Fundamentals and Regulation of Energy Chemical Conversion: Postprint

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Abstract

Energy constitutes a critical foundation for the survival and development of nations and human society, occupying a strategically paramount position in national defense and economic construction. In recent decades, propelled by rapid economic development and surging energy demand, China has emerged as the world' s largest energy producer and consumer, ranking as the second-largest petroleum importer and consumer globally after the United States. The distinctive energy structure of China—characterized by abundant coal reserves, scarce natural gas, and limited oil resources—combined with relatively low energy utilization efficiency, has exerted substantial pressure on sustainable socioeconomic development and environmental conservation. Addressing these challenges hinges substantially upon the advancement of efficient, environmentally benign energy utilization technologies and the development of novel clean energy sources.

Full Text

Preamble

Strategic Priority Research Program (Category B) of the Chinese Academy of Sciences
ChinaXiv Partner Journal: Fundamentals and Regulation of Energy Chemical Conversion

1. Background and Significance

Energy represents a critical foundation for national security and the survival and development of human society, holding a particularly important strategic position in national defense and economic construction. In recent decades, China' s rapid economic growth has led to a surge in energy demand, making it the world' s largest energy producer and consumer, as well as the second-largest petroleum importer and consumer after the United States. China' s unique energy structure—characterized by abundant coal but scarce natural gas and oil—combined with relatively low energy utilization efficiency, has placed enormous pressure on sustainable socioeconomic development and environmental protection. Addressing these challenges depends largely on developing efficient, environmentally friendly energy utilization technologies and exploring new clean energy sources.

Chemistry plays an indispensable role in energy development and utilization, as most energy conversion processes essentially involve transformations between different forms of energy and matter. These conversions between energy and various chemical substances are achieved directly or indirectly through chemical reactions. Energy chemical conversion primarily involves thermal, photochemical, and electrochemical reactions. Therefore, detailed investigations into the dynamic processes and control mechanisms of these important chemical reactions will greatly advance efficient energy conversion technologies and clean energy development. These energy chemical conversion processes occur at material surfaces and interfaces, encompassing crucial scientific questions about chemical reaction dynamics. Driven by heat, light, and electricity—either individually or in combination—these processes present major scientific frontiers for the future development of chemistry: understanding their kinetic principles and achieving better control over energy chemical conversion.

Revealing the dynamic mechanisms of relevant chemical reactions at the atomic and molecular level is key to understanding energy chemical conversion processes and forms the basis for selective regulation of these transformations. Under realistic conditions of combustion, heterogeneous catalysis, and photocatalysis, fundamental questions remain regarding how chemical reactions occur and how catalyst surface/interface structures and active sites evolve dynamically. These questions represent the core focus of this special program. Breakthroughs in addressing these cutting-edge challenges will undoubtedly facilitate the development of new energy conversion processes and help resolve energy and environmental issues facing sustainable economic development.

The Strategic Priority Research Program (Category B) of the Chinese Academy of Sciences, titled "Fundamentals and Regulation of Energy Chemical Conversion,"aims to address major scientific questions and technical challenges in China' s energy chemical conversion processes. The program will develop experimental techniques and methods based on advanced light sources (including extreme ultraviolet free-electron lasers and synchrotron radiation facilities) to achieve high-sensitivity, in-situ dynamic detection of chemical reactions in energy conversion processes. Simultaneously, it will develop new theoretical methods and models to study the dynamic nature of energy conversion chemical reactions at both the microscopic atomic/molecular level and the macroscopic statistical level. Through close integration of theory and experiment, the program will reveal fundamental principles and mechanisms governing three important energy chemical conversion processes—combustion, heterogeneous catalysis, and photocatalysis—and achieve dynamic regulation of these processes by leveraging cutting-edge high technologies. These three processes hold significant scientific importance for chemical science development in energy conversion: combustion chemistry primarily involves gas-phase reactions, while heterogeneous catalysis and photocatalysis feature chemical reactions mainly occurring at material surfaces and interfaces.

Over the next five years, this program will elevate China' s energy basic research to an internationally advanced level, create a world-class energy research platform, and make important contributions to solving fundamental scientific and technical problems in China' s energy sector.

2. Research Content

Based on China' s actual energy needs and targeting major scientific questions in energy chemical conversion, this program will develop experimental techniques founded on a new-generation extreme ultraviolet laser source, create new theoretical methods and models, and achieve dynamic regulation of energy chemical conversion processes through tight integration of theoretical simulation and experimentation. To accomplish these overall objectives, the program has established three research projects.

(1) Combustion Chemistry and Chemical Laser Dynamics

Combustion is fundamentally a gas-phase chemical process, with chemical reactions being the primary controlling factor. Therefore, improving combustion efficiency requires understanding and regulating the nature of chemical conversion. This project will develop high-sensitivity, in-situ dynamic measurement techniques based on a new-generation extreme ultraviolet laser source, combined with Rydberg-state hydrogen atom time-of-flight spectroscopy and ion slice imaging. The research will investigate elementary reaction kinetics relevant to combustion and chemical lasers, enable in-situ dynamic measurements of important combustion systems, and develop combustion and quantum-state particle beam control technologies. A key objective is to control the population of single quantum states in HF chemical lasers to achieve high-power output from HF single-quantum chemical lasers operating in the atmospheric window. The participating institutions are the Dalian Institute of Chemical Physics, Chinese Academy of Sciences, and the University of Science and Technology of China.

(2) Surface and Interface Catalysis for Optimized Carbon Resource Utilization

Catalysis is a highly interdisciplinary field spanning chemistry, physics, and materials science. Developing new catalytic conversion methods and technologies to transform between different forms of chemical energy represents a crucial pathway for improving resource utilization efficiency and reducing consumption. Catalytic reactions are inherently dynamic processes that often require analysis of catalyst microstructures under working conditions to understand their fundamental nature. This project will develop high-sensitivity in-situ dynamic experimental techniques and theoretical simulation methods to investigate the dynamic mechanisms of surface and interface chemical reactions at the atomic and molecular level. The research aims to reveal the microscopic mechanisms by which different active sites regulate C-C bond coupling and C-O/C-H bond activation, and to develop new technologies and processes for catalytic C-C coupling and C-O/C-H activation reactions. These advances will accelerate the development of next-generation industrial technologies for carbon resource conversion (methanol, methane, and syngas). The participating institution is the Dalian Institute of Chemical Physics, Chinese Academy of Sciences.

(3) Efficient Solar Photochemical Conversion

Photosynthesis is the most important chemical reaction on Earth, exemplifying the conversion of solar energy to chemical energy. Elucidating the principles of photosynthesis and its regulation, and mimicking photosynthetic systems to construct artificial systems with photosensitization and catalytic technologies, are essential pathways for achieving efficient solar energy conversion. Focusing on this theme, the project will investigate the structure, function, and regulatory mechanisms of important membrane protein complexes in natural photosynthesis, clarifying the mechanisms of efficient energy absorption, transfer, conversion, and regulation during the primary photosynthetic reactions. This research will provide theoretical foundations for improving crop light utilization efficiency and achieving efficient solar chemical conversion. The project will also mimic Photosystems I and II to construct efficient, low-cost artificial photosynthetic systems for photocatalytic water splitting and CO_2 reduction, enabling efficient solar-to-chemical energy conversion. Additionally, it will develop novel photocatalytic reactions and technologies for producing important chemicals to improve resource utilization efficiency. The project will establish a femtosecond time-resolved X-ray spectroscopic diagnostic system using femtosecond laser pump-probe techniques, providing new ultrafast X-ray spectroscopic tools for photosynthesis research and developing label-free detection methods for biomolecules. Participating units include the Technical Institute of Physics and Chemistry, Dalian Institute of Chemical Physics, Institute of Botany, Institute of Physics, and Institute of Chemistry, all under the Chinese Academy of Sciences.

3. Future Prospects

The "Fundamentals and Regulation of Energy Chemical Conversion" Strategic Priority Research Program is hosted by the Dalian Institute of Chemical Physics and the Technical Institute of Physics and Chemistry, Chinese Academy of Sciences. The program integrates multiple CAS units with strengths in this field, fully leveraging the Academy' s institutional advantages and multidisciplinary integration. These research units possess numerous experienced scientists of all career stages with high scientific literacy, forming a complementary and collaborative research team through years of cooperation.

The current research team comprises ten CAS academicians and thirty-eight recipients of prestigious talent awards including the National Science Fund for Distinguished Young Scholars, Excellent Young Scientists Fund, Thousand Talents Plan, and CAS Hundred Talents Program. This team possesses not only strong scientific research capabilities but also proven expertise in developing high-level experimental apparatus and instrumentation. In recent years, the team has developed dozens of experimental devices and instruments for molecular dynamics research, including universal and specialized molecular beam apparatus, surface photochemistry setups, synchrotron radiation photoionization mass spectrometry and combustion kinetics facilities, ultrafast process experimental systems, kinetic spectroscopy instruments, time-of-flight mass spectrometers, and electron energy analyzers. The team has mastered, applied, and advanced various experimental techniques, including crossed molecular beams, spectroscopy, mass spectrometry, ultrafast spectroscopy, particle detection, and time- and space-resolved detection methods. These capabilities are crucial for modern chemical reaction dynamics research, as many large-scale instruments must be custom-designed and built according to specific research needs, and every major advance in chemical dynamics has been closely tied to the development and application of new technologies and methods.

A comprehensive experimental research facility based on tunable extreme ultraviolet coherent light sources, combining ultrafast lasers with high-energy electron beams, has been completed and commissioned at the Dalian Institute of Chemical Physics. This development provides an excellent opportunity for energy chemistry research. The tunable, high-brightness extreme ultraviolet laser source will substantially enhance detection efficiency for products and intermediates in energy chemical reactions, holding extremely important significance for studying energy chemical processes. This facility shows great promise for becoming a uniquely world-class platform for investigating fundamental scientific questions related to energy and the environment.

(Host Institutions: Dalian Institute of Chemical Physics, Technical Institute of Physics and Chemistry, Chinese Academy of Sciences)

Note: Figure translations are in progress. See original paper for figures.