating these systems with solar heating reduces fossil fuel reliance during material regeneration, contributing to sustainable energy solutions [5, 4, 8, 9].

Tungsten carbide (WC) has emerged as a promising solar selective absorber due to its unique optical properties. Future research aims to improve sintering processes to enhance optical performance and solar energy absorption [2]. In chemical looping, natural ores like ilmenite are gaining attention for their mechanical strength and stability, offering viable alternatives to synthetic oxygen carriers [12]. The influence of strain on oxygen migration barriers in perovskites has been extensively studied, revealing significant enhancements in oxygen mobility, crucial for efficient chemical looping processes [14].

These advancements in material design and performance highlight the potential for ongoing improvements in thermochemical conversion technologies. By leveraging advanced materials and enhancing their functional properties, researchers are significantly increasing the efficiency and sustainability of energy conversion processes, vital for developing innovative technologies such as solar thermochemical CO₂ splitting and optimizing chemical looping systems for methane conversion. These developments are essential for advancing renewable energy production and reducing global greenhouse gas emissions [5, 4, 8, 9].

6.3 Integration with Renewable Energy Sources

Integrating thermochemical conversion technologies, such as solar-driven CO₂ splitting and chemical looping, with renewable energy sources like biomass and solar heating, represents a promising strategy for establishing a sustainable and resilient energy system. This integration facilitates the production of sustainable fuels and chemicals, closing the anthropogenic carbon cycle, enhancing energy storage capabilities, and reducing greenhouse gas emissions, thereby promoting a balanced and efficient energy grid [5, 7, 9, 4, 8]. Technologies like solar thermochemistry and chemical looping can complement and improve the efficiency of existing renewable energy systems, including wind, solar photovoltaics, and bioenergy.

Developing advanced materials and technologies that efficiently harness and convert renewable energy into chemical fuels is key to this integration. The SCAN+U method, which evaluates the electronic structures and oxidation energetics of transition metal oxides (TMOs), shows significant potential for optimizing materials in these processes. Future research should focus on benchmarking this method for various TMOs and exploring its application to other materials, including sulfides, to enhance thermochemical conversion technology performance and scalability [3].

Incorporating AI and automation in experimental setups, particularly within MAPs, represents another promising avenue for advancing the integration of thermochemical conversion technologies with

renewable energy sources. By minimizing physical movements in MAPs, researchers can accelerate material discovery and optimization, enhancing the efficiency and scalability of these technologies [4]. Additionally, optimizing reactor designs and exploring new materials for oxygen carriers are critical for successfully integrating chemical looping technologies with other renewable energy sources. Conducting pilot-scale tests to validate these technologies in real-world applications will be essential for demonstrating their viability and potential impact on the renewable energy landscape [7].

Through the continued development and integration of thermochemical conversion technologies with renewable energy sources, researchers can pave the way for a sustainable and efficient energy system. This innovative approach significantly enhances the performance and reliability of renewable energy systems by enabling efficient solar-driven thermochemical processes, such as converting CO₂ into sustainable fuels. Furthermore, it aligns with global initiatives aimed at reducing carbon emissions and promoting energy sustainability, facilitating the transition to a cleaner energy future. By leveraging advanced technologies like chemical looping and materials acceleration platforms, this strategy enhances energy efficiency and supports scalable solutions for mitigating climate change and achieving long-term environmental goals [5, 7, 9, 4, 8].

7 Conclusion

7.1 Future Research Directions

Advancing solar thermochemistry and chemical looping necessitates a comprehensive approach to refining materials, processes, and technologies. Enhancing solar thermochemical hydrogen generation (STCH) hinges on optimizing the cobalt content in compositionally complex perovskite oxides (CCPOs) and exploring non-equimolar compositions. Such refinements aim to boost performance and efficiency. In parallel, the calcination process of oxygen carriers must be optimized to balance mechanical strength with reactivity, particularly in their interactions with coal ash during extended operations.

Investigating the effects of strain on material properties remains pivotal. Future studies should delve into how strain impacts material characteristics, the role of doping in influencing strain responses, and strategies to maintain effective strain in practical applications. Additionally, exploring alternative materials and configurations could elevate solar reactor performance, fostering more sustainable energy conversion systems.

In chemical looping technologies, optimizing materials and processes is crucial. Pilot-scale tests and the examination of mixed metal oxides can enhance performance and reduce costs, promoting wider adoption in renewable energy systems. In optoelectronics, refining the synthesis of transition metal perovskite chalcogenides (TMPCs), investigating new compositions, and conducting detailed studies on device performance could unlock their potential for next-generation applications.

Finally, deepening the understanding of mechanistic pathways in CO production and refining the synthesis of metal oxides used in chemical looping could markedly improve the efficiency and selectivity of these processes. Addressing these research areas is essential for propelling solar thermochemistry and chemical looping forward, providing sustainable solutions for energy production and carbon emission reduction.

References

- [1] Dawei Zhang, Hector A. De Santiago, Boyuan Xu, Cijie Liu, Jamie Trindell, Wei Li, Jiyun Park, Mark A. Rodriguez, Eric N. Coker, Josh Sugar, Anthony McDaniel, Stephan Lany, Liang Ma, Yi Wang, Gregory Collins, Hanchen Tian, Wenyan Li, Yue Qi, Xingbo Liu, and Jian Luo. Compositionally complex perovskite oxides for solar thermochemical water splitting, 2022.
- [2] Toshiharu Chono, Hisashi Tokutomi, Kazuma Nakamura, and Koji Miyazaki. Reflectance spectral studies of spark plasma sintered tungsten carbide pellet, 2024.
- [3] Gopalakrishnan Sai Gautam and Emily A Carter. Evaluating transition metal oxides within dft-scan and scan+ u frameworks for solar thermochemical applications. *Physical Review Materials*, 2(9):095401, 2018.
- [4] Andrew Wang, Carlota Bozal-Ginesta, Sai Govind Hari Kumar, Alán Aspuru-Guzik, and Geoffrey A. Ozin. Designing materials acceleration platforms for heterogeneous co2 photo(thermal)catalysis, 2023.
- [5] Yongliang Yan, Ke Wang, Peter T Clough, and Edward J Anthony. Developments in calcium/chemical looping and metal oxide redox cycles for high-temperature thermochemical energy storage: A review. *Fuel Processing Technology*, 199:106280, 2020.
- [6] Shanyuan Niu, Huaixun Huan, Yang Liu, Matthew Yeung, Kevin Ye, Louis Blankemeier, Thomas Orvis, Debarghya Sarkar, David J. Singh, Rehan Kapadia, and Jayakanth Ravichandran. Band-gap control via structural and chemical tuning of transition metal perovskite chalcogenides, 2018.
- [7] Submitted accepted and published.
- [8] Lang Qin, Mengqing Guo, Yan Liu, Zhuo Cheng, Jonathan A Fan, and Liang-Shih Fan. Enhanced methane conversion in chemical looping partial oxidation systems using a copper doping modification. *Applied Catalysis B: Environmental*, 235:143–149, 2018.
- [9] Energy environmental science.
- [10] Raúl Pérez-Vega, Alberto Abad, Francisco García-Labiano, Pilar Gayán, Luis F de Diego, María Teresa Izquierdo, and Juan Adán. Chemical looping combustion of gaseous and solid fuels with manganese-iron mixed oxide as oxygen carrier. *Energy Conversion and Management*, 159:221–231, 2018.
- [11] Yan Liu, Lang Qin, Zhuo Cheng, Josh W Goetze, Fanhe Kong, Jonathan A Fan, and Liang-Shih Fan. Near 100% co selectivity in nanoscaled iron-based oxygen carriers for chemical looping methane partial oxidation. *Nature communications*, 10(1):5503, 2019.
- [12] Michael Matzen, Jessica Pinkerton, Xiaomeng Wang, and Yaşar Demirel. Use of natural ores as oxygen carriers in chemical looping combustion: A review. *International Journal of Greenhouse Gas Control*, 65:1–14, 2017.
- [13] P. J. Lloreda-Jurado, Jesus Hernandez-Saz, E. Chicardi, A. Paul, and R. Sepulveda. Pore morphology evolution and atom distribution of doped fe2o3 foams developed by freeze-casting after redox cycling, 2020.
- [14] Tam Mayeshiba and Dane Morgan. Strain effects on oxygen migration in perovskites, 2016.

Disclaimer:

SurveyX is an AI-powered system designed to automate the generation of surveys. While it aims to produce high-quality, coherent, and comprehensive surveys with accurate citations, the final output is derived from the AI's synthesis of pre-processed materials, which may contain limitations or inaccuracies. As such, the generated content should not be used for academic publication or formal submissions and must be independently reviewed and verified. The developers of SurveyX do not assume responsibility for any errors or consequences arising from the use of the generated surveys.

www.SurveyX.cn