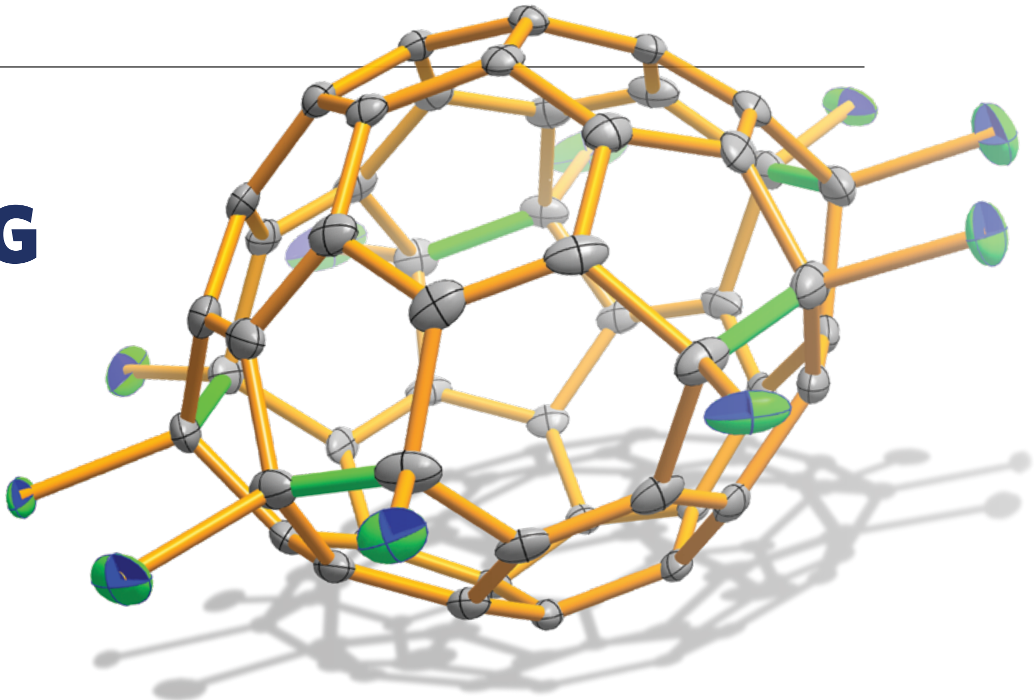
UNLEASHING CHEMICAL POTENTIAL

Chemists at XMU are spearheading new research to find vital solutions.



XMU researchers have developed new fullerene series, including the $C_{50}Cl_{10}$ fullerene.

A founding programme at XMU in 1921, its chemistry department has been a national leader in the field. Thanks to the legacy of the predecessors, including physical chemist and former president of the Chinese Academy of Sciences (CAS), Jia-Xi Lu, and Khi-Rui Tsai, an expert in molecular catalysis and a CAS member, the push for innovation and cooperation is deeply rooted in the culture of XMU's College of Chemistry and Chemical Engineering (CCCE), nurturing generations of faculty members and students.

Dedicated to high-quality education and cutting-edge research, CCCE strives for an inclusive, vibrant and collaborative research environment to address fundamental chemistry problems and urgent societal needs. Carrying on Lu's tradition in physical chemistry, it houses the State Key Laboratory of Physical Chemistry of Solid Surfaces (PCOSS), which has been ranked at the highest level in all national appraisals since its foundation in 1987. PCOSS has profound influence on CCCE's research, ranging from experimental and computational methods for studying complex chemical systems, and synthetic chemistry for making novel molecules and materials, to technological innovations for meeting world challenges.

Tackling complex chemistry

Physical chemists at CCCE excel at harnessing instrumental and computational techniques to study surface and interface chemistries. The globally leading group for Surface-Enhanced Raman Spectroscopy (SERS) has developed operando instrumental methodologies. They also led the construction of China's first Infrared Free Electron Laser (IRFEL) facility, which enables detailed investigation of chemical processes. Beyond revealing molecular reaction mechanisms, research at CCCE also covers chemical dynamics and kinetics, with applications in fuel cells, batteries, and electrochemical nanomachining.

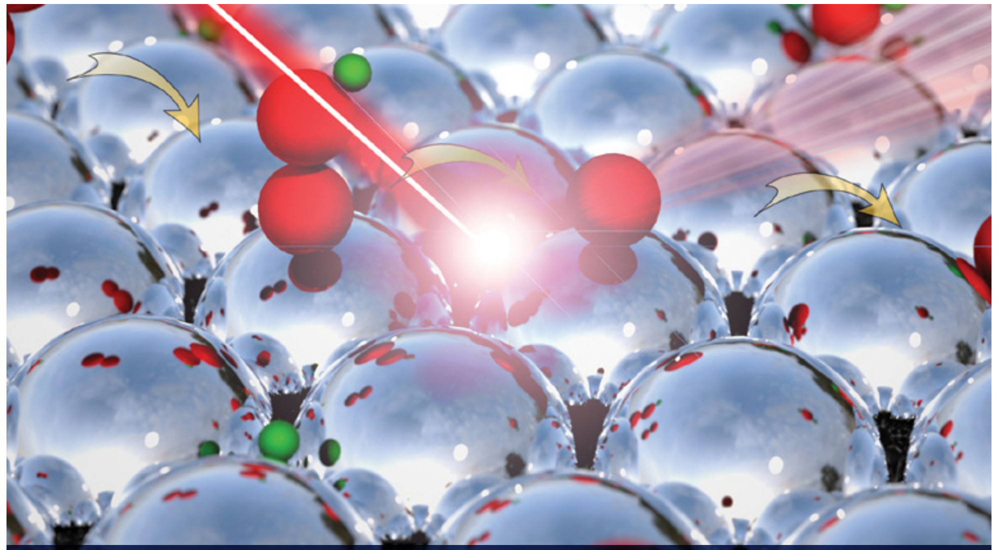
CCCE's analytical chemists develop new methods and devices to solve measurement problems in biomedicine, materials, environmental, and energy sciences. Focusing on improving sensitivity, selectivity, and spatio-temporal resolution of analytical signals from target analytes, they have designed new functionalized molecules and supramolecular assemblies, built new physical and chemo-biological interfaces, and developed novel instruments, providing new tools for biomolecular recognition and sensing, single cell analysis, and disease diagnosis. Particularly, their mass and fluorescence spectroscopy technologies have improved surface-imaging performance. Their novel microfluidic systems allow for biomolecular detections, capturing and releasing circulating tumour cells for liquid biopsy, and enable genetic analysis of foetal cells using peripheral blood samples.

Making advancement in everything from chemical reactions to materials design requires powerful computational tools. An example is the Xiamen Valence Bond (XMVB) software programme for electronic structure calculations. Designed to explore the nature of chemical bonding and mechanisms of reactivity, XMVB is useful for predicting material properties, and is widely used by global researchers. Excited state calculation and quantum dynamics methods developed at CCCE open the door to studying photophysics and photochemistry of complex systems.

Mastering synthetic chemistry

Aiming to develop new synthesis methods to solve challenging chemical problems, inorganic chemists at CCCE are recognized for their achievements in cluster chemistry, and surface and interface chemistry of nanomaterials. They study new carbon, rare earth, and noble metal clusters to improve controllable synthesis and stabilization. Their novel clusters have applications in photovoltaic conversion and catalysis, along with molecular magnetism and chiral recognition. They have also characterized structures of fullerenes, a family of all-carbon clusters with wide applications, and developed new fullerene series. Their continuous combustion method enables the production of tonnes of fullerenes annually.

Engineering nanocrystallites to enhance structural diversity, CCCE inorganic chemists have also proposed a new theory to explain the growth of nanocrystals, and established an effective strategy to control their surface structure. By revealing the molecular mechanisms underlying complex surface and interface behaviours of major functional nanomaterials, they have developed multifunctional catalysts for industrial use. Their hydrogenation metal nanocatalysts, with almost 100% selectivity, can reduce polluting emissions during chemical processes.



Operando and *in-situ* spectroscopic techniques help reveal reaction mechanisms at a molecular level.

In organic chemistry, CCCE researchers have developed methods for efficient, direct, and selective transformations of amides and amines, presenting a new frontier for chemoselective synthesis. Used by researchers across the world, their approach has proved practical and ubiquitous.

They are also pushing limits on the number of metal-carbon bonds that can be built on one metal centre, a central issue to organometallic chemistry. They synthesized 'carbolongs', namely, long 'carbon scarfs', by forming several metal-carbon bonds based on extended carbon chains. These complexes boast diverse properties, including broad absorption of light of different wavelengths, and good photothermal/photoacoustic performance, ideal for use in photoelectric materials and biomedicine.

Driving interdisciplinary innovations

The emphasis on fundamental chemistry has helped CCCE identify emerging fields that cross boundaries with traditional disciplines. It was the first in China to offer undergraduate training in chemical biology, in 2003, and energy chemistry, in 2016.

CCCE's exploration of new catalytic methods and materials for sustainable utilization of carbon resources started with the founding of the XMU Catalysis Institute in 1958, one of China's earliest to focus on energy chemistry. Its recent efforts include transforming C1 molecules with one carbon atom into multi-carbon chemicals of higher value. Their photocatalytic approaches to make use of biomass show promise for producing fuels from renewable carbon resources.

They have also developed *in-situ* electrochemical techniques to monitor electrocatalysts real-time as they operate in batteries. This led to a cheap, noble-metal-free electrocatalyst with record-high power density for fuel cells.

In chemical biology, CCCE researchers are developing tools for in-depth life sciences studies. By exploring phosphorus chemistry, a team proposed important ideas about the origin of life, including the role of N-phosphoryl amino acid in co-evolution of nucleic acids and proteins.

Bridging biochemistry and engineering, another team developed a nano-flow cytometry technology, capable of measuring the count, size, composition, and phenotypes of nanoscale biological particles with enhanced sensitivity and accuracy. The technology has been commercialized, becoming a popular biomedical tool. Other innovations include a single-cell RNA sequencing tool combining microfluidics and DNA barcoding, new magnetic resonance imaging (MRI) probes for *in vivo* deep-tissue imaging, and multifunctional probes within organelles for *in-situ*, real-time optical tracking.

Looking to the future

CCCE researchers also develop instruments to explore the potential of single molecules for next-generation electronic devices. Their intelligent and ultra-sensitive instruments can detect electrical signals of individual molecules.

Another new technology explored at CCCE is liquid gating, which was selected as one of the Top Ten Emerging Technologies in Chemistry by the International Union of Pure and Applied Chemistry in 2020. This new strategy for gating micro/nanopores opens possibilities for designing smart liquid systems in future.

CCCE researchers are also integrating machine learning technologies by developing automated experiments and computational workflows to accelerate materials discovery. ■

CCCE: Sparking chemical brilliance

Global recognition:
Ranked among the global **5‱** in chemistry, according to the Essential Science Indicators (ESI) field ranking

Cross-disciplinary research:
Nine sub-disciplines including inorganic chemistry, organic chemistry, analytical chemistry, physical chemistry, polymer sciences, chemical biology, energy chemistry, chemical engineering, and biological engineering

World-class faculty team:
Seven CAS members, and **20** recipients of the National Science Fund for Distinguished Young Scholars

A leader in chemical education:
Among the **first** to obtain state approval for offering undergraduate, graduate, and postdoctoral programmes