Department of Chemical Sciences

The Department of Chemical Sciences covers two first-grade disciplines (chemistry and chemical engineering) and is divided into five divisions (including seven disciplines): Division I for inorganic chemistry and analytical chemistry, Division II for organic chemistry, Division III for physical chemistry, Division IV for polymer science and environmental chemistry and Division V for chemical engineering. Researches in chemical sciences focus on the change of matters and chemical reactions, and not only maintain close ties with but also intercross and permeate into other disciplines, such as information science, life science, materials science, environmental science, energy science, earth science, space science and nuclear science. Chemical engineering is to accomplish the transfer and conversion of matters and energy by making use of the principles of basic disciplines, and to solve scientific problems in achieving large-scaled production of chemical materials and products.

The mission of the Department is to promote the development of chemistry and chemical engineering, to strengthen original innovation in basic research so as to bring into full play its roles as core science in multidisciplinary research, to improve the overall quality and international status of chemical science and to foster creative talents and groups. It supports research of Pan Molecules to find more types and patterns of molecules at different levels and to control chemical reactions and processes. It encourages multi-level and multi-scale research proposals that take atoms, molecules, molecular aggregation and condensed state as well as those of complex systems as their objects of study. In order to bring the role of chemistry and chemical engineering into full play to address major scientific issues related to the national economy, social development, national security and sustainable development, it encourages research of chemical sciences and chemical engineering conducted in the fields of life, materials, energy, information, resources environmental science and human health. As for the methods of study, it stresses the combination of (1) microscopic and macroscopic research, (2) static and dynamic states, and (3) theoretical research and empirical development of novel experimental methods and analytical technologies. It also encourages the introduction of latest theories, technologies and achievements from other disciplines, aiming at promoting innovation and interdisciplinary studies, and supports the emerging frontiers in research.

In the Eleventh Five-Year Plan period, China will strive hard to hold a major position in the international frontiers of chemical science. To achieve this goal, the Department energetically promotes high quality research in the fields of cutting edge science, lays stress on in-depth and systematic work, and gives priority to those interdisciplinary research projects. It takes effective measures to support original creative researches with high risk. The stress of Young Scientists Fund is to support projects with new ideas. Less attention will be given to the weight of research background in the review process so as to encourage young talents for innovative research. Scientific value will be emphasized

through out the review procedure and the balanced, coordinated and sustainable development of different disciplines will be focused on to enhance the quality of China's basic research of chemical sciences. Moreover, the Department will work hard to reach the developing goals and to carry out the strategic plans suggested by NFSC in the Eleventh Five-year Plan.

Funding for Free Application Projects in Recent Years

Unit: 10, 000 yuan

Scientific division		FY 2005			FY 2006		
		Projects granted		Rate (%) ***	Projects granted		Rate (%) ***
		Number	Funds		Number	Funds	
Chemistry I	Inorganic chemistry	105+11*	2,818	22.97	115+15*	3351	22.03
	Analytical chemistry	96+10*	2,659	22.55	108+13*	3134	20.37
Chemistry II	Organic chemistry	171+16*	4,766	24.90	182+21*	5287	22.26
Chemistry III	Physical chemistry	165+17*	4,465	26.57	184+22*	5385	24.44
Chemistry IV	Polymer science	108+10*	2,904	27.96	120+14*	3502	22.91
	Environmental chemistry	89+10*	2,452	19.11	102+13*	2967	18.76
Chemistry V	Chemical engineering	161+15*	4,267	18.92	178+22*	5222	17.73
Total		895+89*	24,331	22.99	989+120*	28848	21.06
Average amount per project		24.72 (26.39**)			26.01 (28.12**)		

Notes: * The number of projects of Small Fund for Exploratory Studies.

** The average funding of 3-year projects of General Program (not including projects of Small Fund for Exploratory Studies).

*** The rate is calculated on the basis of all projects (including projects of Small Fund for Exploratory Studies).

In FY 2007, the number of projects supported is to be the same as that in FY 2006. The average funding of 3-year project is about 300,000 yuan for Free Application projects and 260,000 yuan for projects of Young Scientists Fund and that of Less Developed Regions.

Division I of Chemistry

Research projects supported by the Division fall into two disciplines: inorganic chemistry and analytical chemistry.

Inorganic Chemistry

The intercrossing and fusion of inorganic chemistry with materials science and life science are current trends in disciplinary development. Great efforts should be made in the following fields: 1) Developing new synthetic methods and ways in the studies of synthesis and preparation; 2) Employing the concept of molecular design and crystal engineering on research related to the synthesis of new compounds and the aggregate state of matters; 3) Emphasizing studies on the composition, assembly and hybridization of inorganic functional materials; 4) Strengthening research on relations between the structure and property of functional inorganic matters and supporting theoretical studies on mesoscopic and microscopic structures; 5) Intensifying in-depth interdisciplinary research on inorganic chemistry and life science, especially chemical study of biological effects of inorganic elements. 6) Developing basic research on new types of metal combined bio-macromolecules, inorganic bionic processes and bioinorganic chemistry beyond molecular level.

In the past few years, the number of proposals for coordinated chemistry, molecular-based materials chemistry and inorganic nano-material chemistry represents a large proportion in General Program projects funded by the Division, which is in line with the development trend of the discipline. These fields will remain key funding areas of the Division. Proposals related to new type inorganic compounds and new synthetic methods, reaction processes and relations between structures and properties are declining. So are those for bioinorganic chemistry and radiochemistry. More proposals in these two fields are expected. New ideas appear in quite a number of proposals while original creativity is still to be encouraged. In general, research on fundamental theories should be strengthened, the consciousness of exploration and creativity should be enhanced, and the depth of research on inorganic chemistry should be increased.

Proposals are encouraged in the following research areas:

- Synthesis, reaction, structures and properties of new inorganic compounds;
- Design and synthesis of functional inorganic materials;
- Theoretical inorganic chemistry;
- Chemistry of informational opto-electronic materials and original-type devices;
- Basis of nano-chemistry;
- New types of functional coordinated complexes;
- Assembly, structure and properties of super-molecular compounds;
- Chemical basis of inorganic biological effects;
- Research on inorganic bionics and metal combined bio-macromolecules;
- Basis of new type inorganic pharmacochemistry and radiochemistry;
- Research areas intercrossing with other related disciplines.

Analytical Chemistry

The development of life science, materials science, environmental science, postgenomic era and bio-informatics poses higher requests on analytical chemistry and provides

opportunities for its development. The research areas include not only inorganic analysis, organic analysis, biochemical analysis, environmental analysis, process analysis, pharmaceutical analysis, cellular analysis, immunization analysis, food analysis, clinical analysis, analysis of traditional Chinese medical herbs, spectroscopy analysis, characterization and analysis of materials, analytical chemistry of nano-particles and chips, but also chemo-informatics, bio-informatics, instrument development, quality control and surface and interfacial analysis. Basic research on new principles, methods, techniques, instruments and key devices related to those areas are supported by the Division.

In recent years, continuous increase was achieved in the number of proposals submitted and projects funded. Based on the situation, the tendencies of disciplinary development fall into: 1) To highlight the research of methodology and the integration of methods to address issues at deep levels; 2) To combine closely with the national security, national needs and economical development; 3) To strengthen the research on new techniques and methods of detection and diagnosis related to human health; 4) To strengthen and emphasize the development of instruments, including not only the development of whole set instruments, but also the improvement of instruments, the escalation of performance, the development of accessories and parts and so on; 5) To stress the studies of mutual action, signal transformation and action mechanism of related materials; 6) To bring into full play the major role of analytical chemistry in the studies of all types of biomics and system biology; 7) To pay attention to the development of pre-treatment technologies of samples.

Research proposals are encouraged in the following areas:

- New technologies and methods of analysis in genomics, proteomics, metabolismics and metallomics;
- Analyses of monomolecular and unicellular as well as real-time and quantitative expression of life information;
- Pre-treatment technologies of samples, and interaction between bio-molecules;
- Analysis of traditional Chinese herbs and screening of active compositions;
- Food analysis and food safety;
- New techniques and methods of pre-warning and diagnosis of diseases;
- Various kinds of probe and sensor techniques, and analysis of spectroscopes and mass spectra;
- Analysis of surface, micro-area and morphology, and analysis of *in site* image formation;
- Analytical chemistry of processes, environment, nano-particles and chips;
- Chemo-informatics;
- Instrument development (including accessories and minimization of instrument);
- Analytical methods and techniques of aviation and space survey;

Analytical methods and techniques involved in the national prestige, national benefit, national security and suddenly occurred events.

Division II of Chemistry

Research projects related to organic chemistry and chemical biology are supported by the Division. The research contents of chemical biology can be found in the guide of other related divisions.

Organic Chemistry

Organic chemistry research covers sources and components, synthesis and preparation, structures and properties, reaction and conversion, as well as functions and reactive mechanism of organic compounds. New theories, methods and reactions in organic chemistry have promoted not only the development of chemical science, but also its intercrossing with life science, materials science and environmental science in a greater extent, which has further pushed forward the progress of organic chemistry. The characteristics of current research in organic chemistry are: 1) The concept of organic molecular design, recognition and self-assembly is affecting many fields of natural science; 2) The intercrossing between organic chemistry and life science has provided new research methods and means for studying and recognizing complex phenomena in life systems; 3) The discovery, manufacture and utilization of new functional organic matters have been making significant contributions to meeting the needs of mankind; 4) Selective reaction, catalytic asymmetric synthesis in particular, has become a hot issue and a cutting edge field in the research on organic synthesis; 5) Green chemistry is turning into an important field of synthesis chemistry; 6) The development and application of new technologies promote the deepening of the mechanism studies of organic reactions.

Continuously supported by NSFC, remarkable achievements have been made in the basic research of organic chemistry in China in such areas as metal-organic chemistry, physical organic chemistry, and asymmetrical syntheses and so on. Among the projects funded by the Division in the past five years, those for organic synthesis chemistry account for 34.3%, metal and element organic chemistry for 14.9%, natural organic chemistry for 11.8%, physical organic chemistry for 13.8%, pharmaceutical chemistry for 7.1%, bio-organic chemistry for 8.5%, organic analytical chemistry for 0.7% and applied organic chemistry for 8.9%. In the future, the following issues are the focus to the development of this discipline. In synthetic chemistry, more attention should be given to research on novelty and high-effectiveness of complex organic molecular syntheses and on natural products and new compounds with important physiological function. In metal-organic and element organic chemistry, emphasis should be placed on fundamental studies of green chemistry in organic chemistry and research on new regents, new methods and catalytic reaction with high selectivity. In physical organic chemistry, support should be further enhanced on in-depth theoretical studies of organic chemistry and on studies of structures and properties of new functional molecules.

Research proposals are encouraged in the following areas:

- New reactions, reagents, techniques and methods of organic synthesis (particularly the reactions of organic synthesis with high selectivity and high efficiency, and green chemistry);
- Super-molecular chemistry, molecular recognition and self-assembly, basic research on the synthesis and their physicochemical properties of new organic functional substances;
- Discovery, synthesis and bionic synthesis of natural organic compounds with physiological activity and relatively new fashioned complex structures;
- Studies with specific research objects on biomedicine, aiming at solving fundamental issues in chemical biology and generating new disciplinary growing points, including mutual recognition and interaction between small molecules and bio-macromolecules (for example, proteins, nucleic acids, polysaccharides, polypeptides and so on);
- Organic synthesis and chemo-biological conversion with high-selection catalyzed by enzyme and mimetic enzyme;
- Other basic theoretical issues in the crossing and linking of organic chemistry with related disciplines (especially those facing national major needs and fundamental scientific issues in organic chemistry).

Division III of Chemistry

Research projects related to physical chemistry and theoretical chemistry are funded by the Division.

Physical chemistry and theoretical chemistry form the theoretical foundation of chemical sciences. Their research subjects cover wide areas from mono-molecules, molecular aggregates to condensed states and from weak mutual action between molecules to the formation of chemical bond. Using modern detective techniques of physical chemistry and methods of theoretic analysis, information about molecular structure and dynamic change can be achieved from ground states to excited states and from steady states to transient states. Research on physical chemistry follows the following trends: combination of macroscopic and microscopic studies, combination of bulk phase and surface/interface, and combination of static and dynamic states. These trends have been furthered into the study on control of chemical reaction, which makes theories in closer combination with practices. As its crosscutting and fusion with materials science, energy science, environmental science, life science and information science, many new disciplinary growing points have been generated. Physical chemistry has played a more and more important role in the development of chemistry and related sciences.

Among the projects funded by the Division in recent years, studies on structural chemistry, theoretical chemistry and molecular dynamics have attracted attention from the international scientific community. Chinese research teams have become competitive in these research directions. Catalysis chemistry is one of the most active branches in

physical chemistry. Research in this field has made more international influence and achieved a higher position in recent years. The number of applications per year in the field of catalysis occupies one third of the total in the Division. The studies on electrochemistry and colloid and interface chemistry emphasize the intercrossing with materials and life science. Some studies have formed their own features. The number of applications and projects funded remains stable. Research fields of chemical thermodynamics (including thermo-chemistry and solution chemistry) have been broadened in recent years owing to the integration with life science and materials science, and employing microcosmic research means in these fields becomes a new developing trend. However, the number of applications is relatively small in the areas of solution structure, dynamic structure, and new methods of spectrum, studies of chiral and biological catalyses, as well as photochemistry, high-energy chemistry and chemo-informatics.

Proposals in physical chemistry should aim at disciplinary frontiers and national goals, and emphasize creative, systematic and in-depth studies. The Division encourages wide intercrossing and fusion with other disciplines to develop new concepts, theories and experimental methods while bringing the features of the discipline into full play. In the selection of research topics, emphasis will be given to basic studies with scientific foresight, exploration and possibility of becoming new disciplinary growing points, as well as those with important theoretical significance and potential for application. Meanwhile, the Division invites researchers of other disciplines to apply for interdisciplinary projects and requests the applicants to describe the correlation with the problems of physical chemistry in their applications.

Research proposals are encouraged in the following areas:

- Regulating and controlling methods of synthesis processes of materials with photo-, electro- and magneto-functions and the fundamental physicochemical process in liquid and solid phases;
- New methods of theoretical chemistry and their applied basic research in the fields of life, materials, environmental and information sciences and so on;
- New catalytic materials, new catalytic reactions, catalytic action and mechanisms of reaction, *in-situ* dynamic characterization techniques, and application research of catalysis in energy, resources and environmental areas;
- Fundamental interface chemistry and its intercrossing with materials and life science;
- Studies of electrochemistry with important potential for application;
- Thermodynamics of complex systems, new ideas and methods in chemo-informatics;
- Physiochemical issues in life system;
- Fundamental issues of physical chemistry in nano-sciences and technologies;
- Methods and techniques of *in site, on-time* dynamic characteristics.

Division IV of Chemistry

Research projects supported by Division IV are related to polymer science and environmental chemistry.

Polymer Science

Polymer science deals with the synthesis, molecular structure, chain structure, aggregation structure, properties and functions of polymers as well as their utilization, and takes synthetic polymer, natural macromolecules and bio-macromolecules as its objects of study.

In the field of polymer chemistry, major research directions are as follows: 1) Methodologies of synthesizing polymers from monomers by mono- and/or co-polymerization, polymerizing reaction with controllable molecular mass and structure of products and the biological synthesis of polymers; 2) Chemical reactions involving polymers, such as chemical change and modification of macromolecules, chemical issues in polymer processing and utilization, degradability after use and chemical or physical-chemical changes of cyclic utilization or regeneration of polymers and biochemical effects of macromolecular; 3) Studies on functional polymers such as polymers with electronic, optic and magnetic properties, and polymers for biomedicine (including sustained-release drug carrier, tissue engineering scaffold material and embedded medical parts), energy transformation, adsorption and separation, catalysis as well as reagents, sensor and molecular recognition. Special attention should be given to the studies of tectonics and stereochemistry of new structural polymers, such as upper-molecular polymers, hyper-branched polymers or dendrimer. Specifically, more studies are needed on new polymerization reactions and the development of polymerization systems with original creativity.

In the field of polymer physics, important topics are: to advance new concepts of condensed state physics of polymers, to improve the studies of structure and phase transformation of polymers and the structure and dynamics of sol-gel formation, and to obtain a deeper understanding of crystal phenomena, liquid crystals and glassy states. Studies should be stressed on aggregation structures for whole systems from single chain, oligo chain to bulky parts before and after shape-forming processing. Attention should be paid to studies on the structure of polymers in restricted space, structures and properties of surface and interface, nano microstructure and size effect of polymer, as well as the dynamic change of polymer structures, morphology and relations of structure with physical property. In addition, more efforts should be focused on the studies of polymer solution and rheology (including rheology of complex fluids and chemical rheology).
The Division encourages interdisciplinary studies between polymer science and information science, life science, physics, materials science and food science, especially those (1) to develop the theory of soft matters, the polymer electronics and the polymer photonics by employing new theories and methods from physics; (2) to find out the

growing points and opportunities of polymer development in the study of natural macromolecules and bio-macromolecules, and (3) to explore new areas and directions for polymer development between the gap of synthetic polymers and naturally existed bio-macromolecules, to emphasize the studies of bio-mimic polymers, super molecular structures, assembling and regulation of ordered structures of macromolecules, and to develop chemical biology of polymer.

FY2006 witnessed a slight increase in the number of applications and a continuous growth in the proportion of middle-aged and young applicants. Many proposals are related to the following areas: controllable radical polymerization, biomedical polymers, bioactive macromolecules, coordinative polymerization, polymers with electronic, optic and magnetic properties, polymers for energy conversion, ion liquid and application of super-critical technique in the polymerization, polymer sol-gel, hybri-structure and materials of inorganic/polymer, transformation and phase change of polymers, structure characterization of polymer, polymer processing, surface and interface of polymers, dendrimers and hyper-branched polymers, and computer simulation of polymers. Meanwhile, proposals for the following research areas are not enough: methodologies of poly-reaction and structural characterization, super-molecular polymers, exchanging-place polymerization of ethylenes, and ion polymerization. When selecting research subjects hereafter, applicants should note the development frontiers of the discipline and be able to extracting core scientific problems in industrial practices, but not blindly follow hot subjects while ignoring subjects received less attention and basic scientific issues unresolved at present in the discipline. Meanwhile, a clear statement of scientific issues studied should be given, emphasizing the scientific value and avoiding a too broad theme in the proposals.

Environmental Chemistry

By interpenetrating with other disciplines, environmental chemistry in China has made great progress in the depth of basic research and the range of fields, constantly forming its own systems. Research in environmental analytical chemistry, environmental pollution chemistry, pollution-control chemistry, pollution ecological chemistry and environmental theoretical chemistry has seen rapid development and is playing an increasingly important role in moving forward frontier of basic research, solving national major environmental problems and so on.

Based on recent proposals submitted to NSFC, the main themes of the discipline fall into existence: behavior, evolving ways and trends, effect and control of chemicals, special pollutants in various environmental media, etc. Research has continuously and systematically deepened, from microcosmic to macrocosmic and from static to dynamic. In the previous 3 years, the number of applications in control chemistry of pollution, environmental pollution chemistry, pollution ecological chemistry and relation between environmental pollutants and health has been increasing year by year. Major research orientations include: 1) New analytical principles, methods and technologies of pollutants and their polluting processes to the environment; 2) Important chemical reaction,

transporting mechanism and species structural changes of pollutants at the interface of different media and their bio-ecological effects, including the formation of fine particles in the air, analyses of resources, interface reaction, affection to human health, and the shift and conversion of pollutants in the interface between water-deposit/soil; 3) Interactions and synergistic effects of pollutants in the environmental system; 4) Technologies and principles of controlling air pollution, renovating polluted water bodies and soils, and new technologies and reusable principles of treating solid waste substances; 5) Forming mechanism, ecologic-toxicology and risk evaluation of pollutants' ecological effects; 6) Relation of structure/effect and dose/effect of pollutants and forecast model of environmental pollution, as well as other studies of frontier and creativity in environmental chemistry. Among them, the ranges or species of environmental pollutants studied are increasing to include heavy metals with different species, species of gaseous state and particles in air, persistent organic compounds, endocrine disrupter compounds, antibiotics and daily chemicals.

Research proposals are encouraged in the following areas:

- Finding of pollutants with important environmental effect or harm, and the probing into newly major environmental issues;
- Separation and analysis of ultra-trace hardly degradable toxic organic pollutants;
- Environmental behavior and microscope mechanism of interface processes of pollutants;
- Molecular mechanism and omics of mutual action between pollutants and organisms, mechanism of polluting formation, complex pollution processes, mechanisms and effects on ecology and health;
- Evolutional process and mechanism of the environmental qualities of regions;
- Air, water and soil pollution control as well as renovating principles and technologies after pollution, and new technologies and reusable mechanism of treating solid waste substances,
- Application of nano-materials in the fields of renovating ecologic environment and pollution controlled as well as their ecological effects;
- New bio-markers, indicators and methodologies of bio-ecological effects and risk evaluation of toxic chemicals exposed for low dosage and long time;
- Environmental behavior and ecologic-toxicology of new toxic pollutants.

Division V of Chemistry

Research projects funded by the Division cover two areas: chemical engineering and technology.

Chemical engineering and technology researches focus on the motion, transfer, reaction and interrelation in the conversion processes of matters. Its tasks are to recognize the transfer of matters in the conversion processes and its effect on reaction and properties of products, to study technologies, flow and equipments for the effective conversion of

substances, and to establish theories and methods of design, scale-up and control for use in industrial production. Specific new ideas, concepts and methods as well as their application in chemical engineering and technology are emphasized.

In recent years, chemical engineering and technology is facing an unprecedented development opportunity. Its research contents are revealing a lot of new changes, which are mainly in the following forms. Studies have been shifted from traditional chemical processing engineering to chemical product engineering, from measurements and correlation of gross properties to observation, measurements and simulation for structure, interface and multi-scales, specially research on optimization and regulation of structures, reinforcement of processes and scale-up rules, from common systems to uncommon and extreme processes, and from incremental improvement of existing methods to exploratory studies of new concepts and systems. It has become a major developing trend of chemical engineering that extracts key scientific issues from complex studying systems and gradually forming systematic theories and key techniques.

The Division gives preferential support to the studies of basic theories and key practical technologies in chemical engineering and industrial chemistry, as well as fundamental engineering issues of sustainable development, which aims at enhancing the overall national strength and creativity. It gives particular consideration to the following two research areas: 1) In light of the national conditions, national needs and goals, great efforts shall be made to explore frontier subjects in new and high technologies of chemical engineering and newly emerged disciplines and to emphasize the crossing of multi-disciplines, specially from which to extracts problems related to chemical engineering, so as to promote the development and creation in scientific ideas and technical means. 2) Under the guidance of national goals and social needs, systematic basic research and accumulation should be enhanced for key technologies in chemical engineering related to national economy and people's welfare, so as to gain systematic understanding on the laws, to develop and consummate the theories on the discipline and to play the guiding role of basic research.

Research proposals are encouraged in the following areas:

- Measurement, computation and stimulation of fundamental data of substantial properties;
- Transfer processes;
- Separation and purification;
- Chemical reaction engineering;
- Chemical systematic engineering;
- Inorganic chemical engineering;
- Fine organic chemical engineering;
- Bio-chemical engineering and food chemical engineering;
- Energy and materials chemical engineering;
- Chemical metallurgy;
- Environmental and ecological chemical engineering.