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Physicochemical Studies of Water and Their Application in Environmental Protection and New Energy Development

Water is the most fundamental and important substance in nature. It has been intensively studied, but there is still much we do not know about it. The sustainable utilization and protection of water resources constitute one of the most formidable challenges to human beings in the 21st century. This is especially true for many developing countries, particularly China.

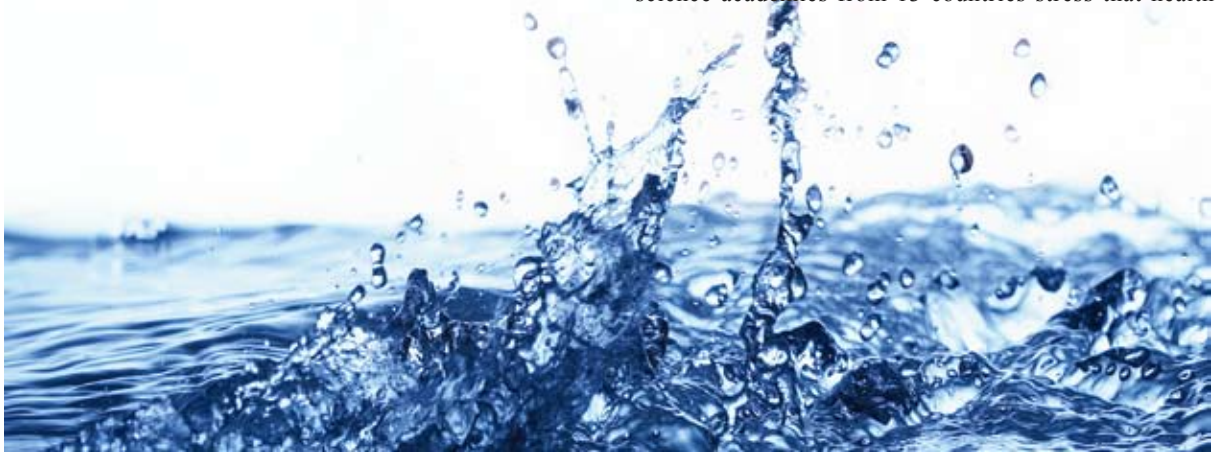
While water can be split into oxygen and hydrogen when absorbing enough energy, it can be produced by burning hydrogen gas, which releases energy. Therefore, water can be used as a carrier and medium for renewable and clean energy sources. Basic research of water science plays a vital role both in water purification for human health and in renewable energy acquisition and utilization for high-tech development. At present, a bottleneck in the large-scale application of water research and development concerning the above-mentioned two aspects is a lack of low-cost, high-efficiency materials and devices. Therefore, breakthroughs are urgently needed in basic research, especially the mechanisms behind the interaction between water and materials interface.

A report was recently completed on the basis of a research project on major issues for the development of basic water science research in China under the auspices of the Academic Division of Mathematics and Physics. The following are major ideas of the report.

1. Importance of Water Studies

With the rapid growth in global population, the environment and water resources on the planet are under huge pressure. Drinking water safety has become a major issue affecting people's life and health, especially for those in developing countries. In China, water pollution has severely hampered its industrial and agricultural development and ecological protection, with grave impacts on living standards and health. The discharge of untreated domestic and industrial sewage has increasingly polluted both surface waters and groundwater. With the growing amount of industrial and domestic sewage in urban and rural areas, and increasing application of pesticides and chemical fertilizers, many drinking water sources have been contaminated. Because of this, it is difficult to safeguard the health of residents who drink directly from surface or shallow water sources. China's access to the WTO and economic globalization are imposing more and more international trade barriers on products containing toxic or otherwise dangerous matter. In part for this reason, China now has a huge water purification and supply industry, with a total annual investment of up to about US$250 million. It is expected to reach $660 million by 2020.

In a joint statement released on May 19, 2011, the science academies from 13 countries stress that health



issues associated with unsafe water have greatly impaired economic activities, social progress, education and public health. It strongly urges governments across the world to develop basic infrastructure for sanitation and maintenance, boost education, and promote low-cost and efficient water treatment technologies and related disease prevention methods.

On January 29, 2011, China's central authorities released a decision on accelerating water conservancy reform and development. As the first drive for systematic reform in the field, the document shows the deep concern of policy-makers over water issues. Promulgated in March of the same year, the Outline of the 12th Five-year Plan for Social and Economic Development also emphasizes the people's wellbeing improvement and leapfrog development. Therefore, we must work hard to make arrangements for accelerating basic research into water science. It will be of strategic importance to improving people's wellbeing, safeguarding national security, achieving the goals of the Outline of medium- and long-term Planning for Science and Technology Development (2006-2020), and upgrading China's economy, frontier science and major engineering projects.

2. Tremendous Challenges Facing Basic Water Science Research

First, although basic water science research has an important bearing on the national economy and people's livelihood, observes the report, it receives inadequate attention in the national strategy. Without systematic organization, guidance and support, research activities in the field are mainly ad hoc, and its disciplinary system is incomplete. In addition, there is a lack of understanding of its strategic role, scope and profundity.

Even as we hear praise of China's economic miracle, its "soft constraints" such as water shortages become more obvious. While maintaining the momentum for economic growth, we should ensure people's health through environmental protection, water pollution prevention and the development of advanced and operational technologies to harness drinking water sources and improve drinking water quality.

To address technological bottlenecks in the safe utilization of water sources for environmental protection and energy development, it is urgent to launch basic research into water science, especially the basic forms and rules of interactions between water and surface/interface. For instance, is it possible to find safe, efficient and long-lasting water purification materials to deal with water crisis? Is it possible to develop low-cost, highly efficient catalysts for producing hydrogen or oxygen compounds using light and water? Specifically, work should be done to find appropriate, low-cost water treatment materials, further upgrade light energy conversion efficiency of semiconducting materials, and reduce the costs of devices for water purification and energy conversion. This research involves a variety of areas, ranging from the microstructure of surface water and interactions between surface materials and water, to the wettability, chemical activity, and stability of new materials and photoelectric splitting mechanisms of surface water. As they fall into different research fields, like surface, chemistry and materials, their solutions need basic research. Studies of water splitting and purification are very complex. Although basic and applied basic water science research accounts for about 10% of the studies in the field, it will impact all sides of the water issue.

There is currently a lack of understanding of the strategic role of basic water science research and of its depth and scope. And investment in the field is limited. Given the strategic role of water issues in China's vigorous development and China's position in the world, this situation must be remedied.

Second, there is a lack of unified planning for the development of fundamental theoretical research in water science and experimental techniques. The planning for fundamental water science research is even replaced by that for water resources.

At present, there is no unified planning and guidance for the development of fundamental theoretical water science research and experimental techniques. A "laissez faire" policy has been adopted vis-à-vis this research, an area of great strategic importance. This will exert a negative or even harmful impact on the development of a science with important bearing on national economic development and people's livelihood and a country at a critical stage of development.

To make things even worse, there is a trend of simply using water resources research and development planning to replace that of basic water science research and development, which is both misleading and dangerous. Basic water science research is different from water resource development research. The former is a necessary discipline providing important basic knowledge for the latter. The development of water resources studies often depends on breakthroughs in basic water science research for renovation of existing water resource engineering treatment technologies, the invention of new sewage treatment technologies and addressing the challenges of water depletion. Strengthening institutions or platforms specializing in basic water science research is urgently needed.

Third, there is a lack of long-term objectives to develop new materials for sewage treatment and water decomposition in basic water science research.

There is no unified planning and long-term goals for major areas in basic water science research and the development of new materials for wastewater treatment. There are no guidelines to bring coherence to the isolated ongoing studies in the field. Aiming at greatly facilitating water pollution control and water treatment for people's wellbeing, the development of basic water science research is needed to lay a solid foundation for potential new applications and technologies, especially for the development of new materials based on an understanding of the interactions between water and substances. It is urgent to develop new materials for water treatment with major applications and to work out relevant long-term development planning and objectives.

Fourth, there is a lack of experimental instruments and means for exploring the physical mechanisms underlying water/materials interface reactions at the molecular and atomic levels.

One major aspect of basic research in this regard is to probe into the interactions between water molecules and other substances. Because these interactions occur through interfaces between them, it is necessary to examine the properties of water on the interfaces and the interfacial properties of water itself (often referred to as "properties of water at interfaces"). To deeply understand these interactions, we need to explore, at the microscopic and even atomic/molecular levels, microstructure, charge distribution and transfer patterns. It is very difficult to study water at interfaces, and because of weak interactions between water and interfaces and among water molecules, the interface structures are easily damaged during the exploration. Therefore, we should made special efforts to develop interface-sensitive and nondestructive experimental methods and means, such as nonlinear optical methods (sum frequency generation vibrational spectroscopy) and advanced scanning probe techniques.

Fifth, there is no overall planning for research and industrial development at the national level in the field. On the one hand, low-level application is emphasized at the expense of conceptual, systematic and methodological breakthroughs from basic research. On the other, some practitioners of basic research tend to go after publishing low-level papers without concern for practical application.

Because of a poor understanding of the strategic role of basic water science research, the lack of national planning for basic research activities, and the lack of guidelines and key knowhow for water treatment materials development, there is no unified national planning and management system for integrating a variety of research activities and related industrial development, ranging from basic research to applied research and development to macroscopic water resources management. Due to the disconnection between the different links, there are no efficient exchanges or mutual promotion between them, which hinders the sound development of water science. In terms of industrial application, for example, there is a lack of conceptual, systematic and methodological breakthroughs from basic research, and a one-sided stress on low-level macroscopic application. Moreover, some researchers seek to publish low-level papers without forming a virtuous cycle of practical application.

Sixth, there is a serious shortage of interdisciplinary professionals, causing insufficient cultivation and retention of personnel in basic water science research.

Water science is a comprehensive branch of science involving many disciplines, such as physics, chemistry, materials, biology and engineering. Because of S&T advances and the complexity of water pollution, researchers in the field need basic knowledge of many such disciplines, which necessitates high requirements for the training of researchers in the field.

At present, water science researchers are mostly graduates in such disciplines as water supply and sewerage, environmental engineering and related engineering fields. While they are trained to solve practical problems in water pollution control with an emphasis on practical knowledge and engineering application, they have insufficient basic knowledge of water science. They generally lack the theoretical background, especially in physics and chemistry, for understanding, analyzing and solving basic problems of water science. It is therefore difficult to conduct high-level research with the current training approach.

3. Recommendations

To accelerate basic water science research in China, says the report, it is necessary to speed up the establishment of a key national research program and a national research platform with basic water science research and applied basic research of environment and energy as its core. This would unify the planning, organization and leadership of China's water science development.

First, to formulate an overall strategy for the development of basic water science research in China and work out medium- and long-term development plans according to national needs.

While formulating national planning for basic water science research, priority should be placed on

the central tasks of coordinating research forces in the field and organizing and leading activities to deal with development issues of this research. Efforts should be made to promote an understanding in many sectors (especially environment, resources, industry and the scientific community) of basic water science research. Channels should be opened to facilitate exchanges, communication and mutual improvement among a variety of key areas, ranging from basic research and materials development to industrial applications and national water resource and water environment management. We should strengthen the cultivation of interdisciplinary professionals with the depth and breadth of knowledge and perspective needed to satisfy the future needs of basic water science research. We should also plan the strategy and objectives for overall development of basic water science research in China and formulate medium- and long-term planning in the light of overall national development.

Second, define clear research directions and strive to make major breakthroughs in selected areas of basic water science research.

We should strengthen research in the following key areas:

(1) Microstructure and dynamic behavior of water on the surface/interface of materials,

(2) Photolysis of persistent organic pollutants in water;

(3) Nano-scale water membranes interface,

(4) Energy transfer process of, and new materials for, photocatalytic decomposition of water.

Third, make great efforts to address key technological challenges.

It urgent to deal with key technological challenges in basic water science research, including:

(1) Nonlinear optical methods, such as sum frequency generation vibrational spectroscopy,

(2) New generation scanning probe technology,

(3) Surface femtosecond two-photon photoemission spectrometry

(4) Combination of femtosecond laser spectrometer and STM technology,

(5) Synchrotron radiation optical methods,

(6) Accurate theoretical computing methods.

Fourth, greatly promote the connection between basic water science research and industrial applications such as clean water and clean energy; strengthen its coordination with disciplines such as climate, geography, energy and nanotechnology; coordinate joint research institutions in basic and applied water science research; establish step by step a unified system from basic research to practical application, and thereby advance the innovation and sustainable development of water science and technology in China.

Efforts should be made to facilitate the integration between basic waterscience research and applied projects, such as clean water and clean energy, and the interdisciplinary cooperation of researchers in water science, climate, geography, energy and nanotechnology.

Importance should be placed on the development of nanotechnologies on the basis interaction at the water interface. We will strive to develop a new generation of efficient and stable visible light-induced nano-catalytic materials through energy band structure design of nanomaterials and surface electron transfer of nanomaterials.

To foster the innovation and sustainable development of water science in China, we should: promote a holistic consideration of water issues; pool research forces in different disciplines, from basic research to applied research; set up a unified system from basic research to practical application; promote a virtuous cycle and exchanges between the many fields involved.

Sixth, enhance training of interdisciplinary research professionals for basic water science research.

As a long-term and difficult task, water science studies should be planned at the national level in a comprehensive way. It is urgent to design and implement a training program for water science studies in such fields as theoretical modeling and simulation computing, surface physics analysis, materials preparation and characterization, optics/electronics measurement and technique, chemistry and environmental sciences. Efforts should be made to introduce high-caliber researchers, build up an echelon of human resources at various levels, and coordinate researchers to undertake large research projects. Its objectives are to train interdisciplinary researchers at different levels, including leading scientists, so as to advance highly-focused basic water science research and China's water environment engineering and new energy industries.

Given the current demand and disciplinary structure of human resources in water science, it is advisable to conduct pilot studies in selected universities, such as Peking University, the University of Science and Technology of China and Fudan University, for the training of future high-level research talents. We should develop an education system featuring the broad theoretical base of physics and chemistry, practical teaching for qualified and innovative researchers, and a training system for bachelor's, master's and doctoral degree holders.