1

Survey of Challenges in Chemistry and Materials Science Research

1.1 Introduction

Chemistry and materials science constitute a profoundly complex and ancient discipline that has faced entirely distinct challenges across different eras. Without delving into the distant past, let us consider the scenario 20 years ago when the author was engaged in undergraduate research within a chemistry laboratory at the University of Science and Technology of China. A formidable challenge at that time was the complete unpredictability of experimental outcomes, which sometimes left the researchers in the dark about the nature of their work. The standard procedure involved mixing prepared solids and liquids in a hydrothermal autoclave, followed by heating in an oven at 180 °C for approximately 24 hours. Subsequently, the mixture was extracted, separated, washed, and prepared for analysis. This involved observations under various electron microscopes to examine the morphology, along with routine completion of other tests, such as X-ray diffraction (XRD) and spectroscopy. Occasionally, tests for lithium-ion battery performance were also conducted. Perhaps one of the most gratifying experiences at that time was observing the artistic beauty of transmission electron microscopy (TEM) images.

Today, we have grown accustomed to the ubiquity of artificial intelligence, big data, and robotics in our daily lives. Looking back at academic papers from the field of chemistry and materials science twenty years ago, especially those concerning nanomaterials, they appear as collections of data interspersed among images, text, tables, and references. During that era, the publication of, or contribution to, an academic paper was often a source of great joy for many. This retrospective underscores not only the dramatic evolution of technology and methodology within the field but also highlights the fundamental nature of scientific inquiry, which remains constant: a quest for understanding and innovation. The transition from manual experimentation and analysis to the integration of advanced computational tools and methodologies has significantly enhanced the capacity for prediction, analysis, and application in materials science. Yet, the essence of discovery, characterized by moments of joy and frustration, the painstaking gathering of data, and the meticulous interpretation of results, continues to define the discipline. This evolution reflects a broader narrative of progress in science and technology, where the accumulation of knowledge and the development of new

AI and Robotic Technology in Materials and Chemistry Research, First Edition. Xi Zhu.

tools mutually reinforce each other, driving the boundaries of what is possible ever forward.

1.2 Energy Form

When we discuss "new energy" today, it is invariably linked to another term, "new materials," and vice versa. The relationship between materials chemistry and energy is one of mutual promotion and complementarity. The generation, storage, transport, and utilization of energy are all reliant on specific functional materials, while more advanced energy systems have enhanced the precision of our observations of the world, significantly propelling the technological progress of materials science. Concurrently, the continuous accumulation of human scientific and technological knowledge further promotes the emergence and application of new technologies. As described by the "materials big data" projects in recent years, combined with the current "generative" artificial intelligence technologies, we seem to have discovered a new domain for more efficient exploration and discovery from existing data toward incremental innovation. Of course, this is predicated on having sufficient computational power, which is itself a part of energy, underscoring the growing importance of technology in the new energy sector. Thus, we observe that today's materials science can be viewed as the process where theory or algorithms drive data through energy to achieve incremental innovation, which represents our primary competitive direction. This improved and expanded version positions the interdependence of new energy and new materials within a broader scientific and technological context, emphasizing the role of computational power and artificial intelligence. It sets the stage for a detailed historical analysis, hinting at the evolution of these fields and their impact on contemporary scientific research and technological development. I will proceed to analyze this process from a historical perspective.

1.2.1 Steam Power

In analyzingthe trajectory of materials chemistry within the broader context of societal development and energy paradigms, it becomes evident that the evolution of this field is deeply intertwined with the predominant energy sources of its respective eras. The progression from a society reliant primarily on human and animal labor to one powered by steam, and eventually to our current age of electricity and emerging renewable energies, has had profound implications for the advancement of materials chemistry.

During the pre-industrial era, characterized by manual labor, the field of materials chemistry was in its nascent stages. The absence of sophisticated instrumentation and analytical techniques meant that researchers' understanding of chemical phenomena was limited to observable reactions and processes that could be achieved without the aid of advanced technology. This period's knowledge base was foundational yet primitive by today's standards, focusing on the basic properties of materials and their simple transformations.

Figure 1.1 The revolutionary invention of the steam engine marked a monumental leap from manual labor to mechanized production, symbolizing a pivotal moment in human history. The Steam Age stands as a crucial milestone in human history, catalyzing industrialization and modernization, reshaping production methods, social structures, and lifestyles, exerting profound and enduring influence on the world.

The Industrial Revolution marked a pivotal shift, with the invention and widespread adoption of the steam engine catalyzing an unprecedented expansion in industrial capabilities and scientific inquiry. The steam engine, a marvel of engineering and materials science, necessitated the development of materials that could withstand high pressures and temperatures. This requirement spurred significant advancements in metallurgy, exemplified by the Bessemer process, which revolutionized steel production by making it more efficient and cost-effective. The ability to produce stronger, more durable materials was not just a technological achievement but also a cornerstone in the edifice of modern industrial society, enabling the construction of railroads, bridges, and machinery that powered the nineteenth century's economic expansion (Figure 1.1).

Furthermore, the steam era's influence extended into the realm of chemical production and analysis. The coal industry, a key driver of the steam engine, became a vital source of raw materials for the burgeoning chemical industry. Coal tar, a byproduct of coal gasification, was the precursor for an array of chemical dyes, initiating a new era in the textile industry and laying the groundwork for synthetic organic chemistry. The development of analytical chemistry was equally crucial, with innovations such as spectroscopy and chemical thermodynamics emerging in response to the industrial and scientific challenges of the time.

The establishment of dedicated research institutions and the systematic approach to materials chemistry research were also hallmarks of this era. The professionalization of chemistry as a distinct scientific discipline, coupled with the enhanced collaboration between scientists and engineers, led to a more methodical and empirical approach to research. This collaborative ethos was instrumental in bridging the gap between theoretical chemistry and its practical applications, fostering a culture of innovation that would pave the way for the next century's scientific breakthroughs. The steam power era's legacy is its role in promoting the global spread of chemical knowledge. The advent of steam-powered printing presses made scientific literature more accessible, while improved transportation facilitated the exchange of ideas and materials between researchers across the globe. This era laid the foundational principles of materials chemistry as we understand it today, setting the stage for the subsequent development of polymers, composites, and nanomaterials that are essential to modern technology.

As steam technology advanced, scientists gained a deeper understanding of thermodynamics, marking a period of significant progress in the field. This era was also characterized by burgeoning theoretical research in reaction kinetics, reflecting an increasing sophistication in the comprehension of the forces and principles governing chemical reactions. Concurrently, the chemical engineering industry experienced sustained growth, driven by these scientific advancements and the demand for industrial applications of chemical processes. In parallel, the field of reaction kinetics emerged, focusing on the rates at which chemical reactions occur and the factors influencing these rates. This area of study is vital for understanding how reactions can be optimized for industrial processes, including those used in the chemical engineering industry. Theories related to reaction kinetics, such as the Arrhenius equation (Arrhenius 1889), which describes how reaction rates increase with temperature, became instrumental in the design and improvement of chemical reactors and processes.

The expansion of the chemical engineering industry during this time can be attributed to the integration of these scientific insights into practical applications. Chemical engineers leveraged the principles of thermodynamics and reaction kinetics to develop processes that are more efficient, cost-effective, and capable of producing materials and chemicals at a larger scale. This not only facilitated the growth of the chemical industry itself but also had a wide-reaching impact on sectors such as pharmaceuticals, energy, and materials science, contributing to the advancement of society as a whole. Thus, the advancement of steam technology and the deepening understanding of thermodynamics and reaction kinetics played pivotal roles in the scientific and industrial growth of the 19th and early 20th centuries, marking a period of remarkable innovation and expansion in the chemical engineering field.

1.2.2 Electricity Power

The transition from steam to electric power marked a revolutionary period in human history, heralding the second industrial revolution. This era, spanning the late 19th and early 20th centuries, was not just about the adoption of electricity as a primary energy source but also about the profound impact it had on materials chemistry. The electrification of society demanded new materials with specific properties, fostering a wave of innovation in chemistry and material science.

An understanding confined solely to gases is significantly inadequate for the field of materials chemistry, which also heavily involves the study of condensed phases such as solids and liquids. These phases arguably represent a more prevalent subject of research. In the domain of solid-state physics, electrons emerge as one of the pivotal research subjects. The study of electrons is indissolubly linked to the understanding of electricity and the socio-economic context of the era. By the late nineteenth century, the exploration and application of electricity had made considerable strides, with the advent of technologies like the light bulb, telephone, and electrical power distribution witnessing a qualitative leap and achieving widespread practical application. Many scientists of that period began to leverage electricity as a tool for scientific investigation. For instance, in 1895, Röntgen (1896) discovered X-rays while experimenting with a Crookes tube – an early experimental electrical discharge tube – during his studies on cathode rays. This discovery underscored the pivotal role of electrical technology in facilitating scientific breakthroughs.

The unveiling of X-rays opened the door to observing the microscopic structure of materials, further broadening the horizons of material chemistry through the advent of quantum mechanics. Quantum mechanics has introduced concepts such as momentum space into contemporary solid-state physics, significantly expanding our cognitive and exploratory scope in materials chemistry. This progression underscores the interdisciplinary nature of materials science, highlighting how advances in one area can propel understanding and innovation across multiple scientific domains. It exemplifies the profound impact of electrical studies and technological advancements on the evolution of materials chemistry, enabling the detailed examination of material properties at the atomic and molecular levels. Consequently, these insights have paved the way for the development of new materials and technologies, underscoring the integral role of a comprehensive understanding of all states of matter – solid, liquid, and gas – in the advancement of materials science and engineering (Figure 1.2).

With the maturation of solid-state physics (Ashcroft and Mermin 1976) and the conceptual framework of momentum space, the intricate relationship between

Figure 1.2 The advent of electricity ushered in an era of unprecedented innovation and connectivity, fundamentally transforming human civilization and laying the groundwork for the modern technological landscape. The Electrical Era represents a paradigm shift in human history, sparking revolutions in communication, transportation, and industry, fostering global interconnectedness, and fostering the birth of countless inventions that continue to shape our daily lives.

structure and properties has been catapulted to the forefront of tangible research inquiries, particularly in the realms of electrical conductivity and band gap analysis. Solid-state physics, as a discipline, seeks to elucidate the physical properties of solids from a microscopic perspective, leveraging quantum mechanics as a fundamental theoretical underpinning. This approach has profoundly enriched our understanding of how the atomic and electronic structures of materials influence their macroscopic properties.

The concept of band theory, a cornerstone of solid-state physics, offers a comprehensive explanation for the electrical conductivity of materials. Band theory posits that the energy levels of electrons in a solid form bands of energy rather than discrete levels. The presence of band gaps, or energy ranges in which no electron states can exist, plays a crucial role in determining a material's conductivity. For instance, insulators are characterized by a wide band gap, preventing electrons from easily moving across the energy barrier, whereas conductors exhibit little to no band gap, facilitating free electron movement and, consequently, electrical conductivity. Semiconductors, pivotal in modern electronics, possess a narrow band gap that allows their conductive properties to be finely tuned through doping or environmental changes.

Moreover, the advent of quantum mechanics has enabled the prediction and manipulation of material properties with unprecedented precision. Quantum mechanics (Griffiths and Schroeter 2018) introduces the principle of wave-particle duality, which asserts that particles such as electrons exhibit both particle-like and wave-like properties. This principle is instrumental in understanding the quantum mechanical behavior of electrons in solids, which directly influences material properties such as electrical conductivity, magnetism, and optical absorption.

The exploration of momentum space, a quantum mechanical construct where positions and momenta are conjugate variables, has further deepened our comprehension of solid-state phenomena. The analysis of electronic states within momentum space facilitates a more nuanced understanding of band structures and electron dynamics, contributing to advancements in material design and application. These scientific advancements underscore the crucial role of solid-state physics in the modern technological landscape. The ability to engineer materials with tailored electrical, optical, and magnetic properties has been a driving force behind the development of advanced technologies, ranging from semiconductor devices and solar cells to quantum computing. The ongoing research into the structure–property relationship not only enriches our theoretical knowledge but also paves the way for the innovation of new materials and technologies that address the complex challenges of the twenty-first century.

During the steam era, the focus was largely on macroscopic physical properties and the statistical behaviors of gases and vapors. This period was marked by the development of thermodynamics, which provided a framework for understanding energy conversion and efficiency in steam engines and other heat-driven systems. The limitations of steam power, however, were evident in its reliance on bulky machinery, the inefficiency of heat engines, and the localized nature of power generation and distribution. The advent of the electrical age represented a quantum leap forward, not just in terms of energy production and utilization, but also in the granularity and precision of scientific research. Electricity offered an unprecedented level of control and versatility, enabling the study of individual atoms and molecules and the electronic properties of materials. This shift was pivotal for the field of materials chemistry, where the focus expanded from the collective behavior of particles in gases to the intricate details of solid materials, including their atomic and electronic structures.

Moreover, the electrical age has brought about significant advancements in energy sustainability and efficiency. Unlike the steam age, which was heavily dependent on coal and other fossil fuels, electrical power can be generated from a variety of sources, including renewable energy such as solar, wind, and hydroelectric power. This diversification of energy sources is crucial for addressing the environmental challenges of the twenty-first century, highlighting the role of electrical power not only in advancing scientific knowledge and technological capabilities but also in promoting sustainable development.

It's essential to emphasize that in the electrical age, the demands of the industrial sector have significantly propelled advancements in materials chemistry. This symbiotic relationship between industrial needs and scientific innovation has led to remarkable progress in materials development, directly influencing the efficiency, sustainability, and capabilities of modern technologies. The industrial demands for better performance, reduced costs, and enhanced sustainability have been key drivers in the evolution of materials chemistry. Industries reliant on electrical technologies, such as electronics, automotive, aerospace, and energy, have continuously pushed the boundaries of what's possible with current materials, urging scientists to innovate and develop new materials with superior properties.

In the electronics industry, for instance, the relentless pursuit of miniaturization and higher performance has driven the development of advanced semiconductor materials beyond silicon, including gallium arsenide (GaAs) and graphene. These materials offer superior electrical conductivity and electron mobility, enabling faster and more energy-efficient electronic devices. The quest for more efficient photovoltaic cells has similarly spurred research into novel materials that can convert sunlight into electricity more efficiently, such as perovskite solar cells, which offer a promising alternative to traditional silicon-based cells with the potential for higher efficiency and lower manufacturing costs.

The automotive and aerospace industries have also been instrumental in advancing materials chemistry, particularly in the development of lightweight and high-strength materials. The shift toward electric vehicles (EVs) and the need for longer battery life have intensified research into advanced battery technologies, including lithium-ion batteries with improved energy density and charging speeds. Materials such as carbon fiber composites and aluminum alloys have become crucial for reducing vehicle weight, enhancing fuel efficiency, and improving performance.

Moreover, the energy sector's shift toward renewable sources has catalyzed the development of materials that can efficiently capture, store, and convert energy. Innovations in materials chemistry have led to more efficient wind turbines, safer nuclear reactors, and more durable hydroelectric power facilities. The advancement of energy storage technologies, including supercapacitors and next-generation batteries, is critical for addressing the intermittency of renewable energy sources and ensuring a stable and sustainable energy supply.

This industrial push for innovation has not only led to the development of new materials but has also necessitated advancements in materials characterization and manufacturing techniques. Techniques such as atomic layer deposition, 3D printing of functional materials, and advanced microscopy and spectroscopy methods have evolved to meet the intricate demands of materials synthesis and analysis, enabling the precise engineering of materials at the atomic and molecular levels.

1.2.3 Other Energy Forms

Following the unprecedented technological progress made through the first two industrial revolutions, the field of materials chemistry has seen significant advancements. Subsequently, there emerged a variety of new energy forms, including nuclear power, lithium-ion batteries, hydrogen energy, and even renewable sources such as hydroelectric and wind power. Cleanliness and environmental sustainability have become the new benchmarks for future energy sources. However, from the perspective of researchers in the field of materials chemistry, the ultimate forms of new energy, regardless of the specific application scenarios, remain thermal and electrical energy. Although fundamentally, new energy sources have not revolutionized the basic modalities of materials science research from a theoretical or experimental standpoint, the development of new energy and its related industries has propelled significant growth in the discipline of materials chemistry, enabling a synergistic empowerment with other societal sectors.

The advent of these new energy sources has introduced complex challenges and opportunities for materials chemistry. The development and optimization of materials for nuclear reactors, for example, require an intricate understanding of radiation resistance, thermal conductivity, and mechanical strength. Similarly, the proliferation of lithium-ion batteries has spurred extensive research into electrode materials, electrolytes, and separators to improve energy density, charge rates, and safety profiles (Figure 1.3).

The development of both renewable and nuclear energy has significantly advanced the field of materials chemistry by creating a demand for new materials with unique properties. These materials are tailored to efficiently harness solar, wind, geothermal, and other renewable sources, as well as to withstand the demanding conditions of nuclear reactors. This dual drive toward sustainable and powerful energy solutions has led to a surge in research and innovation within materials chemistry, focusing on improving energy conversion, storage, and transmission.

Renewable energy development has promoted materials chemistry through the quest for more efficient and cost-effective solar panels, leading to research into novel photovoltaic materials like thin-film technologies, organic, and perovskite solar cells. In wind energy, advancements have been crucial in developing stronger, more durable materials for turbine blades to increase efficiency and lifespan.

(a) (b)

Figure 1.3 (a) Renewable energy: embracing a diverse array of sources like wind, hydro, and solar, renewable energy stands at the forefront of the global shift toward sustainable practices. It offers a promising avenue for reducing greenhouse gas emissions and minimizing our ecological footprint. As a key player in combating climate change, renewable energy not only contributes to a cleaner environment but also supports economic stability by creating jobs and reducing dependency on fossil fuels, encapsulating the dynamic progress and potential of sustainable development. (b) Nuclear power: with its immense potential and controversial implications, nuclear energy represents a double-edged sword, offering vast amounts of carbon-free power while posing significant challenges in terms of safety, waste management, and proliferation concerns, highlighting the complexities of navigating our energy future.

The integration of renewable sources into the power grid has also necessitated advancements in energy storage technologies, with materials chemistry playing a pivotal role in developing advanced electrolytes and electrode materials.

Photovoltaic Materials for Solar Energy. The quest for more efficient and cost-effective solar panels has spurred research into novel photovoltaic materials. Beyond traditional silicon-based solar cells, materials chemists have been exploring thin-film technologies, organic and perovskite solar cells, aiming to increase efficiency, reduce costs, and offer flexible, lightweight options for solar energy generation. This research directly responds to the renewable energy sector's demands for more versatile and efficient solar technologies.

Materials for Wind Energy. Advancements in materials chemistry have been crucial for the wind energy sector, particularly in developing stronger, more durable materials for wind turbine blades. Research into composites and polymers aims to create blades that are not only lighter and stronger but also capable of withstanding harsh environmental conditions, thereby increasing efficiency and lifespan of wind turbines.

Electrolytes and Electrodes for Energy Storage. The integration of renewable energy sources into the power grid has necessitated advancements in energy storage technologies, such as batteries and supercapacitors. Materials chemistry plays a pivotal role in developing advanced electrolytes and electrode materials that offer higher energy densities, faster charging times, and longer life cycles. Innovations in lithium-ion batteries, solid-state batteries, and beyond are directly driven by the needs of the renewable energy sector.

Materials for Hydrogen Production and Fuel Cells. The shift toward hydrogen as a clean energy carrier has promoted research in materials chemistry for efficient hydrogen production, storage, and utilization in fuel cells. Developing catalysts for water electrolysis, materials for hydrogen storage, and proton-exchange membranes for fuel cells are critical areas where materials chemistry contributes directly to advancing hydrogen as a renewable energy source.

Thermoelectric and Piezoelectric Materials. Renewable energy development has also accelerated research into thermoelectric and piezoelectric materials, which convert waste heat and mechanical energy into electricity, respectively. These materials offer potential for energy harvesting in a variety of settings, contributing to the efficiency and sustainability of energy systems.

Similarly, the development of nuclear power has necessitated the creation and improvement of materials capable of handling the extreme conditions of nuclear reactors, such as high temperatures and radiation. This need for specialized materials has spurred substantial research and innovation in materials chemistry, focusing on enhancing the safety, efficiency, and longevity of nuclear energy systems.

Radiation-Resistant Materials. The operation of nuclear reactors involves exposure to intense radiation, which can degrade many materials over time. This challenge led to the development of radiation-resistant materials, including specific alloys and ceramics that can maintain structural integrity and functionality in high-radiation environments. Research in understanding how materials interact with radiation has been a direct outcome of the nuclear power industry's requirements.

High-Temperature Materials. Nuclear reactors operate at high temperatures, necessitating materials that can withstand these conditions while maintaining strength and corrosion resistance. This requirement has driven advancements in high-temperature materials science, including the development of superalloys and advanced ceramics that can perform under the extreme thermal conditions found in reactors.

Fuel Cladding Materials. The development of materials for fuel cladding, which encases the nuclear fuel to prevent the release of radioactive particles, is another area where nuclear power has propelled materials chemistry. Innovations in zirconium alloys, for example, have been critical in creating effective fuel cladding that minimizes corrosion and allows for efficient heat transfer.

Coolant and Moderator Materials. The search for efficient coolant and moderator materials, which play crucial roles in the operation of nuclear reactors by managing reactor temperatures and neutron flux, respectively, has led to significant research in materials chemistry. This includes the development of liquid metals, gases, and graphite with specific properties tailored to nuclear applications.

Waste Management and Containment. The handling and containment of nuclear waste have necessitated advancements in materials capable of safely isolating radioactive materials from the environment for extended periods. This challenge has led to innovations in containment materials, including glass, ceramics, and cements, designed for long-term stability and resistance to radiation and chemical degradation.

Both the renewable and nuclear energy sectors have served as catalysts for significant advancements in materials chemistry, driving the development of new materials that enhance the efficiency, sustainability, and safety of energy technologies. This symbiotic relationship highlights the critical role of materials chemistry in powering the future with a blend of sustainable and reliable energy sources, showcasing the field's extensive contributions to addressing global energy challenges.

These advancements are part of a broader trend where materials chemistry is pivotal in tackling the energy challenges of the twenty-first century. The discipline not only provides new materials but also offers insights into the mechanisms at play within these materials, enabling the design of systems that are more efficient, sustainable, and environmentally friendly. Additionally, the intersection of materials chemistry with other industries has led to a fruitful exchange of ideas and technologies. For instance, developments in photovoltaic materials influence the automotive industry by enabling the creation of lighter, more energy-efficient vehicles. Similarly, advancements in materials for energy storage have significant implications for both the grid and transportation sectors, potentially revolutionizing energy consumption patterns.

In summary, while new energy forms have not fundamentally changed the theoretical or experimental foundations of materials science research, they have greatly expanded the field's scope and impact. The evolution of materials chemistry in response to new energy challenges exemplifies the dynamic nature of scientific inquiry, where advancements in one domain catalyze progress across multiple areas. This interplay between materials chemistry and new energy technologies underscores the field's crucial role in fostering a sustainable and technologically advanced future.

1.3 Data

The advancement of science and technology has significantly increased the precision of experimental testing, fundamentally improving our understanding of the relationships between structure and properties in materials chemistry. Enhanced experimental techniques, such as high-resolution microscopy and sophisticated spectroscopy, allow for detailed observations of materials at the atomic level. These insights are crucial for identifying how structural nuances influence material properties.

Furthermore, the integration of computational models with experimental data accelerates the exploration of new materials, enabling predictions about how changes in structure affect properties before physical experiments are conducted. Techniques like chemical vapor deposition (CVD) and atomic layer deposition (ALD) exemplify the precise control over experimental conditions necessary for synthesizing advanced materials with specific desired properties.

This improvement in experimental precision not only propels basic research but also drives technological innovations, such as more efficient solar panels and batteries with higher energy densities. As experimental methods continue to evolve, they promise to unveil new phenomena, enhancing our understanding of materials and opening up further possibilities for innovation. In essence, the progress in experimental accuracy enriches our material knowledge, catalyzing advancements across both scientific and technological landscapes.

From the era of steam engines to the electrical age, humanity has undergone a transformation in the way we harness energy, thereby accelerating the processes of material production and synthesis. This has naturally accumulated a vast amount of knowledge, transmitted through education across generations. However, due to various reasons, it is inevitable that knowledge will be lost or even inaccurately transmitted during the educational process. For example, the question of what a "dragon" looks like in Chinese mythology is difficult to answer definitively. Therefore, with the widespread adoption of computer hardware technology, transforming knowledge into data and storing it in hard drives can preserve it for many years. The key concepts of "data" and "many years" lead us to the fundamental characteristic of true technology: the ability to traverse time or space. We can express this in more complex terms using the language of physics: the implications of Noether's theorem (Noether 1918).

To illustrate this with a familiar example, consider the camera technology we are now very familiar with, which allows us to see photographs and images from decades ago. Similarly, telephone communication technology enables us to engage in real-time communication with friends thousands of kilometers away or even in space stations, disregarding spatial distance. Nowadays, camera and telephone technologies can be seamlessly integrated into a single smartphone, which is why companies excelling in this field, such as Apple, have become among the world's most profitable companies – a fact that should come as no surprise.

Let's consider the development of materials chemistry and the potential challenges it may face using the logic of time and space traversal. Firstly, chemicals themselves can be a part of smartphones, which is enough to demonstrate the importance of materials chemistry. This conclusion is correct, but the logic may not be. Currently, we generally believe that the emergence of products like smartphones has gone through a progression from non-smart to smart phones. The competitiveness of these products is not solely driven by their material composition. In simpler terms, the logic behind smartphone development is not primarily dominated by materials science.

Take another example, the pharmaceutical industry. The significance of high-quality drugs does not need overstating, and compared to the smartphone industry, the connection to chemistry is more intricate here. In a specific drug development process, numerous chemical molecules are tested based on demand, which is a complex and enduring process. Each chemical molecule in any testing stage may be proven unable to progress to the next stage. There are many blind spots in clinical stages, and selection can only be made based on experimental results. Therefore, drug development is a high-investment, high-risk industry. Thus, whether in the smartphone or pharmaceutical industry, chemical materials are objects of selection rather than having the power of active choice. In simple terms, many industries require the properties of chemical materials, but these properties cannot be mapped directly to structure, necessitating a lot of experimentation. This extensive experimentation itself consumes a lot of time and resources, and even after numerous attempts, the expected results may not be achieved. Meeting the expected results at one stage does not necessarily mean meeting the expected results at the next stage, leading to wasted efforts. Understanding this, you might understand why materials chemistry is not a popular major in universities, especially when a large number of repetitive experiments currently rely on human labor, with low success rates after time investments. Of course, there are also factors such as high personal safety risks and high degree of repetition.

From the described phenomena above, two main problems arise:

1. The ambiguous relationship between structure and performance.
2. Lengthy testing cycles for experimental data.

We see that these are still problems related to time and space. The corresponding solutions are, then:

1. Clarifying the complex relationship between structure and performance.
2. Shortening the testing cycle.

These solutions might seem like they're saying everything and nothing at the same time. Indeed, many problems have similar answers. The answer to the first problem is knowledge, while the answer to the second problem is execution. Interpreted through ancient Chinese wisdom, this is "unity of knowledge and action."

Let's first explore the realm of knowledge. We've elaborated on the journey from the era of steam engines to the current electrical and new energy era over the past 200 years. Throughout this process, the discipline of materials chemistry has been present and has accumulated a vast amount of knowledge and technology. Objectively, it has also promoted the development of other disciplines. However, the primary contributors and holders of this knowledge and technology have been the traditional developed countries such as Europe, North America, and Japan. Most of the powerful materials chemistry giants undoubtedly hail from these countries.

Now, let's briefly examine the situation of materials chemistry in China. Since joining the World Trade Organization in 1999, China's chemical industry has undoubtedly become one of the most important components of the global chemical industry. Chinese universities and research institutes have surpassed the United States in publishing academic papers in the field of chemical materials, becoming the world leader. It took less than 30 years for China to catch up from a relatively backward state, which could not have been achieved without mutual learning and communication with countries worldwide. The most significant aspect we observe is the tremendous change brought about by the transmission of knowledge. We can roughly estimate that China has learned and mastered approximately 200 years' worth of knowledge in just 30 years, leading to enormous economic and academic growth.

Let's carefully contemplate the two numbers and the logic behind them. The process of these 30 years is driven by continuous human effort, whether it's physical laborers or academic workers contributing. The most typical data point is the significant increase in urbanization rate and the expansion of universities, both in terms of the number of students and research personnel. In line with our previous discussion, this is a chemically driven process. However, the essence of the knowledge gained over these 200 years is essentially stock knowledge. In terms of incremental knowledge, cutting-edge biotechnological materials technology still needs to be imported from Western countries. Here, we would not go through the international geopolitical and economic issues. If we merely consider China's materials chemistry industry as a model, we can summarize its characteristics: acquiring a vast amount of knowledge in a short period and naturally predicting its future demand, which is to acquire even more knowledge in a shorter time. It's essential to note that here we are referring to "knowledge," not just "technology."

Let's take a look around. In today's electrified age, a large number of factories, including chemical plants, produce various chemical industrial products in large quantities through automation technology. One reason for this mass production is that mechanization and automation have replaced manual operations with standardized procedures, thereby significantly increasing the number of finished products per unit time and reducing costs. Robots and automation technology are widely used in the industrial sector, enhancing production efficiency and product quality. However, their application in chemical, materials, and biological laboratories is relatively limited. Why is that?

The reason lies in the stark differences between technological implementation in industry and knowledge realization in academia, in terms of quantity and process requirements. One involves the systematic digestion of existing knowledge, while the other entails free exploration for incremental transformation. Thus, even though chemical plants around us started automating and digitizing much earlier than 50 years ago, and despite having more and better-quality experimental testing equipment, the layout of chemical materials laboratories has not changed significantly. As shown in the images below, on the left is a picture of a chemistry laboratory at Beijing Institute of Technology in 1960, and on the right is a picture of a chemistry laboratory at a certain university in 2024. Both images show rows of experimental workbenches, cabinets underneath, and many chemical reagents and drugs on the workbenches. Despite spanning 64 years, there is no significant difference between the two images. We still rely on our graduate students and postdocs to operate chemical containers and obtain experimental data, and the entire process of chemical experimentation has not achieved automated and intelligent assembly-line-style operation (Figure 1.4).

Indeed, we can argue that the complexity and variability of laboratory work, along with the need for flexibility and specialized knowledge, make it challenging to achieve automation. However, from a solution perspective, there is not much difference compared to solving other physical chemistry problems. We start by addressing one point, then move on to handling the relationships between this point and others, and gradually address the relationships between more points. Although the reagent bottles used in chemical experiments are standardized – for example, in my laboratory, we only have three types: 10, 100, and 500 ml bottles – we cannot demand standardization when it comes to the actions of our students. For

(a) (b)

Figure 1.4 The chemistry lab in (a) 1960s (SinaEducation 2010) and (b) 2024.

instance, we cannot insist that they must assemble a 100 ml reagent bottle within one minute, and that the turbulence bubbles in the solution must be uniform. While the latter may be difficult to achieve, the former could be easily realized through automation technology. However, it may not seem necessary to limit the assembly time to one minute until we realize that the time for reagent preparation may have subtle connections with the quality of the final product.

There is another crucial logical issue here. In the history of chemical materials development, many significant discoveries have occurred due to accidentally using the wrong reactants or incorrect amounts of reactants. For example, the discovery of conducting polymers, which began with Hideki Shirakawa's accidental discovery in 1971 (Shirakawa and Ikeda 1971). At the time, he was supervising a group of South Korean exchange students conducting experiments on the synthesis of polyacetylene. Perhaps due to a language barrier, the students mistakenly increased the amount of the designated catalyst, the Ziegler–Natta catalyst, by thousands of times. As a result, they produced a silver-colored polyacetylene film, overcoming the challenge of synthesizing highly crystalline polyacetylene. The lightweight structure obtained provided an excellent foundation for future doping to enhance electrical conductivity. If Shirakawa had used a machine to precisely conduct the experiment, such an important discovery might not have been made. Although this is a relatively specific example, it is certainly not an isolated case. Historically, laboratory practitioners seem to not prefer automated equipment and consider experimental operations as an integral part of the experiment itself. There are two specific issues here.

Firstly, many researchers do not handle multiple experimental tasks and requirements simultaneously. In the same period, many experimenters often only need to focus on a specific project. This may be determined by the project's budget, timeline, and the current research paradigm. Conversely, pharmaceutical companies have different practices. Over 30 years ago, many pipetting workstations were already in operation. Although these workstations generate vast amounts of research data every day, when I deployed such a workstation at a Chinese university in 2023, I found that the doctoral students there did not frequently use the machine. One reason is that they could not handle so many samples at once.

We have learned about the significant differences between university laboratories and corporate laboratories, as well as the reasons why it is more challenging for university laboratories to adopt intelligent and automated equipment: the conflict between academic credit and task division. In a corporate setting, each position has very detailed task division, so there are clear application scenarios for accelerating processes through automation equipment. However, university laboratories are different. Academic credit for research achievements is a crucial indicator, so it is not feasible to distribute tasks or outsource them through assembly-line-style operations. Researchers theoretically need to be familiar with all aspects of the research process, especially many sequential steps. Researchers need to understand detailed information about all aspects to design and correct the next experimental operation. Current experimental automation equipment focuses on the needs of pharmaceutical companies and other discrete experiments within enterprises but does not provide intelligent equipment with a full-process information architecture. Therefore, for specific chemical materials researchers, the use of local automation acceleration equipment, including pipetting workstations, does not significantly promote research efficiency. Therefore, the main reason why the current paradigm of chemical material science research, mainly led by universities and research institutes, has not achieved a paradigm shift is that there is no automation stage, and it must directly enter intelligence.

I mentioned earlier that in the future, whether in China or the world, the chemical materials industry or any other industry will need to master more knowledge in a shorter time. The above paragraph explains why "intelligent" equipment, rather than "automatic" equipment, is the solution for "shorter time." Next, we need to explain what the solution for "more knowledge" is. Suppose a laboratory researcher synthesizes a chemical molecule that contributes to the treatment of a certain disease. Is this molecule knowledge? Of course, it is, but it is far from enough. The full process information including reaction conditions, synthesis pathways, and various experimental details involving this molecule is more critical knowledge, and the amount of knowledge is closely related to the amount of information. Here, we need to mention the difference between patents and papers. In order to protect the intellectual property related to the knowledge, a patent related to molecule synthesis often discloses many process details, which are protected commercially, but still promote knowledge dissemination. Authors and readers of academic papers often focus more on the conclusions themselves and may not deliberately detail the implementation process because they care more about personal academic credit, and academic papers themselves are not a form of protectable intellectual property. Of course, there are many other problems in the academic paper field, such as unreliable conclusions, poor reproducibility, repetitive research, academic integrity, and so on, which can seriously hinder or even mislead knowledge dissemination. There are countless similar events, and dealing with these problems is very difficult. For example, an American scientist misled the work of 100 research groups in China for 10 years with a false paper, and there is currently no organization that can handle such incidents. In comparison, patents are much simpler, and problems can be solved through domestic or international legal means (Figure 1.5)

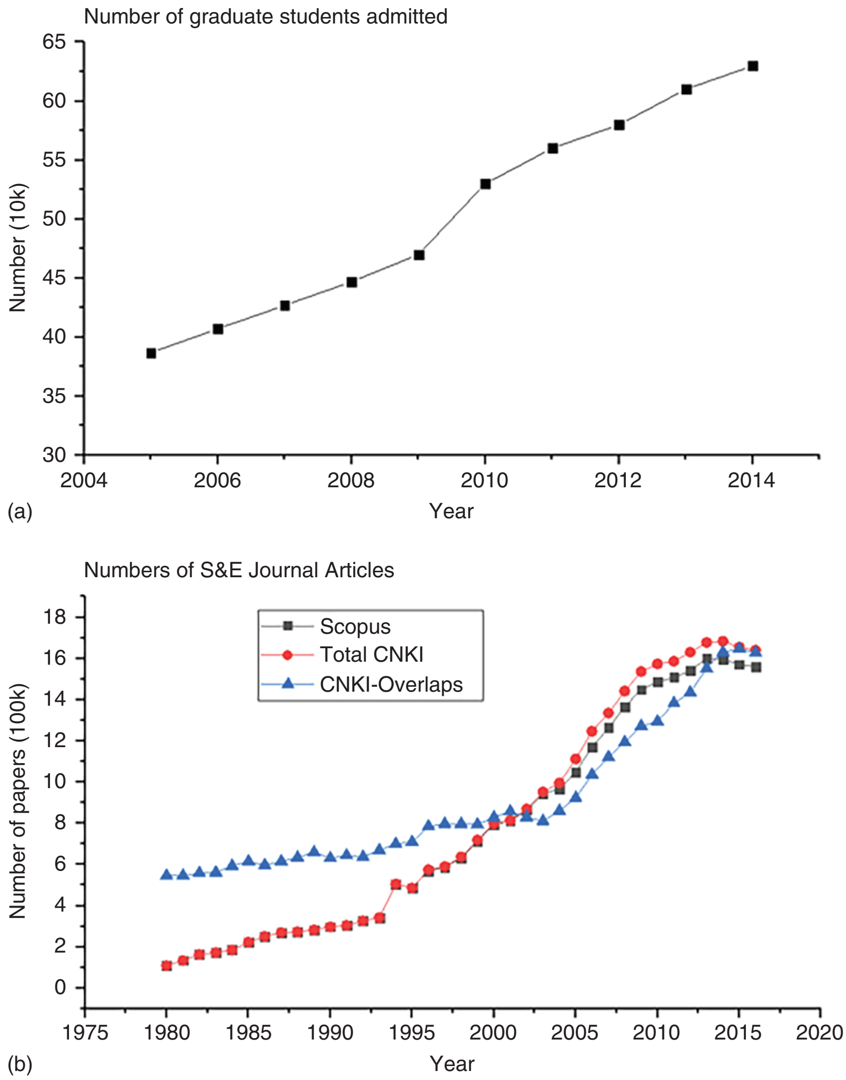

Figure 1.5 (a) The number of graduate students in China has grown since 2004 by about 80% by 2014 (ChinaEducationOnline 2015). (b) The numbers of S&E Journal Articles in Scopus and in CNKI, 1980–2016 (VoxChina 2018).

Let's discuss the issue of the rate of knowledge generation using academic papers as an example. A report (Miyazaki 2023) by *Nature* journal in 2023 stated that China had surpassed the United States in the number of high-quality journals indexed in the Nature Index, with the number of journals in the field of chemical materials surpassing even earlier. There are certainly many reasons why China has achieved this surpassing. Let's take a look at the two charts above. We can observe that the number of graduate students enrolled in China has increased from approximately 360,000 in 2005 to about 640,000 in 2014, an increase of about

80% (ChinaEducationOnline 2015). Meanwhile, the number of scientific and technological papers has increased from about 800,000 in 2005 to about 1.6 million in 2014, a growth of about 100% (VoxChina 2018). We notice that these two numbers are very close, indicating that the increase in the number of papers in China cannot be separated from the expansion of the number of graduate students, including in the field of chemical materials science. If we assume that, on average, an academic paper in the field of chemical materials represents the synthesis or discovery of a new material, then is the rate of discovering new materials meaningful?

Actually, it is not meaningful because it is still too slow! We can do a simple and rough calculation to estimate how many chemical experiments we can conduct. Figure 1.6 summarizes and classifies the total ~2 million papers published in the field of materials science in 2022 through our KnowledgeWorks (Yanheng et al. 2024), divided into 15 categories based on application scenarios, including Energy Storage and Conversion, Catalysis, Environmental Applications, and other familiar categories. Each application scenario can be achieved through a maximum of eight experimental methods. Let's assume there are a total of 1 million reagents, 10 reaction steps, 100 solvents, and up to 4 solvent mixtures, as well as approximately 100 reaction conditions for each of the 10 reaction steps. Calculating this, we find:

$$15 \text{ Applications} \times 8 \text{ Methods} \times (10^6 \text{ Reagents})^4 \times (10^3 \text{ Conditions})^{10} > 10^{100}$$

This means that exploring all known chemical reactions would require a dataset of one Googol (10^{100}), while the amount of data currently explored by humanity is probably less than 10^{10}. Perhaps under the current research paradigm, we can still make many significant discoveries, but the overall conquest still seems far out of reach (Figure 1.6).

This is the biggest challenge in the field of chemical materials science. Currently, it is still driven by human chemistry, much like agricultural societies, where the production of agricultural products is almost entirely linearly dependent on the number of laborers, and a country's overall strength is closely related to its population. Therefore, we often see in some countries that pursue scientific research outcomes, many research teams with hundreds of members, most of whom are graduate students. If we liken the discovery or synthesis of new chemical substances to a treasure hunt

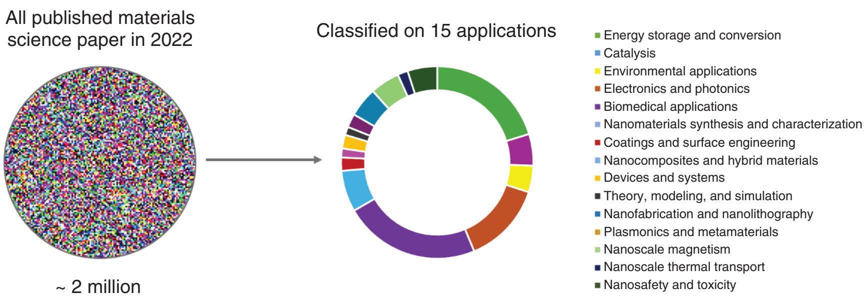

Figure 1.6 There have been ~2 million papers published in materials science since 2022. The papers can be classified according to applications into 15 categories, as shown in the figure. They can also be classified to 8 methods, 10^6 reagents, 10^2 solutions, 10^3 conditions.

game, are players driven by electricity more likely to discover targets faster and more often than players driven by chemical energy? This question is actually difficult to answer because both intelligence and physical strength are indispensable in a treasure hunt game. Electricity may make physical activities easier, but this logic does not necessarily apply to intelligence. So, let's switch to a different analogy: if the same person drives a Tesla and rides a horse, which situation is more likely to discover targets faster and more often? The answer to this question is probably self-evident.

So, can using intelligent machines alone accelerate the discovery of new materials and processes? The answer is also negative. Machines only provide a linear increase in experimental operations compared to human researchers, and this linear coefficient is not particularly large. From my personal experience, it may be around 20 times. The biggest problem with linear relationships is their linear relationship with time, meaning that achieving large-scale knowledge innovation will take a very long time in the future. This is not a reasonable scientific framework; it lacks imagination. Let's imagine a completely new mathematical formula:

$$F_{n+1} = F_n + F_{n-1}$$

Now let's define $n+1$ as tomorrow, n as today, and $n-1$ as yesterday. Let the function F represent the amount of data in a particular industry or chemical experiment. Then this sequence is the famous Fibonacci sequence, with the first few terms being: 1, 1, 2, 3, 5, 8, 13, 21, 34, and so on. The general form is: $F_n = \frac{\phi^n-(-\phi)^{-n}}{\sqrt{5}}$, where $\phi = \frac{1+\sqrt{5}}{2}$. When n is large, F_n is proportional to ϕ^n. Finally, we see an exponential growth relationship.

At first glance, does this look very familiar? Yes, it is indeed the mathematical principle of the famous golden ratio, where the artistry of science is vividly demonstrated. Taking a closer look, it becomes even more familiar. Essentially, this is what current large language models are doing: packaging all historical data for training, starting with F_{n-1}, and then incorporating all incremental data from today onward. For text, video, and other information on the internet, due to relatively uniform data formats and the accumulation of technical expertise in this area, technologies like ChatGPT and Sora have been impressive since their inception. If it were possible to generate new chemical materials with just a prompt word like Sora, how would we need to reconstruct our databases and algorithms?

References

Arrhenius, S. (1889). Über die Dissociationswärme und den Einfluss der Temperatur auf den Dissociationsgrad der Elektrolyte. *Zeitschrift für Physikalische Chemie* 4 (1): 96–116.

Ashcroft, N.W. and Mermin, N. (1976). *Solid State Physics*. Saunders Collage Publishing.

ChinaEducationOnline (2015). The popularity of postgraduate applications slows down and the enrollment crisis begins to spread. Retrieved from https://www.eol.cn/html/ky/report2015/a2.shtml.

Griffiths, D.J. and Schroeter, D.F. (2018). *Introduction to Quantum Mechanics*. Cambridge University Press.

Miyazaki, A. (2023). New Nature Index data shows China on top for natural sciences as US leads on health sciences research. Retrieved from https://www.natureasia.com/en/info/press-releases/detail/8966.

Noether, E. (1918). Invariante variationsprobleme. *Nachrichten von der Gesellschaft der Wissenschaften zu Göttingen, Mathematisch-Physikalische Klasse*, pp. 235–257.

Röntgen, W.C. (1896). On a new kind of rays. *Science* 3 (59): 227–231.

Shirakawa, H. and Ikeda, S. (1971). Infrared spectra of poly (acetylene). *Polymer Journal* 2 (2): 231–244.

SinaEducation (2010). Old photos of Beijing University of Technology: Chemistry Experiment Class in the Laboratory (pictures). Retrieved from http://edu.sina.com.cn/gaokao/2010-07-13/1131258180.shtml.

VoxChina (2018). China's Overwhelming Contribution to Scientific Publications. Retrieved from https://voxchina.org/show-3-99.html.

XU, Y., Ye, S., Liu, R. et al. (2024). Spider Matrix: Towards Research Paper Evaluation and Innovation for Everyone. *ChemRxiv.* doi: 10.26434/chemrxiv-2024-689vs-v4.