# Structure- and Function-Oriented Creation of New Materials: Postprint

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## Abstract

The creation of new materials, particularly functional new materials, constitutes the material foundation of modern civilized society and serves as the driving force for economic and social development, national security, and scientific and technological advancement. Governments and scientists worldwide are committed to researching new materials with diverse special functions and structures. The capability and level of functional new material creation represent a hallmark of national core competitiveness and a strategic high ground for innovation-oriented nations, urgently necessitating the integration of resources, consolidation of strengths, and collaborative efforts to achieve leapfrog development in innovation.

## Full Text

## Preamble

The creation of new substances, particularly functional materials, forms the material foundation of modern civilization and serves as the driving force for economic and social development, national security, and scientific and technological advancement. Governments and scientists worldwide are dedicated to researching new substances with special functions and structures. The capability and level of functional new substance creation represent a hallmark of national core competitiveness and a strategic high ground for innovative nations, urgently requiring resource integration, concentrated advantages, and collaborative breakthroughs to achieve innovative leapfrog development. As noted by Academician Xu Guangxian, the six major inventions of the 20th century —information technology, biotechnology, nuclear science and nuclear weapons, aerospace and missile technology, laser technology, and nanotechnology—all depend on new materials from chemical synthesis. Without chemical synthesis, these technologies would be impossible to realize.

## 1. Project Background and Rationale

The creation of new substances has fundamentally transformed human lifestyles. Over 100 million compounds have been registered with CAS (Chemical Abstracts Service), the vast majority obtained through chemical synthesis. This reflects the powerful vitality and unlimited creativity of synthetic chemistry while greatly satisfying material needs for human survival and social progress. This impact manifests in four key areas: (1) improving living standards through synthetic fibers, plastics, and rubbers that shape modern life; (2) ensuring food security via synthetic ammonia and pesticides that increase crop yields; (3) addressing health challenges through antibiotics and pharmaceuticals that control disease, extend lifespan, and improve health; and (4) providing the foundation for new technologies, such as silicon semiconductors and optical fibers that underlie the information age of electronic communication, high-speed computing, artificial intelligence, and networking. Concurrently, new substance creation has spawned new technologies, materials, and products, constructing next-generation industrial chains. Over 90% of chemicals worldwide are produced through catalytic processes, with the global catalyst and regeneration market reaching $23.2 billion and $24.6 billion in 2013 and 2014, respectively. The fresh catalyst segment alone is projected to grow from $20.5 billion in 2014 to $25.0 billion by 2019, representing a compound annual growth rate of 4.0%.

New substance creation represents a pinnacle of scientific excellence. Nearly half of all Nobel Prizes in Chemistry have recognized discoveries and creations of new substances, including four awards in the past decade alone. This underscores the critical role of theoretical and experimental research in new substance creation for advancing science and productivity. Such research encompasses persistent efforts to achieve specific synthetic targets, exemplified by Haber' s 1918 Nobel Prize for the ammonia synthesis catalyst; targeted synthesis of known structures, as recognized by Woodward' s 1965 Nobel Prize for natural product synthesis; and function-oriented synthesis, highlighted by Tsien' s 2008 Nobel Prize for green fluorescent protein engineering.

To achieve precision creation of new substances, we must pursue function-oriented structural design and structure-oriented precision synthesis. Despite over 100 million registered compounds, those with clearly defined functional applications remain extremely limited, revealing constrained capabilities in controlling function-specific creation and a lack of guiding theories. As Tang Youqi proposed, chemistry' s central task includes elucidating composition-structure-property relationships to design molecules with desired characteristics. Xu Guangxian identified the "quantitative structure-property relationship" as one of chemistry' s four grand challenges for the 21st century. Nobel laureate Noyori emphasized that chemists must strive for "perfect reaction chemistry" —generating only desired products with 100% selectivity and yield, without waste. Therefore, developing function-oriented structural design and structure-oriented precision synthesis is imperative to achieve the ultimate goal of "precision creation of new substances driven by both structure and function."

Strengthening research on structure- and function-oriented new substance creation is essential for China' s transition from a major chemical producer to a chemical powerhouse. The United States, Europe, Japan, and other nations have adopted government-led approaches to mobilize research institutions and enterprises, aiming to shorten creation-to-application cycles and seize the international high ground. China has similarly prioritized this research through programs like the "973" Program, NSFC Major Research Plans, and CAS Key Direction Projects, yielding substantial results. Since 2008, China has led the world in chemistry publications, though its impact lags behind Europe and the United States. This gap stems from the need for breakthroughs in new substance creation, discovery of novel phenomena and functions, and development of original theories and methods. Thus, strengthening structure- and function-oriented research is the necessary path for China' s innovative leap from a major chemical country to a chemical powerhouse.

In this context, the Strategic Priority Program on "Structure- and Function-Oriented New Substance Creation" was launched. On October 29, 2016, the Chinese Academy of Sciences officially initiated this Category B Strategic Priority Research Program, with the Shanghai Institute of Organic Chemistry and the Fujian Institute of Research on the Structure of Matter as supporting units. Chief Scientists Academician Hong Maochun and Academician Ding Kuiling lead a multidisciplinary team encompassing chemistry, physics, materials science, and biology, including 6 CAS academicians, 5 "973" Program chief scientists, 32 NSFC Distinguished Young Scholars, 7 NSFC Innovation Groups, and 71 participants in the CAS "Hundred Talents Program" and "Young Thousand Talents Program."

## 2.1 Two Major Scientific Questions

Function-oriented structural design and structure-oriented precision synthesis have become focal points in new substance creation research. This program addresses two major scientific questions:

(1) How can we achieve structural design for specific material functions? This focuses on the structure-property relationship, revealing the microstructure and properties of functional building units and the synergistic principles governing their interactions.

(2) How can we achieve directed synthesis of specific material structures? This emphasizes the structure-synthesis relationship, elucidating mechanisms of electron transfer, atomic migration, and energy conversion in reactions based on functional building units, along with synergistic effects among these processes.

## 2.2 Three Major Research Areas

To address these questions, this program adopts a functional building unit research strategy (Figure 1 [Figure 1: see original paper]), developing modular chemical synthesis methods. Focusing on inorganic, organic, and inorganic-organic hybrid compounds, we pursue function-oriented structural design and structure-oriented directed synthesis for photoelectric, catalytic, and other functions across three main areas:

(1) Structural design and creation of inorganic compounds. Based on photoelectric functional building units, we establish models for inorganic photoelectric functional building units according to their operational modes of electronic polarization, electronic transition, and ionic polarization in response to photoelectric fields. This enables structural design and synergistic effects of functional building units, facilitating modular inorganic synthesis to create new inorganic substances with photoelectric functions.

(2) Precision synthesis of organic molecules. Targeting functional organic substances for pharmaceuticals and materials, we develop precision synthesis based on functional building unit catalysis. Using organic catalytic functional building units, we develop elementary reactions, create catalytic systems, and design synthetic strategies. We explore synergistic mechanisms between molecular structure and reaction behavior, reveal qualitative and quantitative structure-function relationships, and achieve efficient, concise, and environmentally friendly precision synthesis of functional molecules.

(3) Synthesis of functional inorganic-organic hybrid compounds. Based on synergistic effects, we pursue directed synthesis and assembly of inorganic-organic hybrid compounds. Building upon research on inorganic photoelectric and organic catalytic functional building units, we explore key structural factors enabling complementary advantages between inorganic and organic functional building units, along with the fundamental nature of synergistic effects in electron transfer and energy conversion. We establish new methods for hybrid assembly to achieve directed synthesis of inorganic-organic hybrid compounds with efficient activation/conversion and photoelectric conversion functions.

## 3. Expected Outcomes

The program will focus on challenging issues at the frontier of creating inorganic, organic, and inorganic-organic hybrid functional substances, integrating scientific breakthroughs with team and platform development while emphasizing multidisciplinary collaboration.

(1) Aiming at the key scientific objective of "precision creation of new substances driven by both structure and function,"we will achieve major breakthroughs in creating substances with specific structures and functions. We will take the lead in establishing an international functional building unit

theoretical framework and database application platform, create internationally recognized new reactions for substance creation, discover several phenomena with major disciplinary impact, and lead international development in 2–3 research directions.

(2) Targeting frontiers in national economic development, national security, and public welfare, we will create functional new substances with independent intellectual property rights to catalyze transformative technologies. These include: 1–2 internationally influential "Chinese-brand"photoelectric crystals enabling new-wavelength laser applications; 3–5 superior catalyst systems for comprehensive CO  utilization and efficient hydrocarbon conversion; 2–3 preclinical drug candidates and fluorine-containing functional substances; 4–6 low-cost, high-conversion-efficiency inorganic-organic hybrid compounds for efficient small-molecule activation; 2–3 highly efficient rare earth/transition metal/organic hybrid luminescent materials; and rare earth OLED devices with low decay rates and long lifetimes.

Through successful implementation, this program will cultivate top scientists in functional new substance creation, enhance China' s capabilities and standards, transform contemporary chemistry and materials research approaches, advance disciplinary development, and meet major national needs.

(Supporting Units: Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences; Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences)

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