

Preface to the Series

As Lao Tzu said, “A huge tree grows from a tiny seedling; a nine-storied tower rises from a heap of earth.” Basic research is the fundamental approach to fostering innovation-driven development, and its level becomes an important yardstick for measuring the overall scientific and national strength of a country. Since the beginning of the 21st century, China’s overall strength in basic research has been consistently increasing. With respect to input and output, China’s input in basic research increased by 14.8 times from 5.22 billion yuan in 2001 to 82.29 billion yuan in 2016, with an average annual increase of 20.2%. In the same period, the number of China’s scientific papers included in the Science Citation Index (SCI) increased from lower than 40,000 to 324,000; China rose from the 6th to the 2nd place in global ranking in terms of the number of published papers. In regard to the quality of output, in 2016, China ranked No. 2 in the world in terms of citations in 9 disciplines, among which the materials science ranked No. 1; as of October 2017, China ranked No. 3 in the world in the numbers of both Highly Cited Papers (top 1%) and Hot Papers (top 0.1%), with the latter accounting for 25.1% of the global total. In talent cultivation, in 2006, China had 175 scientists (136 of whom from the Chinese mainland) included in Thomson Reuters’ list of Highly Cited Researchers, ranking 4th globally and 1st in Asia.

Meanwhile, we should also be keenly aware that China’s basic research is still facing great challenges. First, funding for basic research in China is still far less than that in developed countries—only about 5% of the R&D funds in China are used for basic research, a much lower percentage than 15%–20% in developed countries. Second, competence for original innovation in China is insufficient. Major original scientific achievements that have global impact are still rare. Most of

the scientific research projects are just a follow-up or imitation of existing research, rather than groundbreaking research. Third, the development of disciplines is not balanced, and China's research level in some disciplines is noticeably lower than the international level—China's Field-Weighted Citation Impact (FWCI) in disciplines just reached 0.94 in 2016, lower than the world average of 1.0.

The Chinese government attaches great importance to basic research. In the 13th Five-Year Plan (2016–2020), China has established scientific and technological innovation as a priority in all-round innovation and has made strategic arrangements to strengthen basic research. General Secretary XI Jinping put forward a grand blueprint of making China into a world-leading power in science and technology in his speech delivered at the National Conference on Scientific and Technological Innovation in 2016, and emphasized that “we should aim for the frontiers of science and technology, strengthen basic research, and make major breakthroughs in pioneering basic research and groundbreaking and original innovations” at the 19th CPC National Congress on Oct. 18, 2017. With more than 30 years of unrelenting exploration, the National Natural Science Foundation of China (NSFC), one of the main channels for supporting basic research in China, has gradually shaped a funding pattern covering research, talent, tools and convergence, and has taken action to vigorously promote basic frontier research and the growth of scientific research talent, reinforce the building of innovative research teams, deepen regional cooperation and exchanges, and push forward multidisciplinary convergence. As of 2016, nearly 70% of China's published scientific papers were funded by the NSFC, accounting for 1/9 of the total number of published papers all over the world. Facing the new strategic target of building China into a strong country in science and technology, the NSFC will conscientiously reinforce forward-looking planning and enhance the efficiency of evaluation, so as to achieve the strategic goal of making China progressively share the same level with major innovative countries in research total volume, contribution and groundbreaking researchers by 2050.

The series of *Advances in China's Basic Research* and the series of *Reports of China's Basic Research* proposed and planned by the NSFC emerge against such

a background. Featuring science, basics and advances, the two series are aimed at sharing innovative achievements, diffusing performances of basic research, and leading breakthroughs in key fields. They closely follow the frontiers of basic research developments in China and publish excellent innovation achievements funded by the NSFC. The series of *Advances in China's Basic Research* mainly presents the important original achievements of the programs funded by the NSFC and demonstrates the breakthroughs and forward guidance in key research fields; the series of *Reports of China's Basic Research* shows the core contents of the final reports of Major Programs and Major Research Plans funded by the NSFC to make a systematic summarization and give a strategic outlook on the achievements in the funding priorities of the NSFC. We hope not only to comprehensively and systematically introduce backgrounds, scientific significance, discipline layouts, frontier breakthroughs of the programs, and a strategic outlook for the subsequent research, but also to summarize innovative ideas, enhance multidisciplinary convergence, foster the continuous development of research in concerned fields, and promote original discoveries.

As Hsun Tzu remarked, "When earth piles up into a mountain, wind and rain will originate thereof. When waters accumulate into a deep pool, dragons will come to live in it." The series of *Advances in China's Basic Research* and *Reports of China's Basic Research* are expected to become the "historical records" of China's basic research. They will provide researchers with abundant scientific research material and vitality of innovation, and will certainly play an active role in making China's basic research prosper and building China's strength in science and technology.



Academician of the Chinese Academy of Sciences
Beijing

Preface

As the foundation and precursor of modern science and technology, materials science is an internationally recognized core field. Materials science is intertwined with national economy, engineering and technology, and national security, which is critical to the national economic and social development. Developed countries have prioritized novel materials as a key area in the development of science and technology to maintain their economic and technological leadership.

The invention and application of new materials are milestones of human civilization, and the development of materials science has contributed to the advancement of human society and civilization. People have long expected a new paradigm of materials engineering to guide the search for new materials, i.e., to predict material properties based on known scientific laws or to design and prepare new materials with specific functions according to the properties required, thereby shortening new materials' development cycles. So far, to develop new materials, scientists have mastered the correlations between macroscopic properties and structures (molecular and spatial structures) of materials, further explored the intrinsic laws, and systematically discussed such relationship based on quantum and structural chemistry.

Materials' functional properties are primarily derived from their optical, electrical, magnetic, thermal, and mechanical effects or combinations of these effects (e.g., photovoltaic, electro-optical, acoustic-optical, magnetoelectric, and thermoelectric effects); and their research and development has shifted the focus from a single-functional to multifunctional one. It is well-known that a material's photoelectromagnetic (PEM) properties are mostly influenced by its electron, spin, and orbital motion, but its electronic structure is primarily determined by its atoms and their spatial arrangement. In materials science research, crystalline materials are the

main constituents of solid materials, with ordered and stable structures, various intrinsic properties, rich physical connotation, clear structure-effect relationship, and ease of control. Modern technology has enabled us to achieve the function-directed structural design, chemical synthesis, and material preparation to obtain materials and devices with the desired application properties. Therefore, we can build a solid theoretical basis for the function-directed design and preparation of crystalline materials by further deepening and improving our understanding of the scientific nature of crystalline materials as well as the materials' structure-effect relationships and their implications, which can lead to the discovery and preparation of completely artificially designed revolutionary new materials and promote the rapid development of national economy and science and technology.

After several generations of efforts in crystalline materials research, China has achieved exceptional results in structural design and crystal growth of nonlinear optical (NLO) crystalline materials and has been leading the international development efforts in this field since the 1980s. Chinese scientists have invented high-performance nonlinear optical crystalline materials such as beta-barium borate (BBO), lithium triborate (LBO), potassium beryllium borate fluoride (KBBF), highly magnesium-doped lithium niobate crystals (LN), and L-arginine phosphate (LAP), which are famously known as made-in-China crystals with independent intellectual property rights. Chinese scientists also proposed the anionic group theory, dielectric superlattice theory, dual matrix structure model, anionic ligand structure model, and crystal growth defect mechanism, all of which have been added to the international knowledge bank of crystal growth theories and laid a solid foundation for the development of the field. In the meanwhile, Chinese scientists has pioneered the research of dielectric superlattices and paved the way for new optoelectronic functional materials and devices by combining dielectric microstructure and modern crystal growth technology from both theoretical and experimental perspectives, which is an achievement that has gained worldwide attention.

With the increasingly intensified international competition in crystalline materials, especially the increasing relevance of various crystalline materials in vital technologies related to national security, it is imperative to carry out basic research on new functional

crystalline materials systematically. However, China generally has few new functional materials with independent intellectual property rights and is conducting too many follow-up studies. The dependence of high-tech industries on foreign technologies is greatly affecting the country's overall competitiveness, particularly in national defense and high technology, which are extremely restricted by developed Western countries. Therefore, China should strengthen the research of new functional crystalline materials to reverse the passive situation in the research of new crystalline materials, develop its independent characteristics in the research of crystalline materials within the shortest time possible, achieve breakthroughs in crystalline materials, innovate a number of new materials with independent intellectual property rights, and reach a new height in nonlinear optical crystalline materials in particular.

Materials research not just necessitates a solid understanding of materials science but also relies on various disciplines, including chemistry, physics, and information sciences. Chemists have advantages in the design, controllable preparation, structural control and optimization, and physicochemical characterization of materials, especially in the discovery of new chemical compounds, exploiting the source of new materials research; physicists specialize in the study of new phenomena and properties of materials and their mechanisms, playing an irreplaceable role in the discovery and application of new materials; materials scientists who are the key to the development of new materials from preparation to practical use are responsible for the preparation of materials and focus on optimizing material properties, as well as provide key engineering technologies in the process of materials application; information scientists take the results of new materials research and closely integrate them with major national needs and applications, making the practice of materials more possible. The Major Research Plan "Structural Design and Controllable Preparation of the Function-Directed Crystalline Materials" (hereinafter referred to as the Plan) thereby aims to develop interdisciplinary cooperation among chemistry, physics, materials, and information sciences to discover new materials, propose new theories, develop new methods for materials design and synthesis, implement applications of materials, and closely integrate the results with national economic and social development, thus shortening the research cycles of materials, meeting major national needs, and

accelerating the process of enhancing comprehensive strength of China's materials research.

To conduct cutting-edge research on functional crystalline materials, we must, on the one hand, study the molecular and spatial structures of materials thoroughly, and on the other hand, extensively study the macroscopic physicochemical properties of materials and combine quantum chemistry and solid-state energy-band theories to study the electronic structures of materials to seek and determine the structural motifs or other factors that play a dominant role in the functional properties of crystalline materials. We can develop performance-adapted models to predict the physicochemical properties of compounds, validate functionally dominant structural motifs, and further modify and optimize structural motifs for the design and regulation of material properties using theoretical simulations.

The Plan, guided by national demand and the function of materials, focuses on exploring the relationships between structures, compositions, and properties of crystalline materials, and proposes new mechanisms and models for new materials exploration; the Plan designs and regulates material structures in response to the demand for material functions, and conducts controlled preparation of a batch of new crystalline materials with specific functions, to establish a new materials research theory, new preparation technology, and new material system for independent innovation, and to open up an important source of knowledge innovation and technological innovation. The discovery of the intrinsic relationships between the optical, electrical, magnetic and composite properties of crystalline materials as well as their spatial and electronic structures, will reveal structural motifs that determine the macroscopic functions of crystalline materials and their integration in space, and provide a theoretical basis for the design and preparation of function-directed crystalline materials. Furthermore, practical applications have put forward many new requirements for photoelectric conversion materials, nonlinear optical crystalline materials, laser and fluorescent crystalline materials, ferroelectric and microwave dielectric materials, etc.

The overall scientific objectives and breakthroughs of this Plan are to discover the intrinsic relationships and laws between the optical, electrical, magnetic, and composite properties of crystalline materials and their spatial and electronic structures,

to reveal the functional motifs that determine the macroscopic functions of crystalline materials and their integration in space, and to provide a theoretical basis for the design and preparation of function-directed crystalline materials. Three key scientific issues were raised during the research period: (i) the identification of key structural motifs for the functions and physical properties of crystalline materials; (ii) the relationships and laws of material functions, physical properties, and their microstructures; (iii) the controllability of the design and preparation of crystalline materials based on functional motifs. The research has been conducted in six areas: the study of functional characteristics and structural primitive relationships of crystalline materials; the synergy and structure-effect laws among functional motifs; the calculation, simulation and functional optimization of crystalline materials; new methods for the design, synthesis and controllable preparation of crystalline materials; new methods for the analysis and characterization of microstructures of crystalline materials; and the functions and applications of crystalline materials. We have made important breakthroughs in the following three aspects: (i) development of a functional motif theory to guide crystalline materials development with optical, electrical, magnetic, and composite functions, thus creating a new disciplinary growth point at the intersection of physics, chemistry and materials science; (ii) establishment and development of research methods for controlled crystalline materials synthesis and assembly, detection and characterization of functional motifs, and simulation and prediction of material properties based on the functional motif theory; (iii) acquisition of a number of crystalline materials that have international influence on and a leading position in related technologies and industries. In particular, we have obtained a series of high-performance material systems in laser crystalline materials and nonlinear optical crystalline materials, further enhancing the originality of crystalline materials research in China.

This important research initiative has seen a dramatic improvement in the structural design and controllable fabrication of function-directed crystalline materials, starting with functional motifs. We are leading international research efforts in magnetic molecular materials, ferroelectric molecular materials, functional molecular metal-organic framework (MOF) materials, and nonlinear optical crystalline materials.

We have made great progress in crystalline transparent ceramic laser materials, energy conversion materials, novel iron-based superconductors, bionic materials, etc. Meanwhile, we have developed new nonlinear optical theories of single-atom polarizable orbitals, and have been the first to discover a number of new deep-ultraviolet nonlinear optical crystalline materials. During the Plan, 4,016 research papers were published, including 7 in *Science*, 3 in *Nature*, and 31 in *Nature* research journals; 536 invention patent applications were submitted, 308 of which were granted, including 8 PCT (Patent Cooperation Treaty) patents; 273 guest lectures were given in China and abroad, including 163 international guest lectures; 10 second-class awards of the National Natural Science Award, 2 second-class awards of the National Technical Invention Award and 1 award in Chemistry from The World Academy of Sciences (TWAS) were received.

In terms of talent cultivation, through this Plan, 8 project experts or leaders have been elected as academicians of the Chinese Academy of Sciences, 23 have been awarded the National Science Fund for Distinguished Young Scholars by the NSFC, and 6 have been awarded the Excellent Youth Fund by the NSFC, creating a research team with strong international competitiveness and influence. A new model of research and collaboration on crystalline materials has been established to create an internationally influential research team for interdisciplinary, interpenetrating, and coordinated research in physics, chemistry, and materials science.

We have maintained and developed our strengths in crystalline materials research during this Plan, and proposed strategies and suggestions, which have been adopted by the NSFC and the Ministry of Science and Technology, laying a solid foundation for future development.

HONG Maochun

Academician of the Chinese Academy of Sciences

Fuzhou