Beijing Synchrotron Radiation Facility

As a part of Beijing Electron Positron Collider (BEPC) project, Beijing Synchrotron Radiation Facility (BSRF) (http://english.bsrf.ihep.cas.cn) was constructed almost in parallel with BEPC and has been opened to users since 1991. After the upgrading project of BEPCII, BSRF runs in 2.5GeV full-energy injection and 250mA beam current in the dedicated mode of synchrotron radiation. The intensity of hard X-ray has increased one magnitude and the stability was also improved greatly.

Currently, there are 3 experimental halls (12#, 13#, 15#), 5 insertion devices, 14 beamlines and 14 experimental stations at BSRF. The synchrotron radiation light of BSRF covers the energy from vacuum ultraviolet to hard X-ray, and supports many kinds of experimental techniques, such as X-ray topography, X-ray Imaging, Small Angle X-ray Scattering, Diffuse X-ray Scattering, Biological Macromolecule Structure, X-ray Fluorescence Analysis, X-ray Absorption Fine Structure, Photoelectron Spectroscopy, Circular Dichroism Spectra, Soft X-ray Calibration, Mid-energy X-ray Optics, High Pressure Structure, LIGA and X-ray lithography, which can be applied to lots of fundamental and applied researches, such as Condensed Matter Physics, High
Pressure Physics, Chemistry, Material Science, Biology, Geoscience, Environmental Science, Microelectronics, Micromachining, Metrology, Optics and Probing Technique.

The accumulated experimental time for the dedicated mode of synchrotron radiation is at least three months per year. Additionally, six beamlines (Mid-energy X-ray Station, Soft X-ray Absorption Spectroscopy Station, Photoelectron Spectroscopy Station, Vacuum Ultraviolet Station, Small Angle X-ray Scattering Station and Macromolecular Crystallography Station) could also run while BEPCII was working for high energy physics, which is called as coupling mode and supplies more experimental time to users. Totally, BSRF could supply beamtime to upwards of 500 experiments for over 1000 users from more than 100 institutes and universities at home and abroad.
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2011 Operation of BSRF

Two rounds of dedicated synchrotron radiation running were offered in 2011. The first round was from 8th June 2011 to 15th July 2010; the second round was from 1st November 2011 to 30th November 2011.

In the first round of dedicated synchrotron radiation running, 799.38 hours’ effective beamtime was offered to users, 278 proposals from 83 research institutes at home and 7 research institutes abroad were supported and 14 beamlines were all running. The nano-meter imaging facility of 4W1A-X ray imaging station was opened to users; XAFS experimental mode was opened to users in the dedicated SR running for the first time, which supplied more beamtime to users. Additionally, PAL was shut down in 2011 due to a upgrading and according to the commitment between IHEP and PAL, 9 proposals were supported in this round.

In the second round dedicated synchrotron radiation running, 656.71 hours’ effective beamtime was offered to users, 221 proposals from 76 research institutes at home and 3 research institutes abroad were supported and 13 beamlines were running except 4B9B Photoemission Spectroscopy station which was started upgrading in July. In this running, In this running, at 4B7A-Middle energy Station, an acceptance test was successfully conducted on the project of the Upgrading of BSRF Middle Energy Station Experimental Facility. The Small Angle X-ray Scattering Experimental Platform was tested at the 1W2A-Small Angle X-ray Scattering Station. After the tests, both projects were proved to meet with their design requirements. Another two pre-research projects of CAS scientific facilities were also tested at the Facility.

The Vacuum Ultraviolet experimental station (VUV), mid-energy X-ray experimental station, Soft X-ray Optics Station and Photoemission Spectroscopy Station and biological macromolecule station kept open to users in the coupling mode and have supplied experimental time for 98 proposals. The successful running in the coupling mode gained more beamtime for BSRF. Furthermore, it’s more convenient to arrange the beamtime for the users and significant to the urgently needed national research items.
Fig.1 (left) Users were doing experiment with the help of the workers of 4W1A X-ray Imaging station; (right) Users from KAIST were doing experiments at 1W2A-SAXS station.

Fig.2 (left) An acceptance test was conducted on the project of the Upgrading of BSRF Middle Energy Station Experimental Facility; (right) The small angle X-ray scattering experimental platform was tested at the 1W2A-Small Angle X-ray Scattering Station.

Fig.3 (left) Proposals areas of BSRF in 2011; (right) User distribution in China
GIXRD has played an important role in the characterization of organic thin-film transistors

As an alternative to well-established amorphous silicon electronics for low-cost, large-area, and flexible applications, organic thin-film transistors (OTFTs) have made great achievements in the past two decades. Building on this rapid progress, organic circuits have been successfully demonstrated in various areas such as electronic papers, sensors, and radio frequency identification cards (RFID). A promising development for OTFTs, driven by the urgent demand for ultra-low-cost printed and ambient electronics, is the realization of all-solution-processed complementary circuits composed of both p-channel and n-channel devices. Compared with those exciting reports on solution-processed p-channel transistors with mobility approaching 1.0 cm$^2$V$^{-1}$s$^{-1}$, only a few solution-processed n-channel OTFTs showing mobilities exceeding 0.1 cm$^2$V$^{-1}$s$^{-1}$ have been fabricated, despite many innovative studies of material design and device engineering. This uneven development makes the fabrication of high-performance, solution-processed n-channel organic transistors one of the biggest remaining challenges. Due to the intrinsic nature of electrons being trapped by oxygen, the low air-exposed performance and stability is a key issue for n-channel OTFTs, especially for solution-processed ones. Therefore, most reported solution-processed n-channel OTFTs suffer from relatively low performance (with mobilities < 0.2 cm$^2$V$^{-1}$s$^{-1}$) and stability for the bottom-gate devices where the active layer exposed to air, which presents an obvious contrast with the excellent result for solution-processed top-gate devices. Recently, researchers in Key Laboratory of Organic Solids, Institute of Chemistry and Laboratory of Materials Science, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences make great progress in this field. They developed a bottom-gate device based on a core-expanded naphthalene diimide fused with 2-(1,3-dithiol-2-ylidene)malonitrile groups (NDI2ODDTYM2) presenting a high electron mobility of up to 1.2 cm$^2$V$^{-1}$s$^{-1}$ in air (Fig.1). More excitingly, the outstanding stability of NDI2OD-DTYM2 enables the devices to both endure the high temperature annealing treatment during fabrication and to maintain high performance even when operating at high environmental temperatures ($\leq$120 ° C) under ambient conditions.

Fig.1 a) Illustration of the chemical structure of NDI2OD-DTYM2, fabrication processes, and device structure of n-channel OTFTs. b) Optical images of an all-solution-processed flexible organic oscillator fabricated under
In order to discuss the relationship between the performance and the structure, grazing incidence X-ray scattering (GIXRD) is used as an important method to investigate in detail the microstructure of the film. The in-plane structure of the annealed NDI2OD-DTYM2 film was investigated using GIXRD in Beijing Synchrotron Radiation Facility (BSRF) to probe the crystalline planes, which were oriented perpendicular to the dielectric layer. The annealed film at 170 °C showed a short π-stacking distance of 3.47 Å (Fig. 2). This π-stacking distance is comparable to the values reported for the excellent naphthalene tetracarboxylic-diimide-based semiconductors. The close packing of the π -planes, together with the protection afforded by the long-branched N-alkyl chains, inhibits the ingress of oxygen, which effectively reduces the occurrence of electron trapping. This, combined with the low energy of the lowest unoccupied molecular orbital (LUMO), is responsible for the excellent device performance and outstanding device stability.

Fig. 2 In plane grazing incidence X-ray characterization of NDI2OD-DTYM2 film annealed at 170 °C.

This result was published in *Advanced Materials* (*Adv. Mater.* 2011, 23, 2448-2453) and was selected as cover. It was also selected as the Hot Topic paper in the field of Organic Electronics.

**Article:**

Well-aligned Zn-doped tilted InN nanorods grown on r-plane sapphire by MOCVD

Indium nitride (InN) is a promising material for high efficiency infrared emitters, detectors, high frequency electronic devices because of its excellent characteristics. Nanostructure materials, a new class of materials with particular properties and superior applications, have received much interest in recent decades. A team from Key Laboratory of Semiconductors Materials Science, Institute of Semiconductors, CAS, has gained insight into the research of InN nanorods. Their research has been published on April 7th 2011 in Nanotechnology*.

Well-aligned tilted Zn-doped InN nanorods have been grown successfully on r-plane sapphire in a horizontal metal-organic chemical vapor deposition system. All of the nanorods are symmetrically tilted in two opposite directions. The nanorods are single-crystalline and have exactly the same epitaxial orientation as the a-plane InN film. The nanorod has a new cross sectional shape of an axial symmetry pentagon and the axis of symmetry is the c-axis of the crystal. Zn dopant plays a crucial role in the growth progress, being an important factor in controlling the morphology of the InN nanomaterials and their properties.

The HR-XRD measurement was taken at Beijing Synchrotron Radiation Facility (BSRF). The chi scan of the m-plane InN nanorod gives

out a strong peak at 32° which indicates that the parallelity between the m-plane of the nanorod and the film is very good. So the tilted angle between the substrate normal and the nanorod is about 32°, which can be also said that the nanorods have the same crystal orientation as the a-plane InN film grown on the substrate.
This research provides a scientific foundation for growing nanorods on the film with different dopant, understanding the uniform tilt angle and in-plane projection directions and the m-direction growth.

**Article:**

Preparation of Quasi-Free Standing Graphene with a Super Large Interlayer Distance by Methane Intercalation

Graphene is regarded as a new fantastic material because of its single atomic thickness, high symmetry and relativistic charge carrier behaving like massless Dirac Fermions. Since its discovery, preparation of high quality graphene as host materials for devices has become a key factor for its further development. However, Graphitization process of multilayer graphene is inevitable, if the number of graphene layers (NGL) increases without any further proper measures. Preparation of graphene in multi-layer behaving like a quasi-free standing monolayer remains elusive.

Qingsong Huang and coworkers present a route to graphene epitaxially grown on SiC (0001) by exposing sample to hydrogen, which is accompanied by intercalation of hydrogen and related organic molecules under high temperatures, much different from those in previous works performed under low temperatures (below 600 °C), leading to a uniform intercalation in the cooling process after heat decomposition. When the NGL increases more than 1 ML, the penetration (intercalation) of methane atoms to interspaces of two adjacent layers happens, so that the interlayer distance between two adjacent layers (IDTL) will be enlarged by this intercalation, even more than the distance of AA stacking (3.4693 Å). This abnormally large distance can decouple the two adjacent layers, and make each layer quasi-free standing. This intercalation by methane and methyl group (–CH3) species is much better than that by the high density of rotational faults in the EG on SiC (000-1), where the graphitization should be inevitable with increasing of the NGL.
By utilizing the XRD method at Beijing Synchrotron Radiation Facility (BSRF), the inter-distance of the two adjacent layers (IDTL) can be characterized accurately. Despite of the NGL changing, the XRD-peak positions are almost kept unchanged, which represents the intercalation can be performed effectively and uniformly in random layers, even the NGL of film is different. Furthermore, with the NGL increasing, the reduction of IDTL can be attributed to the graphitization process. Without intercalation, the graphitization process will proceed very quickly because of the interlayer coupling. Here, the IDTL has a minimum value, no less than the radius of intercalation species, so that the charge carriers of graphene can be kept like massless Dirac Fermions because of the abnormally large IDTL by the intercalation of methane, regardless of the number of graphene layers. Thus, the preparation of graphene will become simple, effective and promise in application. It can also be expected that, graphene can be observed with naked eyes, just like a sheet of paper as host materials. For more detail please refer to the article published in J. Phys. Chem. C.

The research results provide an effective route to the graphene in high quality, which makes the graphene to be decoupled from its adjacent layers and to be used widely and prepared easily in large scale. Synchrotron radiation sources have helped us to unveil the inter-distance between two adjacent layers accurately, by which the abnormally large IDTL has been disclosed and makes the coupling between the adjacent layers very weak. The synchrotron radiation techniques can reveal not only the relationship between the inter-distance of the IDTL and the number of layers, but also the misorientation between the adjacent layers. The synchrotron has played an important role in structurally characterizing graphene.

**Article:**

Photoluminescence Properties of several Tb$^{3+}$ active phosphors under VUV excitation

Hg-free lamp is a green environmental-protective lighting energy now due to not containing harmful mercury vapor to people. In recent years, much of the investigation on this is being carried out. The excitation resource in Hg-free lamp mainly emits vacuum violet (VUV) photon of 147 and 172 nm, so exploring luminescent materials with strong absorption around these wavelengths is an important aspect to improve the luminescent efficiency of Hg-free lamp. A team from Laboratory of Function and Environment Materials in School of Physical Science and Technology of Lanzhou University has carried out much investigation on this subject, and a novel white-emitting luminescent material in one host under VUV excitation was identified. The corresponding research has been published on Journal of The Electrochemical Society, J. Am. Ceram. Soc., Electrochem. Solid St., Mater. Res. Bull.

The team explored some new VUV phosphors with phosphate as host. And the phosphate is an excellent host material for rare earth ions to dope owing to its high physical and chemical stability, strong absorption to VUV photon, and environmental-friendly characteristics. On one hand, the photoluminescence properties of Tb$^{3+}$, Ce$^{3+}$, Mn$^{2+}$ ions were single or multi-doped in these hosts were investigated, and the excitation spectra in VUV-UV region and the emission spectra under 147 nm excitation were measured. The emitting color was tuned by varying the content of activator, finally white-emission was achieved. The energy-transfer relationship among multi-doped ions was also studied in this paper. On the other hand, they studied a VUV luminescent material with oxide as host, and Tb$^{3+}$ with short decay time was chosen as activator. The VUV-UV excitation and emission spectra were measured, the quenching concentration of Tb$^{3+}$ in this host was investigated, and the f-d transition of Tb$^{3+}$ located at long-wavelength direction was also interpreted.

Excitation and emission spectra using synchrotron radiation at BSRF and the CIE chromaticity diagram. In the excitation spectrum, Tb$^{3+}$ doped sample shows a broad and strong excitation band between 100 and 250 nm, which is beneficial to the emission wavelengths of Hg-free lamp; and two excitation peaks in UV region are found, which indicates this spectrum can match the light distribution in PDP and Hg-free lamp; from the CIE chromaticity diagram, it shows the luminescent color of the sample can be changed by varying the concentration of the three activators, and white emission has been achieved under certain concentration ratio.
The research result of this paper enriches the rare earth ions doped luminescence materials, and provides material for realizing white emission in single host. The energy-transfer relationship among multi-doped ions under VUV excitation is rarely reported, and we provide some theoretical basis and practical evidence for this.

**Article:**


Synchrotron helps unveiling the mechanism underlying thermoelectricity of La$_2$CuO$_4$ ceramics

As one of the key materials for national strategic development for energy resources, thermoelectric (TE) materials are renewable energy-related materials based upon either thermo-voltaic (Seebeck) effect or electro-refrigeration (Peltier) effect. TE-devices made with thermoelectric materials have been applied as essential elements in many cutting-edge technologies (e.g. space shuttles, scientific instruments). It was suggested that the TE-devices should be ubiquitously invested in market and readily applied in civil lives if their efficiency can achieve the Carnot efficiency of 30%. On one side thermoelectric materials with high performance can be used to generate power with waste heat (from factories, automobiles, human activities, etc); one the other side the solid state thermoelectric materials are environment-friendly and will not cause secondary pollutions. Henceforward, thermoelectric materials researches are becoming one of the hottest areas for materials scientists in 21st century.

Solid-state thermoelectric oxides belong to a family of novel thermoelectric materials. They features in relatively higher thermopower (Seebeck coefficient) and easier manipulation of transport property of charge-carriers simply by tuning the ingredients and site occupation for specific atomic sites. As a good antiferromagnetic insulator, La$_2$CuO$_4$ is known to exhibit superconductivity as the lanthanum site being substituted with alien atoms, e.g. Strontium. Besides, this family of materials possess d$^9$ electronic configuration for copper ions, which renders it as a three dimensional Mott insulator. The German physicist J. Georg Bednorz and Swiss physicist K. Alexander Müller from IBM Zurich Research Laboratory were awarded Nobel Prize in physics in 1987 for their contribution in the discovery of superconductivity in ceramic materials (e.g. La$_2$CuO$_4$). The transport property (e.g. superconductivity) in those materials with copper oxide layer had been the hottest area in condensed matter physics. The Professor Ce-Wen Nan and Professor Yuan-Hua Lin’s group from Tsinghua-university discovered that the pure and lanthanum-site-rare-earth doped La$_2$CuO$_4$ ceramics exhibit excellent thermoelectric performances and are promising candidate for thermoelectric applications at high temperatures.

By using the X-ray absorption spectroscopy provided by 4W1B endstation of Beijing Synchrotron Radiation facility (BSRF), they in collaboration with staffs of BSRF studied the local structure of copper-site doped La$_2$CuO$_4$. Combining the macroscopic measured transport properties such as electrical conductivity, Seebeck coefficient, etc, it is revealed that copper-site doping affects the transportation of charge carriers thus rendering increment of electrical resistivity. Moreover, the small-polaron conduction mechanism is adopted to illustrate the metal-to-insulator transition with increasing temperature.
This work provides interpretation of high temperature transport property of La$_2$CuO$_4$, the parent for high temperature superconductors; and addresses the origin of the doping-induced-conduction-transition at atomic scale. In addition, the application of X-ray absorption fine structure spectroscopy is expanded to the functional materials, providing guidance for improving thermoelectric performances and optimizing technical route. Meanwhile, the merits of synchrotron-based spectroscopy have been demonstrated.

**Article:**

Luminescence and microstructures of Eu$^{3+}$-doped Ca$_9$LiGd$_{2/3}$(PO$_4$)$_7$

In the RE doped compounds with a $\beta$-Ca$_3$(PO$_4$)$_2$ structure, the crystallographic site-occupancy of RE in host lattices has a strong influence on the luminescence mechanism and applications, but there is nearly no report. The nature of a monovalent ion plays a critical role in the luminescence properties. The composition change from Ca$_9$Gd(PO$_4$)$_7$ to Ca$_9$MGd$_{2/3}$(PO$_4$)$_7$ is accompanied by an increase of the luminescence intensity of Gd$^{3+}$ by about 5 times for M = Na$^+$ and a decrease of the luminescence intensity by about 4 times for M = Li$^+$. Among these kinds of phosphates, the luminescence spectra of Eu$^{3+}$ ions (under a laser excitation $\lambda_{ex} = 337.1$ nm, $T = 290K$) have been briefly reported by Lazoryak et al. only in Eu$^{3+}$-concentrated Ca$_9$MEu$_{2/3}$(PO$_4$)$_7$ (M = Li$^+$ and Na$^+$). A team from College of Chemistry, Chemical Engineering and Materials Science of Soochow University study the red-emitting phosphors of Eu$^{3+}$-doped Ca$_9$LiGd$_{2/3}$(PO$_4$)$_7$. Different from the work by Lazoryak et al., some new results were obtained in the present investigation. Their research has been published on Dalton Transactions.

The team identified that the excitation spectra in $^7F_0 \rightarrow ^5D_0$ transition show two broad spectra, which indicates that there are at least two kinds of Eu$^{3+}$ sites in the lattices. The luminescence intensity of Ca$_9$LiGd$_{2/3}$(PO$_4$)$_7$:Eu$^{3+}$ was greatly enhanced in comparison with that of Ca$_9$Gd(PO$_4$)$_7$:Eu$^{3+}$. Moreover, an efficient red-emitting phosphor could be expected because of the weak concentration quenching of Eu$^{3+}$ luminescence.

![Fig.1 The excitation and emission spectra of Ca$_9$LiGd$_{2/3}$(PO$_4$)$_7$ measured by the synchrotron radiation VUV light.](image)

Excitation	Emission

Intensity (a. u.)

Wavelength (nm)

Ca$_9$LiGd$_{2/3}$(PO$_4$)$_7$ measured by the synchrotron radiation VUV light.
Fig.3 and Fig.4 are the emission spectra of Ca$_9$LiGd$_{2/3}$PO$_4$:Eu$^{3+}$ (x = 0.35) excited by wavelengths from the synchrotron radiation VUV and UV light respectively. The luminescence intensity of Ca$_9$LiGd$_{2/3}$PO$_4$:Eu$^{3+}$ (b) was greatly enhanced in comparison with that of Ca$_9$Gd(PO$_4$)$_2$:Eu$^{3+}$ (a). The inset shows there is no concentration quenching.

The research provides the scientific community clues to understand the luminescence mechanism and applications, synchrotron sources have helped the team to unveil the crystallographic site-occupancy of RE in host lattices. And synchrotron sources have helped the team to verify the luminescence intensity of Ca$_9$LiGd$_{2/3}$(PO$_4$)$_2$:Eu$^{3+}$ was greatly enhanced in comparison with that of Ca$_9$Gd(PO$_4$)$_2$:Eu$^{3+}$.

**Article:**
Fuping Du, Rui Zhu, Yanlin Huang, Ye Taob and Hyo Jin Seo. Luminescence and microstructures of Eu$^{3+}$-doped Ca$_9$LiGd$_{2/3}$(PO$_4$)$_2$. Dalton T., 2011, 40,11433-11440.
Enhancement of light-emission efficiency of ZnO light-emitting-diodes by Ag localized surface plasmons

ZnO has substantial advantages including large exciton binding energy (60 meV) and direct wide band gap (3.37 eV) and has been regarded as one of the most promising candidates for ultraviolet (UV) light-emitting diodes (LEDs). However, there are many practical challenges that must be resolved before it leaps from lab to market-place. The most crucial one is to improve the light-emission efficiency with which the LEDs are more effective at converting electricity into light. A team from Key Lab of Semiconductor Materials Science in Chinese Academy of Sciences, has demonstrated that exploitation of localized surface plasmons (LSPs) is a feasible way to enhance the efficiency of ZnO LEDs. Their research has been published on November 3rd, 2011 in *Applied Physics Letters*.

LSPs are collective excitation modes in metal nanoparticles (NPs), comprising an electromagnetic field coupled to oscillations of the conduction electrons. When the emission energy of semiconductor and the SP energy are similar, the luminescence efficiency of light-emitting materials and devices can be enhanced significantly by the resonance coupling between them. Although LSPs in principle can improve the light emission of LEDs, there has been no report concerning the LSP-enhanced electroluminescence (EL) in ZnO-based LEDs structure. For effective exciton-LSPs coupling, the NPs must locate in close proximity to the emitter. The strategy the team adopted is to incorporate Ag NPs in the vicinity of the active layer, but not the commonly used one, i.e., on the top of the device. The ultraviolet/violet near band edge emission of the device is significantly enhanced while the green defect-related emission is suppressed as compared to the LEDs without Ag NPs. A maximal 2.5-fold enhancement of electroluminescence was observed.

TR-PL spectra of the ZnO LEDs with and without Ag NPs measured at RT. The decay time is determined to be ~25 ns for the LED without Ag NPs, while it is reduced to ~6.4 ns after introducing Ag NPs. The data were collected at beam line 4B8 of BSRF with the exciting wavelength of 200 nm.

Synchrotron sources helped the team to uncover the microscopic origin of the enhancement in
light-emission efficiency. Time-resolved photoluminescence (TR-PL) measured at beam line 4B8 of Beijing Synchrotron Radiation Facility (BSRF) reveals that the decay time (i.e., the effective exciton lifetime) is greatly reduced from 25 ns to 6.4 ns after introducing Ag nanoparticles. This is because the exciton energies can transfer to the Ag LSPs for emission, creating an alternative recombination channel. The internal quantum efficiency (IQE) of the ZnO with exciton-LSP coupling can be described as \( \eta = \frac{k_{\text{rad}} + k_{\text{sp}}}{k_{\text{rad}} + k_{\text{non}} + k_{\text{sp}}} \), where \( k_{\text{rad}} \) and \( k_{\text{non}} \) are the radiative and nonradiative recombination rates of ZnO, respectively, and \( k_{\text{sp}} \) is the exciton-LSP coupling rate. Due to \( k_{\text{sp}} \) is very fast compared to \( k_{\text{rad}} \) and \( k_{\text{non}} \), the PL decay rate are largely enhanced. This new recombination path increases the spontaneous radiative recombination rate, and thereby the IQE of ZnO is significantly improved. The resultant enhancement factor of radiative recombination rate determined from the corresponding decay time is around 3.9, which is in accordance with the maximum EL enhancement ratio of 4.2 observed at 410 nm with a current of 6 mA.

The research provides a promising method to enhance the performance of ZnO-based LEDs. “However, the results at this stage are preliminary. We still have a long way to go to solve all the problems on commercializing ZnO-based LEDs, and synchrotron radiation is surely helpful for that. It is lucky that we start well.” Said XingWang Zhang, the team leader and the professor of Key Lab of Semiconductor Materials Science, Institute of Semiconductors, Chinese Academy of Sciences.

**Article:**

Preparation and characterization of porous carbon Spheres with controlled micropores and mesopores

Porous carbon materials as a major candidate for hydrogen storage have attracted many scientific interests because of its light weight, abundant natural precursors, low cost, and high surface area. Tailored pore system of the porous carbon materials for hydrogen storage is an urgent matter. Functional materials group from the department of Physics in University of Science and Technology Beijing has developed a simple and effective synthesis strategy for porous carbon spheres whose microstructure was modified by controlling the synthetic condition. The microstructure of the carbon spheres was investigated and published on the Journal of Alloys and Compounds in September 2011.

The porous carbon spheres were prepared by carbonizing the resorcinol–formaldehyde (RF) xerogel spheres at a high temperature under an argon atmosphere. In the synthesis, Commercial opaque polymer (OP) hollow spheres were used as templates and microreactors for polymerization of resorcinol and formaldehyde monomers. Resorcinol-formaldehyde was used as the carbon source. The carbon dioxide activation was applied to further control the pore structures and textures of the porous carbon spheres which closely associated with the hydrogen storage properties. Small angle X-ray scattering (SAXS) technique at Beijing Synchrotron Radiation Facility (BSRF) was applied to analyze the microstructure as shown in the following Figure and Table. Finally, the framework of resulting carbon sphere is hollow structure with a cavity of about 200 nm diameter. The wall of hollow carbon sphere is also porous with average pore diameter of 5~26 nm, porosity of 0.52~0.91, and specific surface of 210~670 m²/cm³ and 747~1606 m²/g. The pore characteristic of the hollow carbon spheres is alterable with the carbon source concentration, which can be used to modify the pore structures of the hollow carbon spheres. An appropriate treatment of CO₂-activation can improve further the network structure of the carbon spheres and increase their specific surface area.
Pore structure of carbon spheres from different carbon source concentration, determined by SAXS using synchrotron radiation as the x-ray source with a long-slit collimation system at the Beijing Synchrotron Radiation Facility (BSRF). The structure of resulting carbon spheres is mesopores with average pore diameter of 5~26 nm, porosity of 0.52~0.91, and specific surface of 210~670 m²/cm³ and 747~1606 m²/g. For AC-xx series, the variation trend of the average pore size, porosity, and the specific surface is in rough accordance with that of CS-xx series, but the average pore diameter and porosity is lower, the specific surface is higher. It indicates that smaller pore is apt to result in higher specific surface. CO₂-activation produces a large number of micropores reducing the average pore size and induces collapse of larger mesopores resulting in fall of porosity. The specific surface of the carbon spheres estimated is up to 1606 m²/g, which is higher than the surface area of 1405 m²/g for the activated carbon G212.

<table>
<thead>
<tr>
<th>Sample</th>
<th>RF precursor content</th>
<th>Deviation</th>
<th>(R_g) (nm)</th>
<th>(d_p) (nm)</th>
<th>(a_c) (nm)</th>
<th>(\varphi)</th>
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This research provides a new effective and simple approach to tailored porous carbon materials synthesis. The obtained porous carbon spheres remain promising candidates for cryogenic hydrogen storage. Synchrotron radiation SAXS technique is very helpful for us to unveil the microstructure of pore systems in materials.

**Article:**

Structure and charge transfer dynamics of the PTCDA/Au(111) interface probed by resonant photoemission spectroscopy

Organic semiconductors have attracted widespread interests due to their promising applications in organic electronic devices such as organic panel displays and photovoltaic cells (OPVCs). In these devices, the molecular orientation and interfacial coupling, which are found to markedly affect the charge transfer process, determine the device performance. For example, lying-down orientation could improve the charge transfer timescale. Ultrafast charge transfer at the organic/substrate interfaces is necessary to compete effectively against various loss processes and increase the efficiency of solar energy conversion.

Synchrotron-based core-hole clock implementation of resonant photoemission spectroscopy (RPES) and near-edge X-ray absorption fine structure spectroscopy (NEXAFS), is a novel technique and has been successfully utilized to probe the ultrafast charge transfer dynamics at organic/inorganic interfaces using the core-hole lifetime as an internal reference clock. This method allows the quantification of the delocalization of electrons from unoccupied molecular orbitals to a substrate with fs or sub-fs timescale. In addition, angular dependent NEXAFS has been found to be a powerful tool for characterizing the adsorption geometry of planar aromatic molecules on a solid substrate. Surface Science group from University of Science and Technology of China (USTC) had investigated the molecular orientation and charge transfer dynamics at PTCDA/Au(111) interface using angular dependent NEXAFS and core-hole clock spectroscopy. PTCDA molecules are found to be lying-down on the substrate with high degree of orientational order. The charge transfer timescale at the PTCDA/Au(111) interface is much larger than the C 1s core-hole lifetime of ca.6 fs, indicating weak electronic coupling between PTCDA and the gold substrate due to the absence of chemical interaction and/or bonding. It turns out that gold may not be an ideal electrode for PTCDA-based organic device applications owing to the slow charge transfer dynamics at this specific interface. The research results have been published on November 1st 2011 in Journal of Chemical Physics.

Good evaluation on the application of core-hole clock spectroscopy on organic/metal interface was provided by referee of Journal of Chemical Physics: “This paper contributes some much needed data for those attempting to apply the core-hole clock principle to organic molecules on metal surfaces. This is a really challenging area, much more so than the application of resonant photoemission to molecules on wide band gap semiconductors such as TiO2.”

The research revealed the nature of interactions and the influence of molecular orientation on charge transfer dynamics at PTCDA/Au(111) interface. In addition, this research results lay a solid foundation for the application of core-hole clock technique at organic/inorganic interfaces. The photoemission spectroscopy endstation at 4B9B beamline of the Beijing Synchrotron Radiation Facility (BSRF) where the experiments were carried out is upgrading now. The new endstation will
include a *Scienta* R4000 analyzer for ARPES and multi-function chambers. More high level researches on the new apparatus are highly expected.

**Fig.1** Angular dependent C $K$-edge NEXAFS spectra for monolayer (a) and multilayer (b) PTCDA molecules on the Au(111). The inset shows the measurement geometry. The spectra show that the intensities of the $\pi^*$ resonances enhance with decrease of incident angle, whereas the $\sigma^*$ resonances show the opposite dependence.

**Fig.2** RPES spectra for monolayer (a) and multilayer (b) PTCDA on Au(111). The bottom spectra are corresponding VB spectra measured with photon energy of 60 eV and the spectra on the left side is their respective NEXAFS spectrum. The fact that significant resonant features can be clearly resolved in both monolayer and multilayer PTCDA on Au(111) suggests that the photo-excited electrons are considerably localized in the molecules without obvious charge transfer to the substrate within the core-hole lifetime.

**Article:**

**Surfactant molecular aggregates in green solvents**

In recent years, supercritical CO$_2$ (SC CO$_2$) and ionic liquids (ILs), considered as unconventional and green solvents, have received much attention. The SC CO$_2$ solvent is readily available, inexpensive, nontoxic, and nonflammable. More importantly, its physical and chemical properties can be easily adjusted by varying the operating pressure and temperature. ILs are also an interesting class of tunable solvents with essentially zero vapor pressure, wide electrochemical window, nonflammability, high thermal stability, and wide liquid range. The researchers from the Institute of Chemistry, Chinese Academy of Sciences have developed a series of novel surfactant molecular aggregates by using SC CO$_2$ and ILs.

The creation of emulsions or microemulsions with SC CO$_2$ and IL is very interesting. The IL/SC CO$_2$ emulsion \cite{1} and CO$_2$-in-IL microemulsion \cite{2} were successfully formed. And, meso-micro porous metal-organic frameworks were also well prepared as shown in Figure 1. These novel surfactant systems show flexible and controllable characteristics, for example, the properties of CO$_2$ phase can be tuned by controlling the pressure of CO$_2$; the properties of IL phase can be tuned by changing the kind of ILs because of the tunable and designable features of ILs. Therefore, the system composed of the two green solvents is environmentally friendly. SAXS technique was used to reveal

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**Fig. 1** Surfactant molecular aggregates in SC CO$_2$ and ILs.
the nanoscale structure and confirmed that the size of micelles in microemulsion is indeed tuned by the pressure of CO₂.

The micellization of amphiphilic molecules is generally tuned by adjusting the temperature and pH value, or adding solid and liquid additives (salt, cosurfactant, etc.). However, the researchers found that the compressed CO₂ can induce the micellization of Pluronics at 15 °C [3]. Different from the common micelles with hydrophobic cores, this kind of CO₂-induced micelle, interestingly, has an amphiphilic core, and hydrophobic and hydrophilic domain coexistent as shown in Figure 1. SAXS results demonstrate that the micelles are spherical and their size can be tuned by the pressure of CO₂.

The formation of nanoscale multiple emulsions is very difficult. To induce the formation of nanoscale double emulsion, the ultrasonic and microfluidic homogenization and specially designed surfactants are generally needed. The researchers found that the compressed CO₂ can induce the formation of not only water-in-oil-in-water multiple nanoemulsions [4], but also water-in-oil-in-water double nanoemulsions [5] (see Figure 1). Especially, the formation or devastation of these multiple nanoemulsions can be reversibly controlled by the CO₂ pressure.

These surfactant molecular aggregates in SC CO₂ and ILs have potential applications in material synthesis, chemical reaction and extraction.

**Article:**


**Triggering Mechanism in Phase Transitions of Phospholipids**

Phospholipids are the most ubiquitous structural elements of biological membranes. The vast majority of lipid molecules are comprised of a hydrophilic headgroup, a glycerol backbone, and two hydrophobic hydrocarbon chains. Due to their amphiphilicity, phospholipids represent an important class of soft matter and can self-assemble into various ordered structures. Although numerous efforts have been made to unveil the various aspects (such as phase stability, phase diagram, and morphology) of the phase states of phospholipids, some long-standing and challenging questions still remain. For instance, one of these key questions is to know which part of the amphiphilic molecule triggers the phase transition.

A research group led by Prof. Zhi-Wu Yu in the Department of Chemistry, Tsinghua University has tried to seek the answer by investigating the phase behavior of the most important and widely used phospholipid, dipalmitoylphosphatidylcholine (DPPC). The results have been published on an American Chemical Society journal, Journal of Physical Chemical B, on June, 6 2011. Their strategy was to combine calorimetry and synchrotron radiation small angle X-ray scattering techniques to obtain macroscopic and structural information on phase transitions. And, by using FTIR and image analysis, they analyzed the rearrangement paces of different groups/portions of DPPC during the phase transitions.

The figure gives the small- and wide-angle X-ray scattering (SAXS and WAXS) results collected at the beamline 1W2A of the Beijing Synchrotron Radiation Facility (BSRF). The SAXS results show that the four phases (crystalline L_{c}', gel L_{β}', ripple P_{β}', and liquid crystalline L_{α}) are all lamellar-structured. By combining the electron density calculation, not only the repeat distance but also the interlamellar water layer thickness can be obtained. The WAXS data provide information on the packing states of the lipid tails. These X-ray scattering data are crucial for the characterization of the different phase structures. Particular efforts have been devoted to studying the isothermal crystallization of DPPC at 3 °C. From the image analysis data, it can be seen that the packing state of CH_{2} in the lipid tail region changes prior to the interfacial C=O region. Because the lipid head does not change during the phase transition, they deduced that the lipid tails trigger the isothermal crystallization.

Studying the role of the individual groups/portions of an amphiphilic molecule played during the phase transformation can be termed as the “regional cooperativity issue”, which can provide new insights into the triggering mechanisms of phase transitions. The regional cooperativity issue opens a broad window for us to challenge important questions including the kinetics, polymorphism, metastability, and reversibility of the phase transitions of amphiphiles.
**SAXS (A) and WAXS (B) results of DPPC in the four phase states (crystalline L\textsubscript{c'}, gel L\textsubscript{β'}, ripple P\textsubscript{β'}, and liquid crystalline L\textsubscript{α}) collected at the beamline 1W2A of Beijing Synchrotron Radiation Facility (BSRF). (C) The corresponding electron density calculation results of the L\textsubscript{c'} and L\textsubscript{β'} phases. (D) and (E) give the FTIR and image analysis results during the isothermal (3 °C) crystallization process of DPPC. δCH\textsubscript{2}: the bending vibration of CH\textsubscript{2} reflecting the packing state change of the lipid tail region, νC=O: the stretching vibration of C=O group reflecting the conformation/hydration change of the lipid interfacial region.**

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**Article:**

In situ XAS study on the mechanism of reactive adsorption desulfurization of oil product over Ni/ZnO

Ni/ZnO is an ideal adsorbent for the reactive adsorption desulfurization (RADS) to produce oil products with ultra-low sulfur content. Though many efforts have been made to reveal the mechanism of RADS, however, current evidences still cannot give a detailed understanding on the transfer mechanism of the sulfur species from oil to the sulfur acceptor, the role of hydrogen in desulfurization, as well as the structure evolution of the adsorbent during the desulfurization process. In this work, the RADS of a model oil n-nonane containing dibenzothiophene (DBT) was conducted over a Ni/ZnO adsorbent. The fresh and spent adsorbents were characterized by X-ray diffraction (XRD), X-ray absorption spectroscopy (XAS), and X-ray photoelectron spectroscopy (XPS); the evolution of Ni/ZnO adsorbent structure during desulfurization was monitored by in situ XAS in Beijing Synchrotron Radiation Facility (BSRF), Institute of High Energy Physics (IHEP), Chinese Academy of Sciences (CAS). Efforts were then made to elucidate the state of active nickel species, the role of hydrogen in desulfurization, the adsorbent structure evolution during the desulfurization process, and the possible reaction mechanism for the RADS process. The results are newly published in Appl. Catal. B: Environmental, 2011, 106(1–2): 26–38.

To get a better insight into the evolution of Ni/ZnO adsorbent structure and the transfer of sulfur species from DBT in the feed oil to the adsorbent during the RADS over Ni/ZnO, the desulfurization of the model oil containing DBT was carried out in an in situ XAS cell at 350 °C and 3.0 MPa in the stream of H2–He mixture; meanwhile, a series of XAS spectra were collected in the transmission mode at an interval of 40 min, as shown in Fig. 1.

As shown in Fig. 1(I), a series of in situ Ni K–edge XANES spectra are compared with those of fresh calcined NiO/ZnO and the reference samples NiO, Ni, Ni3S2 and NiS. Ni species in the fresh calcined adsorbent is NiO; after carrying out the RADS for 40 min on stream, its white line intensity is greatly decreased and the spectrum becomes quite similar to that of metallic Ni, suggesting that most of NiO is quickly converted to Ni in the reductive reaction atmosphere. During the whole RADS period, metallic Ni is the dominant Ni species and bulk Ni3S2 species is indiscernible even after 660 min on stream, suggesting that a complete sulfidation of Ni is difficult under current reaction atmosphere. Fig. 1(II) presents the in situ Zn K–edge XANES spectra of the calcined NiO/ZnO adsorbent during the RADS of the model oil in hydrogen. A change in the chemical state of Zn is also observed during the RADS. Compared with the spectra of the reference samples, it was found that the intensity of the dominant peak attributed to ZnO decreases gradually along with time on stream (TOS), meanwhile the peak attributed to ZnS becomes distinct and its intensity increases incessantly. The gradual evolvement of the XANES spectra with increasing TOS indicates a smooth progression from ZnO to ZnS.
The quantitative components of Ni species in the adsorbent, estimated from PCA and LCF of the XANES spectra, indicate that the main Ni-containing components in the adsorbents during the RADS are NiO, Ni and Ni$_3$S$_2$. The content of NiO decreases successively with the TOS, while that of Ni increases at first, and then remains stable until 480 min on stream and thereafter decreases with the TOS. On the other side, the content of Ni$_3$S$_2$ remains almost unchanged before 120 min on stream due to the balance between sulfidation and regeneration; after that, it increases gradually with the TOS for the RADS. Meanwhile, the main Zn components in the adsorbent are ZnO and ZnS; the content of ZnS increases successively, accompanied by a gradually decrease of ZnO content with the TOS. It should be mentioned that the sulfidation rate of ZnO to ZnS decreases with TOS and becomes very low at the later period of the RADS reaction, properly due to the limitation of H$_2$S diffusion into the bulk of unreacted ZnO through a previously formed ZnS layer.

Current results suggest that the in situ XAS is an efficient technique in characterizing the structure evolution of a catalysts or adsorbent during the reaction process. Considering also the results of catalytic tests for the RADS, it was found that the desulfurizations under nitrogen and hydrogen are different in the reaction mechanism. In nitrogen, the desulfurization over Ni/ZnO is realized through physical and chemical adsorption; a severe decrease in the desulfurization activity of Ni/ZnO is observed with the TOS and the desulfurization capacity is very low. In hydrogen, the desulfurization turns to be a reactive adsorption process and Ni/ZnO exhibits a high desulfurization activity and capacity.

Among the nickel species (NiO, Ni, and Ni$_3$S$_2$) detected in the adsorbent, the metallic nickel is the principal active sites for the RADS over Ni/ZnO. Hydrogen plays an important role in the RADS; it facilitates the decomposition of DBT on the active Ni species, the formation of Ni$_3$S$_2$, and
thereafter the transfer of sulfur from Ni$_3$S$_2$ to ZnO. Metallic Ni as the active nickel species is preserved until most of ZnO is converted to ZnS.

These observations support the three-step sulfur transfer mechanism for the RADS over Ni/ZnO in hydrogen (Fig. 2): DBT in the model oil is first decomposed on surface Ni of Ni/ZnO to form Ni$_3$S$_2$, then Ni$_3$S$_2$ is reduced in the presence of hydrogen to form H$_2$S and the active nickel species is liberated from Ni$_3$S$_2$, and lastly H$_2$S is stored in the adsorbent accompanied by the conversion of ZnO into ZnS. It seems that the presence of hydrogen is favorable and even essential for all three steps. Because the nickel species and zinc species are well contacted in the coprecipitated adsorbent and the in situ intermediate H$_2$S species are highly active, the sulfur transfer is efficient during the RADS process in the presence hydrogen.

Fig. 2. Proposed mechanism for the RADS of DBT-containing model oil over the Ni/ZnO adsorbent in hydrogen.
One-step impregnation: a new method for introducing Co\(^{2+}\) into ZrO\(_2\) with little change of the Brönsted acid sites

Sulphated metal oxides with both Brönsted and Lewis acid sites are widely used as solid acid catalysts and/or supports in organic synthesis, transformation reactions, and NO\(_x\) removal. Of particular interest is sulphated zirconia (the first impregnation), which possesses more acid sites than other sulphated metal oxides. To further improve the properties of sulphated zirconia, active component transition metal cations have been introduced into sulphated zirconia by impregnation (the second impregnation). However, this conventional two-step impregnation method often decreases the number of Brönsted acid sites, since these sites are preferentially occupied by the cations introduced, such as Co and Pd. As Brönsted acid sites play a crucial role in both the anchoring other active components and in catalytic reactions, such a decrease would cause deteriorations the intrinsic properties of solid acid materials. Thus, designing and implementing new methods for the introduction of transition metals into sulphated zirconia while minimizing the consumption of Brönsted acid sites is of particular importance. A team from Environmental Catalysis and Heterogeneous Atmospheric Chemistry of Research Center for Eco-Environmental Sciences developed a one-step impregnation method, by which the transition metal Co\(^{2+}\) cations were successfully introduced into zirconia with little consumption of Brönsted acid sites. Their research has been published on April 25\(^{th}\), 2011 in Journal of Catalysis.

The sulphation of Zr-Co hydroxides was employed to introduce Co species and to increase the number of acid sites. The number of Brönsted acid sites on sulphated Zr-Co oxide prepared by this method was much larger than that on zirconia prepared by the two-step impregnation method. As a result, sufficient Brönsted acid sites are left available for the introduction of a second active component and subsequent catalytic reactions. Specifically, a sulphated Zr-Co hydroxides supported Pd catalyst is further prepared by the impregnation method. As expected, this catalyst showed high activity towards the selective catalytic reduction of NO\(_x\) with methane.

Using X-ray Absorption Spectroscopy (Zr and Co K-edge), they provide the direct evidence of the entrance of Co into the lattice of cubic zirconia to form a substitutional solid solution.

As a new and simple approach, the one-step impregnation method provides significant advantages for the design of catalysts that require Brönsted acid sites and for further introduction of other active components.

**Fig.1 Possible structure of Co introduced zirconia with different methods**
High-Pressure Studies on CeO₂ Nano-Octahedrons with a (111)-Terminated Surface

High-pressure studies on nanostructured material have attracted great enthusiasm because of the appearance of many novel high-pressure behaviors in the nanomaterials. The phase transition pressure and process of nanomaterials strongly depend on their grain size, shape, and structure. However, previous studies have been focused on the size effect which has a strong influence on the critical pressures for phase transitions, phase transition routines, and even amorphization processes. Thus, it requires an in-depth exploration on the high-pressure phase transition and the phase transition mechanism of nanomaterials with special morphologies. Bingbing Liu and her co-workers from State Key Laboratory of Superhard Materials Jilin University have pay insight into high-pressure studies of CeO₂ nanomaterials with special exposure surface by in situ high-pressure synchrotron X-ray diffraction. Their research has been published on March 3rd, 2011 in the Journal of Physical Chemistry C.

![Fig.1](image)

Fig.1 (a) In-situ high-pressure Raman spectrum of samples, (b) In-situ high-pressure synchrotron X-ray diffraction spectrum of samples, (c) Variation of relative d spacing (d/d₀) for the CeO₂ nanoctahedrons and (d) TEM image of CeO₂ nano-octahedrons released from 55 GPa to ambient condition

The team have been performed In situ high-pressure X-ray diffraction and Raman spectroscopy on well-shaped CeO₂ nano-octahedrons enclosed by eight (111) planes. High-pressure X-ray diffraction experiments were carried out using a synchrotron X-ray source (λ = 0.6199 Å) of the 4W2 High-Pressure Station of Beijing Synchrotron Radiation Facility (BSRF). A phase transition
from an initial fluorite-type structure to a $\alpha$-PbCl$_2$ phase in CeO$_2$ nano-octahedrons has been observed at above 33 GPa. The transition pressure is slightly higher than that for bulk CeO$_2$ (at 31 GPa) and much higher than that for 12 nm CeO$_2$ nanocrystals (at 23-27 GPa). Furthermore, such transformation is complete at 38 GPa for both bulk and 12 nm CeO$_2$ nanoparticles but far from completion for CeO$_2$ nano-octahedrons even at 55 GPa. The TEM image on the sample after decompression from 55 GPa clearly shows that the nano-octahedrons preserve the starting shape. Such distinct high-pressure behavior in CeO$_2$ nano-octahedrons is believed to be due to their intrinsic geometry. Further analysis shows that the lower compressibility of the exposed (111) planes in the CeO$_2$ nano-octahedrons may be the critical factor to elevation of the phase transition pressure and the sluggishness of the transition. Indeed, the characteristics of synchrotron radiation at BSRF such as more brilliant synchrotron beams and smaller synchrotron spots would surely help to obtain strong diffraction lines of sample avoiding the interferences beyond sample chamber.

This research has used the exposure (111) planes as a detector to explore high-pressure phase transition behaviors of CeO$_2$ nano-octahedrons. This work exhibited the special morphologies played an important role on the high pressure behaviors of nanomaterials.

**Acknowledgment:**

This work was supported financially by the NSFC (10979001, 51025206), the National Basic Research Program of China (2011CB808200), the Cheung Kong Scholars Programme of China. This work was performed at 4W2 beamline, Beijing Synchrotron Radiation Facility (BSRF), which is supported by the Chinese Academy of Sciences (grant no. KJCX2-SW-N20, KJCX2-SW-N03).

**Article:**

Bo Liu, Mingguang Yao, Bingbing Liu, Zepeng Li, Ran Liu, Quanjun Li, Dongmei Li, Bo Zou, Tian Cui, and Guangtian Zou, High-Pressure Studies on CeO$_2$ Nano-Octahedrons with a (111)-Terminated Surface, *J. Phys. Chem. C.*, 2011, **115**, 4546–4551.
Structural Properties and Halogen Bonds of Cyanuric Chloride under High Pressure

In his Nobel Prize lecture, Odd Hassel particularly referred that there are Cl···N charge-transfer interactions which was widely studied by scientists later in cyanuric chloride crystals. As can be seen in figure 1, the molecules of C3N3Cl3 are forming planar layers parallel to the ab-plane. Within the layers, each molecule is linked to six neighbor molecules by halogen bonds. Owing to its outstanding structure, cyanuric chloride can be considered as a model system for studying the structural properties of halogen-bonded crystals under high pressure. Bo Zou’s group from State Key Laboratory of Superhard Materials at Jilin University has made an in-depth research in study the changes of crystal structure and halogen bonds under high pressure. The research result has been published in The Journal of Physical Chemistry B.

For studying the changes of cyanuric chloride under high pressure, this group carried out a high pressure experiment at BSRF, the highest pressure reached in this study was about 30 GPa. Representative X-ray diffraction patterns of cyanuric chloride at various pressures are shown in Fig. 2 (left). With the increase of pressure, it is evident that all the diffraction peaks shifted to higher angles, indicating a decrease in unit cell volume. We note that the shift of the (002) diffraction peak has the largest value, due to the high compressibility along the c-axis. These compressional behaviors could be explained by taking into account the layered crystal packing. The planar cyanuric chloride molecules were connected together by multiple halogen bonds to form a layered structure in the ab-plane, while the main interaction between the different layers was π-π stacking interaction. Therefore, the small compressibility of the a-and b-axes was explained by the strength of the multiple intermolecular halogen bonds between molecules. Because of weak π-π stacking interaction between layers, the c-axis was the most compressible one as expected. As pressure increased, the peaks became broader and less intense and some merged together. From the above observations and analysis, we can conclude that there is no obvious phase transition that occurred up to 30 GPa.
To understand the experimental results, the research group analyzed the changes of the crystal structure and the halogen bond under high pressure based on ab initio calculations. The crystal structure of the cyanuric chloride and the structure of halogen bond are shown in Fig. 2 (right). From the figure, we can see that a halogen bond is always along the b axis, and its bond angle maintains 180 ° under high pressure, while the bond angle of another halogen bond decreases gradually with increasing pressure. This indicates that the cyanuric chloride molecular rotates around the b axis under high pressure, which leads the originally nearly flat-shaped halogen bond network structure to become fish-scale arrangement.

In this study, synchrotron radiation light source provides sufficient experimental data for the stability of crystal structure under high pressure, which demonstrates the halogen bond in the cyanuric chloride crystal is an effective intermolecular interaction, especially the cooperation of multi-halogen bond. This research is important for understanding the changes of weak interaction of halogen bond under high pressure and the stability of halogen bond system under high pressure.

Article:
The measurement of differential EXAFS modulated by high pressure

The modulation and demodulation technique is the base of radio broadcast, as well as the information transmission and communication of modern computers. In physics, the modulation method has been applied to study the spectroscopy of semiconductors since the 1960s. Modulation spectrum, which is to measure small changes of sample under the periodic perturbation of external fields, can substantially increase the contrast of micro-structures that are difficult to discover on the static spectrum. Due to the unique characteristic of high resolution and high sensitivity, it is drawing more and more attentions. Modulation technique was also been introduced into the experiments of X-ray Absorption Fine Structure (XAFS) at the end of 20th century. The results from the present investigation indicate that modulated XAFS is able to detect femtometer-scale atomic displacements, and shows a sensitivity of 100 times better than conventional EXAFS.

We have established a novel experimental technique the pressure-modulated XAFS is firstly established on 1W1B XAFS station, Beijing Synchrotron Radiation Facility (BSRF). The technique is based on the dynamic Diamond Anvil Cell (dDAC). Pressure modulation system is built up on the basis of dDAC equipment. The working principle of the system is that the distance between two diamonds in DAC is controlled by the periodic motion of PZT position, and then the pressure on the sample varies according to the small adjustment of the distance of diamonds, as shown in figure1.

Fig1. (a) Photograph of the dDAC. (b) Several periods of pressure change on ZnSe in a dDAC at 4.8 GPa. Solid squares denote the pressure measured by ruby fluorescence. The dashed line is a periodic 1 Hz ramp wave applied to three actuators.
Moreover, we have developed the relatively complete pressure-modulated XAFS technique based on the modulation system of dDAC, from the experimental devices, and measuring method to data analysis. We have detected 0.001Å atomic displacement change by this method, which shows a precision of one order of magnitude better than conventional EXAFS (figure 2).

![Fig.2 Zn K-edge DiffEXAFS signal of ZnSe upon various pressure differences.](image)

Combining the XAFS, high pressure condition and modulation method, the pressure-modulated XAFS technique unites the characteristic of modulation and the ability of XAFS to probe local structure. The method can in situ study the local structure variation of materials under dynamic high pressure condition, for example to study a pressure-induced phase transition process in detail, or to investigate the difference of dynamic modulation and static process, and so on. Furthermore, the dynamic DAC can be used not only in the measurement of x-ray absorption spectrum, but also in the experiment of diffraction, infrared absorption, raman spectroscopy and so on.

**Article:**

**XAFS study of nanoparticle structure and adsorption complexes at metal oxide-water interface**

Magnetite (Fe₃O₄) nanoparticles have shown great potential for sorption of arsenic in contaminated soil and water because of the small particle size, large specific surface area, and high sorption capacity and affinity. To prevent nanoparticles from aggregating, and thus, to enhance sorption capacity and soil deliverability, starch has been chosen to act as a stabilizer in preparation of the Fe₃O₄ particles. However, a molecular level understanding has been lacking. A team from Research Center for Eco-Environmental Sciences (RCEES), CAS, has gained insight into bridge this knowledge gap. Their research has been published in August, 2011 in Environmental Pollution.

The team synthesized magnetite nanoparticles by co-precipitation method, using starch as a stabilizer. They found that the adsorption characteristics of starch-stabilized magnetite nanoparticles (SMNP) and their particle sizes could be manipulated by adjusting the concentration of starch. Starch can not only control the particle size of SMNP, but the adsorption affinity for arsenate. Such information is critical for predicting arsenic fate and transport in the environment as well as for guiding the design of more effective nano-scale sorbents for arsenic removal.

The presence of starch leads to the formation of more effective adsorbing sites on magnetite particle surfaces. Arsenate is adsorbed on starch stabilized magnetite nanoparticles mainly as inner-sphere bidentate and monodentate complexes. The coordination numbers of As-Fe binding increases with increasing starch concentration, which indicates that the arsenate is more firmly adsorbed at higher starch concentrations. The XAFS analyses were performed on the beam line 4W1B of BSRF.

The research finds the application of starch as a stabilizer in preparation of the Fe₃O₄ particles is able
to effectively reduce particle aggregation, and thus, particle size, resulting in much greater specific surface area and adsorption sites. XAFS spectroscopy was employed to examine the local structure of the arsenate complexes and the local structure of the average Fe atoms. Synchrotron-based XAFS can yield chemical and structural information for specific elements in a variety of unmodified—even hydrated—samples of surface species. The information provided by XAFS includes an element’s oxidation state and coordination chemistry (in the form of the average number, distance, and atomic species of elements surrounding the element of interest). Synchrotron capabilities hold great promise for more sophisticated studies and increased understanding of metal transformations at water-mineral interfaces. We hope that we can carry out time-resolved XAFS experiment in the near future to study dynamic chemical systems in non steady-state environments, and, for instance, the elucidation of the structure of intermediates involved in chemical processes.

Article:

Meiyi Zhang, Gang Pan*, Dongye Zhao, Guangzi He, XAFS study of starch-stabilized magnetite nanoparticles and surface speciation of arsenate, *Environ Pollut.* 2011, **159**(12), 3509-14.
A 5-coordinated adsorbed Zn found at water-TiO₂ interfaces

The local structure of aqueous metal ions on solid surfaces is central to understanding many chemical and biological processes in soil and aquatic environments. Differences in surface coordination structure may greatly affect the local chemical properties, long-range interactions, surface reactivity, and bioavailability of metal ions in the aquatic environment. Conclusive diagnosis of the surface coordination structures of metal ions on the atomic scale is helpful for the understanding of the toxicity and environmental impacts of the pollutants. A team from Research Center for Eco-Environmental Sciences (RCEES), CAS, has gained insight into the coordination structures of hydrated Zn(II) on TiO₂ surfaces obtained by XAFS spectroscopy. Their research has been published in January, 2011 in Environmental Science & Technology.

The team identified the local coordination structure of hydrated Zn(II) at water-TiO₂ interfaces using EXAFS and XANES spectroscopy combined with DFT calculations. A 5-coordinated geometry of adsorbed Zn(II) on TiO₂ surfaces was reported for the first time. They found that the multiple coordination structure was due to the coexistence of 4-coordinated and 5-coordinated adsorption states. The spectral and theoretical diagnosis of coordination properties would terminate the pending controversy and hypothesis about the coordination chemistry of Zn(II) cation, and may lead to re-examination on pollutants from atomic scale.

Zn(II) may occur in 4, 5, and 6-oxygen coordinated sites in different adsorption states, and the coexistence of different adsorption states formed the multiple coordination environments. The XAFS analyses were performed on the beam lines 4W1B of the Beijing Synchrotron Radiation Facility (BSRF).

The research provided a new interpretation of the EXAFS data using DFT calculations and experimental XANES analysis for metal ion adsorption on oxide surfaces. The coordination
complexity of adsorbed Zn(II) suggested a potential new development of surface complexation models that can take into account the microscopic coordination structures in describing macroscopic relationship between equilibrium concentrations in solution and on solid surfaces. The atomic-level identification of surface coordination geometry helps improve our understanding of the toxicity and environmental impacts of metal ions, because the change of metal coordination structure may produce a significant impact on its speciation and transport in the environment.

Article:

New insights into the sorption mechanism of cadmium on red mud

Cadmium (Cd), as a highly mobile and toxic trace element, has been exerting a great pressure on environmental safety due to its increasingly higher input flux from anthropogenic sources. Appropriate remediation technologies for the contaminated environments become necessary. It is known that the fate of Cd is controlled by its sorption reactions and speciation in the environment. Therefore much attention has been paid to its sorption reactions and speciation in immobilizing materials for remediation. A research group from the Chinese Agricultural Academy of Sciences has successfully applied red mud, a byproduct of aluminum production from bauxite, to immobilize Cd by significantly decreasing the labile fraction of Cd on red mud and gained new insights into the sorption mechanism of Cd on red mud with the use of synchrotron intermediate energy X-ray absorption near edge structure (XANES) spectroscopy. Their research has been published on March 2nd, 2011 in Environmental Pollution.

The research group has been working on the remediation of heavy metal-contaminated soils and proposed in-situ chemical immobilization as a sustainable remediating method for low to medium contaminated soils. However, understanding how the contaminant interacts with and competes for sorption sites in immobilizing materials is a prerequisite for predicating accurately the fates of contaminants and remediating effectively the contaminated soils. Effectiveness and mechanism of cadmium sorption on original, acidified and ball milling nanoparticle red muds were investigated using batch sorption experiments, sequential extraction analysis and XANES spectroscopy.

Cadmium $L_3$-edge (3538 eV) XANES spectra were collected at the 4B7A beamline of the Beijing Synchrotron Radiation Facility (BSRF), China. Based on the principle component analysis and linear combination fitting analysis, the Cd LIII-edge XANES spectrum indicated the formation of inner-sphere complexes of Cd similar to $\text{XCdOH}$ (X represents surface groups on red mud) on the red mud surfaces although outer-sphere complexes of Cd were the primary species.

This work shed light on the potential application of red mud to remediate Cd-contaminated soils and illustrated the promising tool of XANES spectroscopy for speciation of multicomponent systems of environmental relevance. Due to the lower sensitivity of both the intermediate energy X-ray and lower concentrations of Cd in the samples, the EXAFS data of the sorption samples displayed poorly and thus failed to provide the fine structure information of the complexes, which still needed further investigation. Brighter beamline and updated analyzing chamber (with helium) will be helpful for the speciation analysis of environmental samples.
Cadmium $L_{III}$-edge XANES spectra (a) and corresponding first derivatives (b) of sorption samples on different red mud (RM) and reference compounds: A, CdCO$_3$; B, CdO; C, Cd(OH)$_2$; D, Cd(NO$_3$)$_2$; E, Cd(OH)Cl; F, RM$_{nano}$+1.0 mmol/L Cd; G, RM$_{nano}$+6.0 mmol/L Cd; H, RM$_a$+1.0 mmol/L Cd; I, RM$_a$+6.0 mmol/L Cd; J, RM$_o$+1.0 mmol/L Cd; K, RM$_o$+6.0 mmol/L Cd and the LCF results (open circles).

**Article:**

*Lei Luo, Chenyan Ma, Yibing Ma*, Shuzhen Zhang, Jitao Lv, Mingqi Cui, New insights into the sorption mechanism of cadmium on red mud. Environmental Pollution, *Environmental Pollution* 2011, **159**, 1108-1113.
Transformation of arsenic in offshore sediment under the impact of anaerobic microbial activities

The stability of sedimentary arsenic significantly depend on many processes, such as adsorption, desorption, oxidation, reduction, dissolution, precipitation or co-precipitation. And thus the arsenic species will changed between different speciation with those chemical processes and redistributed in different phases. Although the arsenic speciation under microbial activity was controlled by many factors, the redox conditions within the sediment appear to directly affect arsenic speciation. Microbial activity strongly affects the redox conditions in sediment, speciation transformation of iron and sulfate, and thus ties to the stability of arsenic in sediments. It is important to shed more light on the behavior and the fate of arsenic in offshore sediment of seawater systems. A team from Institute of Applied Ecology, Chinese Academy of Sciences has gained insight into the fate and pathways of arsenic speciation conversion from oxyhydroxide-associated to sulfide-associated forms. Their research has been published on December 15th, 2011 in Water Research.

In present work, the fate of arsenic was discussed based on quantitative analysis of aqueous and solid arsenic and iron, and qualitative characterization using X-ray absorption near edge spectroscopy (XANES). It is proposed from XANES evidence that orpiment-like mineral is the major As sulfide phase precipitated. This indicates that the arsenic in offshore sediment has undergone a transformation process from oxyhydroxide associated arsenate to sulfide associated forms due to anaerobic microbial activities. Arsenic was released and reduced upon development of anoxic conditions but was resequestered by authigenic minerals later.

Left: Arsenic XANES spectra (A) arsenate. (B) arsenite. (C) arsenopyrite. (D) realgar. (E) orpiment. (F) as-received sediment. (G) the sediment incubated at 30 °C for 20 days. (H) the sediment incubated at 30 °C for 60
days (I) the sediment stored in tightly sealed bottle at 4 °C for 1.5 year. Right: Sulfur XANES spectra (A) disordered mackinawite. (B) pyrite. (C) arsenopyrite. (D) realgar. (E) orpiment. (F) elemental sulfur. (G) ferrous sulfate. (H) ferric sulfate. (I) the sediment incubated at 30 °C for 20 days. (J) as-received sediment.

Arsenic K-edge XANES spectra were collected on beamline U7C (XAFS station) at National Synchrotron Radiation Laboratory (NSRL) of China. Sulfur K-edge XANES spectra were collected on the mid-energy X-ray station at Beijing Synchrotron Radiation Facilities. In present work, it is obtained the transformation of As and S in offshore sediment under the anaerobic microbial activities. Sulfate was transformed from S (+VI) to S(0), S(-1) and S(-II), while the formation of orpiment-like mineral was the major mechanism for As sequestration in an estuarine sediment.

The present work documented a transformation process of Fe oxyhydroxides associated As to sulfide associated As upon environment shifting from oxic-suboxic to anoxic-sulfidic condition in a sulfur-rich system, e.g. offshore sediment.

The authors proposed that the arsenic speciation and behavior under microbial activity depend strongly upon specific environmental conditions, the fate was probably different with different scenarios. Realgar was identified as the dominant As species in the aquifer sediment infiltrated with marine water of San Francisco Bay (O’Day et al., 2004), whereas the fate of arsenic in the sediment of Jinzhou Bay in China is the orpiment-like mineral.

Article:

Liying Xu, Zhixi Zhao, Shaofeng Wang, Rongrong Pan, Yongfeng Jia*. Transformation of arsenic in offshore sediment under the impact of anaerobic microbial activities. Water research, 2011, 45, 6181-6188.
Characterization of the thermo-reduction process of chalcopyrite at 65 °C by cyclic voltammetry and XANES spectroscopy

Dissolution of chalcopyrite in most of the hydrometallurgical practices is by using of the oxidative decomposition treatment. However, some researchers reported reducing of chalcopyrite to the more dissolvable copper sulfide chalcocite (Cu$_2$S) may be a feasible alternative treatment. Chalcocite, bornite and metal copper have been proposed as the reduction products of chalcopyrite by electrochemical studies, and the formation of chalcocite has been confirmed in chalcopyrite bioleaching. It is noteworthy that the formation mechanism of these intermediates is difficult to identify by traditional composition analysis method that usually are not able to provide the formation information of these intermediates, and though electrochemical methods can provide the the intermediate reactions information, they cannot provide the direct evidence of the formation of them. A team from School of Minerals Processing and Bioengineering of Central South University, by using of Fe L$_3$-, Cu L$_3$- and sulfur K-edge XANES spectroscopy, had characterized the formation of these reduction products on the chalcopyrite electrode surface which was reduced under special potentials and revealed the transformation conditions of chalcopyrite reduction products. Their research has been published in Hydrometallurgy in April of 2011.

Fe, Cu L$_3$-edge and Sulfur K-edge XANES spectra of the massive chalcopyrite electrode potentiostatic reduced at 0, -0.2 and -0.5 V for 240 s, respectively. The results confirmed the formation of bornite and chalcocite
The team identified the formation of bornite, chalcocite and metal copper on chalcopyrite electrode surface during chalcopyrite reduction, and the formation of them follow the order of the decrease of the applied potential. The reduction of chalcopyrite to bornite in 0.1 to -0.1 V, and it is the initial and rate-limited step of the successive reduction of chalcopyrite. When the potentials continued moving toward negative direction, the reduction of bornite and chalcopyrite to chalcocite took place in the potential range of -0.1 to -0.56 V. When the applied potential was negative than -0.5 V, the reduction of the remaining chalcopyrite and chalcocite on the electrode surface to elemental copper took place in this negative potential.

The research showed the sulfur K-edge XANES based on synchrotron sources can help to reveal the oxidative and reductive mechanism of sulfur-containing compounds. Instanteous formation of the oxidized and/or reduced compounds can be examined if some in-situ detection facilities are assembled to the synchrotron facilities, which can provide more information and help to reveal the redox mechanisms of the sulfur-containing compounds.

**Article:**

Sulfur oxidation activities of pure and mixed thermophiles and sulfur speciation in bioleaching of chalcopyrite

In contemporary era, the research and development of bioleaching have been always focused on achieving effective recovery of valuable metals by improving the efficiency of bioleaching microorganisms, which may be determined mainly by sulfur oxidation activities of sulfur-oxidizing microbes and the speciation of intermediate compounds formed during bioleaching processes. However, the correlation between sulfur oxidation activities of sulfur-oxidizing microbes and the speciation of intermediate compounds has remained elusive. A team from Key Lab of Biometallurgy of Ministry of Education of China, School of Minerals Processing and Bioengineering, Central South University has gained insight into sulfur oxidation activities of thermophiles and sulfur speciation in bioleaching of chalcopyrite. Their research has been published on November 26th, 2010 in Bioresource Technology.

The team identified the mixed thermophiles, with contributing significantly to the raising of leaching rate and accelerating the formation of leaching products, had a higher sulfur oxidation activity than the pure culture, and jarosite was the main passivation component hindering the dissolution of chalcopyrite, and elemental sulfur seemed to have no influence on the dissolution of chalcopyrite. In addition, The team supported that covellite might be converted from chalcocite during the leaching experiments, and the elemental sulfur may partially be the derivation of covellite and chalcocite.

Sulfur K-edge spectra of chalcopyrite leaching with mixed thermophilic archaea using synchrotron radiation at BSRF: Besides the features of chalcopyrite in Fig. a, the spectra presented a new peak at 2.4804KeV that could be assigned to sulfate ions. And the chalcopyrite peak kept declining when the sulfate ions peak kept increasing. The fitted XANES spectra of the surface residues at day 6 suggests that the surface residue mainly contained chalcopyrite, jarosite, covellite and chalcocite with the fraction of 47.5%, 38.2%, 13.5% and 0.7%, respectively.
The research provides the scientific community clues to promote the understanding of the synergistic effect of the thermophiles as well as bioleaching mechanism by the mixed thermophilic culture, and to devise an efficient way to enhance the yield of chalcopyrite bioleaching. In their works, Sulfur K-edge X-ray absorption near-edge structure (XANES) of BSRF was proved to be a particularly useful technique to investigate the variations in the sulfur species, ranging from sulfide, sulfite, and sulfate; in addition, it is able to differentiate various sulfides based on the shape and the position of the XANES features, thus providing useful site-specific information for sulfur species of catalysis.

Article:

Reconstitution and structural analysis of the yeast box H/ACA RNA-guided pseudouridine synthase

Box H/ACA RNA-protein complexes (H/ACA RNPs) are ancient molecular machines conserved from archaea to eukaryotes that mediate pseudouridine synthesis, eukaryotic ribosome biogenesis and vertebrate telomere formation. Although studies of archaeal H/ACA RNP has led to a rather detailed understanding of its structure and mechanism of action, the assembly and architecture of eukaryotic H/ACA RNP remain unclear. The laboratory of Dr. Keqiong Ye, at the National Institute of Biological Science, Beijing, has reconstituted functional yeast H/ACA RNP, analyzed its assembly, activity and structure and found many eukaryotic-specific structural features of H/ACA RNP. Their results were recently published in *Genes & Development* on November 15, 2011.

The difficulty in expression and purification of recombinant H/ACA proteins has hindered the structural and functional analysis of H/ACA RNPs for a long time. The Ye’s group has successfully obtained well soluble recombinant H/ACA proteins by utilizing a co-expression and co-purification strategy and reconstituted functional yeast box H/ACA RNPs. Taking advantage of this reconstitution system, they identified that the protein-RNA interaction occurring at the upper stem region of eukaryotic H/ACA RNA is dispensable for the activity, revealing a major difference in the functional organization between archaeal and eukaryotic complexes. Although eukaryotic H/ACA RNAs have a conserved two-hairpin structure, they found that each isolated single hairpin of yeast H/ACA RNA is able to form an independent structural and functional unit.

They crystallized a ternary H/ACA protein complex of Cbf5, Nop10 and Gar1 and collected a high-quality 1.9 Å x-ray diffraction dataset at Beijing Synchrotron Radiation Facility beamline 3W1A. The structure determined by molecular replacement reveals many eukaryotic-specific features of H/ACA RNP. The core domain of yeast Gar1 contains a C-terminal extension that forms hydrophobic contacts with the thumb loop of Cbf5 (Fig. 2). Related biochemical analyses show that the extension of Gar1 regulates substrate turnover and likely facilitates Gar1 to replace the assembly factor Naf1, which binds at the same site of Cbf5 during H/ACA RNP biogenesis in vivo.

Mutations in human Cbf5 (dyskerin) have been shown to lead to a rare inheritable disease dyskeratosis congenita (DC). The eukaryotic-specific N-terminal extension of dyskerin is a hot spot of DC mutation. The structure of yeast Cbf5 reveals that the extension forms an extra structural layer on the PUA domain, providing an improved model to understand the mutational effect (Fig. 3).

This work using biochemical experiments and X-ray crystallographic analyses in BSRF provides novel insight into eukaryotic H/ACA RNP structure. The future work is to determine the structure of fully assembled yeast H/ACA RNP in various functional states and to understand the structural adaptation of H/ACA RNP during evolution.
**Figure 1.** Crystal structure of the yeast Cbf5-Nop10-Gar1 complex and comparison with archaeal H/ACA RNP structure.

**Figure 2.** Yeast Gar1 possessed a conserved C-terminal extension (orange) that contacts the Cbf5 thumb loop (green) via hydrophobic interactions and regulates substrate loading and release.

**Figure 3.** The N-terminal extension of yeast Cbf5 (magenta) forms an extra structural layer on the PUA domain and harbors many dyskeratosis congenita mutation sites (orange balls).

**Article:**

ATRX ADD domain links an atypical histone methylation recognition mechanism to human mental-retardation syndrome

ATR-X (alpha-thalassemia/mental retardation, X-linked) syndrome is a human congenital disease whose clinical manifestations are α-thalassemia and mental retardation. Approximately 50% of the missense mutations in affected persons are clustered in the ADD (ATRX-DNMT3-DNMT3) domain of the syndrome’s key gene ATRX. However, the function of ATRX ADD (ADD_{ATRX}) domain has remained elusive. In collaboration with Dr. Yang Shi at the Harvard Medical School, a group led by Dr. Haitao Li from the Center for Structural Biology, Tsinghua University conducted structural and functional studies on ADD_{ATRX} and demonstrated that ADD_{ATRX} is a new type of histone H3-binding module that is able to combinatorially sense the methylation state at both H3K4 and H3K9. This work has been published in *Nat Struct & Mol Biol* in June, 2011.

Recognition of H3K9me3 by ATRX ADD

At beamline 3W1A of Beijing Synchrotron Radiation Facility (BSRF), Dr. Li group achieved 0.93Å atomic resolution co-crystal structure of ADD_{ATRX} bound to H3K9 trimethylated (H3K9me3) peptide. The structure revealed the following new mechanisms in the recognition of histone lysine methylation:

1) ADD_{ATRX} adopts an atypical polar pocket for H3K9me3 readout, in which recognition of trimethyllysine is notably contributed by a set of unconventional “C-O” hydrogen bonds. Such a polar pocket is distinct from the classical “aromatic cage” that has been widely reported for
trimethyllysine binding.

2) The H3K9me3-binding pocket is formed at the interface of a GATA-like finger and a PHD finger of ADD_{ATRX}. The usage of a “composite” pocket for histone methylation readout highlights the strategy of module integration to create a functional reader pocket.

3) Effective binding of H3K9me3 by ADD_{ATRX} not only depends on trimethylated H3K9 but also on non-methylated H3K4 as well as a free amino terminus, representative of a combinatorial readout mode of histone H3 methylation.

ATRX is the key etiologic factor for ATR-X syndrome. This work identified ADD_{ATRX} as an important H3K9me3 “reader”, which is essential for the recruitment of ATRX to heterochromatic regions like pericentromeric heterochromatin or telomere for optimal chromatin remodeling function excelled by ATRX. This study has revealed a unique histone-recognition mechanism underlying the ATR-X etiology, and may have also provided a new avenue for therapeutic intervention in ATR-X syndrome.

The synchrotron radiation light source at BSRF played a vital role in the structure determination of the ADD_{ATRX}–H3K9me3 complex. It is the high intensity and small beam size of the synchrotron radiation light that allows the complex structure determination at atomic resolution and enables the elucidation of such an atypical histone methylation recognition mechanism to the public.

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Article:

SARS CoV nsp16/nsp10 protein complex: A unique ribose 2’-O-methyltransferase

The 5’-cap structure is a distinct feature of eukaryotic mRNAs, and eukaryotic viruses generally modify the 5’-end of viral RNAs to mimic cellular mRNA structure, which is important for RNA stability, protein translation and viral immune escape. SARS coronavirus (SARS-CoV) encodes two S-adenosyl-L-methionine (SAM)-dependent methyltransferases (MTase) which sequentially methylate the RNA cap at guanosine-N7 and ribose 2’-O positions, catalyzed by nsp14 N7-MTase and nsp16 2’-O-MTase, respectively. A unique feature for SARS-CoV is that nsp16 requires non-structural protein nsp10 as a stimulatory factor to execute its MTase activity. Yet a team composed of researcher from Wuhan University and Nankai University has gained insight into the mysterious structure and biochemical feature of nsp16/nsp10 protein complex. Their research has been published on October 13th, 2011 in Plos Pathogens.

Previous work of this team indicate that nsp10 may function as a stimulatory factor for nsp16 and is required for the 2’-O-MTase activity of nsp16. Now they proved that nsp10 assists nsp16 to bind substrate for its methyltransferase activity, include capped RNA substrate and the methyl donor S-adenosyl-L-methionine (SAM), also they present structure of nsp16/nsp10 complex. They show that nsp16 possesses the characteristic fold of the class I MTase family, comprising a seven-stranded β-sheet surrounded by α-helices and loops. But differences between nsp16 and other methyltransferase which can exert methyltransferase alone, is that nsp16 possesses a shorter αD helix. This feature makes the SAM binding cleft of nsp16 seems more flexible and lower its SAM binding activity, this can explain why nsp16 needs another protein to promote its activity. They also find one hydrogen bond forms between Lys-93 of nsp10 and Ser-105 of nsp16, and two salt bridges exist between His-80 ND1 and NE2 from nsp10 with Asp-102 OD2 from nsp16, these interactions sustain one wall of SAM binding cleft of nsp16, and thus promote the SAM binding activity of nsp16.

SARS-CoV nsp16 is the only 2’-O-MTase currently known that needs a stimulatory subunit for exerting its methyltransferase activity. These mechanisms could be explained based on the crystal structure of nsp16/nsp10 complex, and confirmed by mutational analysis. mRNA capping and methylation play important roles in mRNA stability, processing, transport and protein translation and thus The MTase active site has been suggested as a drug target for developing antiviral drugs, However, the MTase fold is structurally conserved between viral and cellular MTases, and it is thus difficult to obtain antiviral compounds with high specificity targeting MTase active sites. For this reason, it looks more promising to target the interface of nsp16 and nsp10, which is unique to coronaviruses.
Structure of nsp16/nsp10 protein complex, determined at 2.0 Å resolution using synchrotron radiation at BSRF.

Article:
3D configuration of mandibles and controlling muscles in rove beetles based on micro-CT technique

The rove beetles (Insecta, Coleoptera, Staphylinidae) are mainly predators. They use the mandible of their mouthparts to bite food. According to previous morphological studies, three different types of mandibles and heads can be recognized. Presently, the relationship of the head shapes and the robustness of mandibles in rove beetles as well as in other beetle groups is a matter of debate. The group Molecular systematics and evolution of beetles, Institute of Zoology, CAS studied the relationship between the shape of the mandible, the development of controlling muscles, and the morphology of the posterior part of the head. The results has been pressed on the issue of Analytical and Bioanalytical Chemistry, on May 22, 2011.

We selected three rove beetle species in this study which are *Noddia sp.*, *Creophilus maxillosus*, and *Hesperosoma sp.* We reconstructed the three dimensional (3D) structures of their head capsule, mandible and mandible muscles using Xray tomography. From the analysis we found an interesting result connected with the adductor muscles. They are short muscles originating from the posterolateral angle of the head of *Noddia sp.*, whereas the angles with the apodeme are approximately 40°. The muscles are long muscles originating from the posterolateral angles of the head of *Creophilus maxillosus* and the angles with the apodeme are approximately 30°. In addition, there are no adductor muscles originating from the posterolateral angle of the head except for the mandible abductor muscle in *Hesperosoma sp.*
We studied the mandible, muscle and skeleton in 3D, which may explain the relationships of different structures more precise. It will also greatly promote the studies of structure and functions, the phylogenesis, as well as evolution of different structures.

Article:

Nanoprobes: Quantitatively Detecting the Femtogram Level of Arsenite Ions in Live Cells

Recently, arsenite (As) have been applied to treat the acute promyelocytic leukemia (APL) successfully. Further research revealed that the apoptotic effects of arsenic are not restricted to APL cells but also can be observed in other malignant cells in vitro.

There are at least three different molecular mechanisms are proposed but not uniform. Note that all these molecular mechanisms are contrary with each other and they all focused the pathway of bio-molecular triggered by As, no solid information of arsenite in live cell are supplied to match these molecular mechanisms, therefore it is hard for researchers to figure out the right molecular mechanism to understand how did arsenic kill cancer. A group from Institute of High Energy Physics designed a kind of fluorescent nanoprobes to high sensitivity detection the drug arsenic ions in live cells. The research has been published on June 2nd, 2011 in ACS nano.

The team designed the fluorescent nanprobe, single-strand DNA wrapped single-wall carbon nanotubes (ssDNA-SWCNTs, the ssDNA is labeled by the dye molecule), which can detect arsenite ions via an emission decrease method. The mechanism of the nanprobes was studied by the SRCD in BSRF and AFM as follows. For the nanprobe, the SWCNT is wrapped by ssDNA, and the ssDNA is labeled by the 50-hexachloro-fluorescein phosphoramidite (HEX). Arsenite ions could strongly bind the G/T bases of ssDNA and decrease the π-π interaction between ssDNA and SWCNTs. This makes some ssDNA dissociate from the SWCNTs and further adapt condensed conformation in solution. Such condensed conformation of ssDNA will cause the HEX to interact with G/T base-binding arsenite ions, and further induce metal ions quenching the emission of HEX.
Thus, the nanoprobes can detect arsenite ions via an emission decrease method. With the help of a confocal microscope and cryo-electron microscopy, the lysosome target of the arsenite ion and nanoprobe is well described in high spatial resolution. In a live cell, trace arsenite ions could interact with nanoprobes and significantly decrease the emission of the nanoprobes. This result supported that high dosage arsenic will push the cancer cell apoptosis more quickly as more As is concentrated in the cell. For the first time, our studies provide a method to detect artificial metal ions via spatial and quantity parameters in live cells. This study also gives clear proof that the target organelle of arsenite is lysosome, and this strong proof can help the molecular researcher determine the right molecular pathway of As-induced cancer cell apoptosis.

**Article:**

Microglial activation, recruitment and phagocytosis as linked phenomena in ferric oxide nanoparticle exposure

Microglia as the resident macrophage-like cells in the central nervous system (CNS) play a pivotal role in the innate immune responses of CNS. Understanding the reactions of microglia cells to nanoparticle exposure is important in the exploration of neurobiology of nanoparticles. Here we provide a systemic mapping of microglia and the corresponding pathological changes in olfactory-transport related brain areas of mice with Fe$_2$O$_3$-nanoparticle intranasal treatment. We showed that intranasal exposure of Fe$_2$O$_3$ nanoparticle could lead to pathological alteration in olfactory bulb, hippocampus and striatum, and caused microglial proliferation, activation and recruitment in these areas, especially in olfactory bulb. Further experiments with BV2 microglial cells showed the exposure to Fe$_2$O$_3$ nanoparticles could induce cells proliferation, phagocytosis and generation of ROS and NO, but did not cause significant release of inflammatory factors, including IL-1β, IL-6 and TNF-α. Our results indicate that microglial activation may act as an alarm and defense system in the processes of the exogenous nanoparticles invading and storage in brain.

The micro-distribution mapping of iron in the rat brain after nanoparticle intranasal exposure was achieved by synchrotron radiation micro-beam X-ray fluorescence (SR-μXRF) at the Beijing Synchrotron Radiation Facility (BSRF) 4W1B beamline, with space resolution of several micrometer and detection limit of ng/g range. The incident beam was focused approximately 20 × 30 µm by a Pb collimator with two cross-slices. A monochromatic X-ray with photon energy of 16.5 keV was used to excite the samples. Samples were mounted on XYZ translation stages and the sample platform was moved by a 2D stepping motor along the X directions of 40 µm and Z directions of 60 µm for each step.

In the study, we observed the activated microglial cells in olfactory bulb, hippocampus and striatum, accordingly with the storage route of Fe$_2$O$_3$ NP shown by SR-μXRF images and the alteration regions of the pathological reports. The most number of activated microglia were found in the olfactory nerve layer (ONL) and glomerular layer (GL), which was consistent with the transport pathway of Fe$_2$O$_3$ NPs along the olfactory nerve layers.
Biological effects of Fe$_2$O$_3$ nanoparticles on central nervous system. (A) Fe distribution in mouse olfactory bulb tested by SR-$\mu$XRF. (B) Immunofluorescence staining of CD11b in mouse olfactory bulb. Arrows in the box on the top right corner show CD11b-immunoreactive microglia presenting “resting face” with a small cell body in the fine, ramified processes in control mice; in the Fe$_2$O$_3$ nanoparticles group mice, microglia present “activated face” with stouter cell processes. The Fe$_2$O$_3$ nanoparticles induced microglial proliferation and activation mainly concentrated in the olfactory nerve layer (ON) and glomerular layer (GL). (C) The mediation role of microglia for the protection or neurotoxicity of brain after intranasal exposure of Fe$_2$O$_3$ nanoparticles.

**Article:**
Co speciation in blue decorations of blue-and-white porcelains from Jingdezhen kiln by using XAFS spectroscopy

Blue-and-white porcelain is well-known for its skillful techniques and great artistic merit all over the world. It usually designates white porcelain decorated with blue pigment, which is usually cobalt oxide under the glaze. So far, blue-and-white porcelain have been attracting more and more researchers to investigate its manufacturing techniques, the provenance of cobalt blue pigment ore, the dating and authentication, and so on. Coloring origin of the blue color in blue-and-white porcelain is one of these hot topics. Previous studies pointed out there were two factors that influenced the tone of blue color in blue-and-white porcelains. One was the transition elements which contained in the blue decorations, including cobalt, iron and manganese. The content of these elements and their ratio had a large influence on the blue color. Manufacturing techniques, such as pretreatment of the raw materials, the temperature, atmosphere and time during the firing, was another factor. And the latter influence the blue color by controlling the oxidation state and chemical environment of these transition elements. Thus, a thorough knowledge of speciation of transition elements (i.e. oxidation state, chemical environment) is not only crucial for understanding the coloring origin of blue color but also provide an important information for discussing issues about the manufacturing techniques, the provenance of cobalt pigment ore, the cultural exchange between the east and west.

Since the layer of blue pigments was between the glaze and body, little is known about the elements’ oxidation and chemical environment which is directly correlated to the origin of blue color. X-ray absorption fine structure (XAFS) is an atomic probe and has demonstrated its power to investigate the oxidation and local structure of transition element at the molecular scale in recent years. For further understanding the coloring origin of blue decorations, Lihua Wang, supervised by Changsui Wang, from Department of Scientific History and Archaeometry, Graduate University of the Chinese Academy of Sciences carried out Co K-edge XAFS measurements at BSRF to characterize the oxidation state and chemical environment of Co element contained in blue decorations of blue-and-white porcelains manufactured by Jingdezhen official kiln during the Yuan and Ming dynasties. XANES spectra showed that cobalt was present as both divalent and trivalent ions and the ratios of $\text{Co}^{2+}/\text{Co}^{3+}$ were almost similar for all samples with different historical periods. EXAFS analysis indicated that cobalt atom was situated in both octahedral and tetrahedral sites. Considering the empirical optical absorption in visible region, it was assumed that divalent ions located at tetrahedral sites made the main contribution to the blue color. Their research has been published in Journal of Analytical Atomic Spectrometry in September of 2011 (J. Anal. At. Spectrom., 2011, 26, 1796-1801).
Figure (left) Normalized Co K-edge XANES spectra for blue-and-white porcelain shards as compared with reference materials. (right) $k^3$-weighted, phase uncorrected FT of all blue-and-white porcelains and reference materials.

**Article:**

1W1A-Diffuse Scattering Station

(1) Operation

During the periods of dedicated synchrotron radiation running in 2011, X-ray diffuse scattering experiment station provided X-ray diffraction (XRD), X-ray reflection (XRR), grazing incidence X-ray diffraction (GIXRD) and grazing incidence small-angle X-ray scattering (GISAXS) for 39 research projects. The users came from several institutes of Chinese Academy of Sciences and universities in China, in addition to users from Pohang University of science and technology. The research projects distributed over various fields, including wide-band gap semiconductor thin films, iron-based superconductors, soft condensed matters, polymer thin films, nano-porous materials and so on.

(2) Improvement of beamline and station

In this year, facilities in the optics hutch and the experimental hutch were upgraded in chief as the following aspects: (1) To eliminate the effects of solidified In/Ga spots on the bent crystal and improve the fill of the liquid In/Ga as a thermal conductive medium filled between the bending support and the crystal, a new designed monochromator was installed. (2) A 2D detector (Mar345) was equipped in the experimental hutch (as shown in Fig.1), while the detector adjustment stages was designed and employed for the implementation of grazing-incidence small angle X-ray scattering and grazing-incidence X-ray diffraction on characterization of polymer thin films.

Fig.1 Photo of the 2D detector employed in GIXRD setup

(3) Research highlights

In this year, using the in-plane GIXRD method, researchers from institute of chemistry determined the parameters of intermolecular $\pi-\pi$ stacking of materials for all-solution-processed high-performance n-channel organic transistors (Fig.2). Their article was published in *Adv. Mater.*
Researchers from Changchun Institute of Applied Chemistry, exploiting 2D GIXRD technique, characterized the microstructures of an organic electronic material, and their article was published in *Adv. Mater.* (2011, 23, 2850-2854).

**1W1B-XAFS Station**

(1) **Operation**

During this calendar year, there are two synchrotron radiation beamtimes for users. One is from Jun 8 2011 to July 15 2011; the second is from Nov 2 2011 to Nov 30 2011. The 1W1B-XAFS facility has shown good performance with 99% of efficiency. Users are from national universities and science research institutes. There are 45% users in environment and life science; 15% in chemical engineering; 40% in material science. This year, new instrument improvements are based on high temperature cell and micro focus XAFS technology. Novel applications of XAFS are in Single-atom catalysis study (Nature Chemistry 2011, 3, 634–641) and the Coordination Structure investigation at the interface of water-TiO₂ (Environ. Sci. Technol. 2011, 45, 1873–1879).

(2) **Improvement of beamline and station**

- **Design of In Situ High Temperature Cell and Application in Temperature-Dependent XAFS measurements**

Temperature plays important role in the state of matter, which can induce novel optical, electronic, catalysis and magnetic properties. The temperature dependent structure is under continuous interest. Here, based on the beamline and experiment station of 1W1B-BSRF, facile high temperature cell for temperature-dependent XAFS was presented (Fig.1). It can be used in transmittance and fluorescence XAFS measurements. Owing to the optimized electro-circuit and the heating element, it is easy controlled from room temperature to 1273K, and in situ XAFS study of catalyst can be performed under vacuum or realistic gas condition. Now its applications are in situ study the structure of catalysis, liquid metal and ferroelectric materials. Here (Fig.2), ceria is as an example, its oxygen-storage capability and structure are associated in the in situ XAFS study.
Micro-focus technique and application in high pressure XAFS

Glass capillaries have unique properties for guiding X-rays in experiments with micrometer precision. It can provide the microstructure evidences of functional materials, nature mineral and tissues and cells with spatial distribution. Design considerations of such optics are presented for X-ray applications involving high-pressure experiments at the 1W1B-BSRF. For high-pressure experiments in diamond-anvil cells, polycapillary optics provide 70-80 µm diameter beams for X-ray absorption fine-structure applications.
Fig. 3 a: Glass capillaries  b: Design for high pressure XAS measurements

c focus point (73*75µm) ; d Measured vertical FWHM (µm) of the polycapillary focused microbeam (about 75µm)

e, f  Compared XAFS with and without capillaries focus optics at 7KeV and 13KeV

The results indicate that the XAFS data quality has been improved based on the capillaries focus optics. The XAFS data distortion by diamond diffraction effect is much reduced.

(3) Experiments and data analysis training program

XAFS is one of most used station in synchrotron radiation, applied in material, energy, biology, medical, environments. High quality data collections and analysis are very important in the common research platform. On the needs of users in BSRF, we took six months to prepare and organize the experiments and data analysis training program. It is successful and has much help for new users.
In 2011, SAXS station was opened to users in parasitic and dedicated modes. During the first half year in 2011, 1694h were supplied to 23 user’s projects from 14 institutions. From June 8 to July 15, the first dedicated running of SAXS station provided 820h of beam time to 20 user’s projects came from 14 institutions. From November 1 to December 1, the second dedicated running of SAXS station provided 680h of beam time to 24 user’s projects distributed in 16 institutions. In 2011, SAXS station supplied 3194h of beam time in all for users. The experimental modes included normal SAXS, WAXS, SAXS/WAXS, and GISAXS. In-situ heating, stretching, and time-resolved environments were used.
In 2011, SAXS/WAXS mode was opened to users, which can satisfy the partial requirement to acquire simultaneously the experimental data of small angle scattering and wide angle diffraction. At present, 2D-SAXS /1D-WAXS and 1D-SAXS / 1D-WAXS experimental methods are provided. The detectors are 2D CCD and/or 1D gas detector. The sketch map and the corresponding SAXS and WAXS patterns of some carbon fibers are shown in Fig.1.

Fig.1 Sketch map of 2D-SAXS/1D-WAXS and 1D-SAXS/1D-WAXS experimental methods, as well as the corresponding SAXS and WAXS patterns of some carbon fibers.

(2) Improvement of beamline and station

In 2011, the following equipment improvements were performed: A scatterless slit was equipped at SAXS station, which can stop efficiently the parasitic scattering from beamline, improve greatly the signal-to-noise performance of scattering data, and upgrade further the quality of experimental data. A new beamstop with photoelectric diode was also installed in the SAXS camera, which can monitor the intensity and stability of the direct beam and the function used as beamstop is still kept. Utilizing the scatterless slit and the new beamstop, the experimental efficiencies were greatly improved. Fig.2 shows the photographs of the scatterless slit and the new beamstop.

Fig.2 Photographs of the scatterless slit (left) and the new beamstop with photoelectric diode (right).

In November 25-26, 2011, nine experts came from other synchrotron radiation facilities and universities, as well as other research institutes of Chinese Academy of sciences had a performance
test for the SAXS beamline and station. The expert group got the consensus of opinion. They deem that the SAXS experimental platform works in multi-experimental modes with various sample environments. It can supply steady experimental support and advanced SAXS techniques for users.

**1W2B, 3W1A-1W2B, 3W1A-Biological Macromolecule Crystallography Stations**

(1) Operation

Beamline 1W2B and 3W1A are mainly designed for macromolecular crystallography X-ray diffraction experiments, including the multi-wavelength anomalous dispersion experiments. Meanwhile, beamline 1W2B can be used for the X-ray absorption fine structure experiments and opened to users in the dedicated SR mode for the first time. Thus, more beamtime was supplied to users and the beamtime demand pressure of 1W1A-XAFS station was reduced. In 2010, the coupling mode of beamline 1W2B has been accommodated and afforded for users officially.

(2) Improvement of beamline and station

- Gas Mixture Proportion (GMP) has been established in the XAFS experiment platform at 1W2B beamline. By using the gas regulation system, the gas mixture proportion of the ionization chambers can be adjusted in the real time, and benefit of which the best results of the different samples can be got.

![Figure 5.1.7-1 GMP of the 1W2B ionization chambers.](image1)

![Figure 5.1.7-2 The contrast of the experiment data in different GMP](image2)

- The MX beamline Real-Time Station Monitoring System has been further improved. The key part monitoring of the beamline has been completion online, and the data will be writing to the database on real time. Through this system the beamline fault diagnosis can be done effectively and the normal state of the beamline can be restored easily.

![Figure 5.1.7-1 GMP of the 1W2B ionization chambers.](image1)
(3) The Automation Control System of the 1W2B beamline has been constructed initially. In the base of the original mechanical and electrical control, the moving parts of the beamline can be integrated into a control interface, and they also could achieve the local control. In the future it will realize the remote control and the experiment operation.
(3) Research Highlights

- ATRX is a human "ATR-X syndrome" key cause of protein, which is more common in boys. The clinical manifestations has the a-the Mediterranean anemia, and the intelligence retardation, etc. The clinical genetics research in the patients has already identified hundreds of ATRX wrong mutations, in which it is about 50% of mutations in ADD zinc finger structure enrichment domain. Li Haitao who is from Tsinghua University, together with the other institutions researchers from Harvard Medical School and Rockefeller University etc. have analyzed the ATRX biochem and ADD protein structure domain crystal structure, and found that it has the function of the protein with group H3. At the same time they have also found that the H3 ninth of lysine three methylation (H3K9me3) can help a combination of the two, and the fourth lysine three methylation (H3K4me3) will hinder the combination of both. At the molecular level one of the pathogenic mechanism of the ATRX mutations causing the "ATR-X syndrome" has been illustrated, and it provides an important further treatment the etiology of the foundation for human "ATR-X syndrome".


- H/ACA RNA protein complex is a commonly found in eukaryotes and the kind of conservative molecules bacteria, which are mainly the false uracil mediated RNA modification. At the same time, it participates in the eukaryotes ribosomes assembly and the vertebrate telomere synthesis. At present the archaea H/ACA complex structure has a detailed understanding, but on eukaryotic complex structure it has been still known very little. Prof. Ye Keqiong, one researcher from NIBS, firstly use the recombinant protein and RNA expression in vitro to assemble a catalytic
activity of yeast H/ACA compound. By using this reorganization system, the author has analysed the H/ACA complex assembly method, catalytic activity and three-dimensional structure in depth. Their analysis contains three of the protein component of the complex crystal structure. They analyzes the structure and function of complex relationship, and found many eukaryotes H/ACA compound the special structure characteristics.

**Article:** Li, S., Duan, J., Li, D., Yang, B., Dong, M., Ye, K., Reconstitution and structural analysis of the yeast box H/ACA RNA-guided pseudouridine synthase. Genes Dev. 2011, 25: 2409-2421

**3B1- LIGA and X-ray Lithography Stations**

X-ray Diffractive Optical elements were utilized in National Key Facilities.

At BSRF X-lithography/LIGA experimental station, high resolution lithography tool was used to fabricate a series of x-ray diffractive optical elements by Institute of Microelectronics, CAS. Free standing 1000 lp/mm single order diffraction gratings and 2000 lp/mm transmission gratings were manufactured and used for several kinds of spectrometers in national key facilities by successfully depressing the high diffraction orders with the meeting to their theoretical analysis. Using these elements scientists from China Academy of Engineering Physics got good experimental results. Based on above outstanding results, our user was invited to join in Eleventh Five-year Plan Major national science and technology exhibition.

![Single order diffraction grating](image1)

![Diffractive optical elements](image2)

**4W1A-X-ray Imaging Station**

(1) Operation

After three years upgrade project, X-ray imaging station is open for all the uses on 2011. The new station can provide three experimental methods which are crystal diffraction topography, micrometer-resolution CT method and nanometer-resolution CT method. During the dedicated
operation for synchrotron radiation from Jun.5 to Jul.15, 2011, there are total 25 user projects carried out at X-ray imaging station with 28 days beamtime. In which there are 7 crystal diffraction topography projects, 7 micrometer-resolution CT projects and 11 nanometer-resolution CT projects. During the dedicated operation for synchrotron radiation from Oct.29 to Nov.30, 2011, there are total 17 user projects carried out at X-ray imaging station with 20 days beamtime which are all nanometer-resolution CT projects.

(2) Improvement of beamline and station

To insure the stability of the beam on the sample in nanometer-resolution imaging facility, a set of auto-feedback beam adjustment system was developed to correct the beam drift of the secondary source in the vertical direction of nano-imaging beamline. Finally, a case is employed to test and verify the feasibility of this method and it is expected to eliminate the influence to nano-resolution imaging due to the instability in the vertical direction of synchrotron radiation beam.

Fig.1 Auto-feedback beam adjustment system.

(3) Research highlights

Since the opening of the nano-imaging facility, more than twenty users from universities and scientific research institutes all over the world have done many experiments based on the nano-imaging technology. The research subjects are covered microsystems research of insect, acarid high-resolution structure, cell structure, drug carrier microsphere structure, catalyst particle structure, cosmic dust structure, metal doped fiber, metal nano-particles, textile fiber element distribution, fuel cell electrode microstructure, etc. It is approved that the synchrotron radiation nanometer-resolution CT technique is a powerful tool to study the microscopic world and has the widespread application prospect following the optical microscope and the electron microscope. In these researches, we can see that nanometer-resolution CT technique provides a huge amount of useful experimental data. The slice results shown in Fig.2 give a perfect description of the fine structure and distribution of sperm
in the spermatheca cochleate duct which helpful to reveal the process of the sperm transfer (cooperating with Institute of Zoology, CAS). By stacking sequences of x-ray microscopy slices, the 3D reconstruction technique provided an excellent view of the spermatheca cochleate duct of female and the flagellum of male in the species *Aleochara verna* which revealed structural details with nano resolution that were invisible by conventional microscopy, see Fig.2 and Fig.3.

Fig.2 The 3D (right) and 2D (left) reconstruction of the proximal part of spermatheca duct. The triquetral structure marked by arrows in the duct is supposed to be the spermatozoa.
Fig.3 The 3D reconstruction of apex of flagellum (upper) and distal part of spermatheca duct (nether).

Another subject is implemented to observe the 3D structure of large hole inside the microsphere and the variety after sealing the surface hole of the microsphere using nanometer-resolution CT (cooperating with Institute of Process Engineering, CAS), see Fig.4. The result shows that the sealing process just has influence to the surface of the microsphere. The inner of the microsphere has no change and maintains multiple cavity structure. This research results will be a foundation for the future drug-embedded experiments.

Fig.4 The slice images of polylactic acid microsphere with large hole before sealing (left) and after sealing (right).

4W1B-Micro-X-ray Fluorescence Analysis Station

(1) Operation

In 2011 there are two dedicated beamtime operations. From June.8th, 2011 to July.15th, 2011, 22 user programs have been carried out in the first run with effective beamtime of 842hrs. From Nov. 1st, 2011 to Nov. 30th, 2011, 18 user programs have been carried out in the second run with effective beamtime of 653hrs. During the two operations, both μ-XRF and μ-XAS microscopic techniques are available to users. Owing to the double crystal monochromator and capillary lens, the two techniques are facilitated to switch from one to the other. It is worth mentioning that the operation in 2011 has the least problems due to beamline ever since.

Owing to the stability and reliability of the beamline, the users has achieved plenty of breakthroughs in physics, chemistry, environmental sciences, mineralogy sciences, biomedicine, materials sciences, forensic sciences, archaeology, public safety and other scientific area, etc. For instance, large scale tissues from faunas and floras are investigated either by non-destructive -compositional μ-XRF and mapping analysis, or by speciation and valence analytical μ-XAS technique. The XRF mapping method sees more novel applications in various areas including: the metal toxicity in marine organisms, inhomogeneous distribution of elements in austenite magnetic
(2) Experimental Techniques and methods development, user support

In 2011, the XRF endstation developed high pressure physics study using μ-XAS technique and acquired high quality μ-XAS spectra. This experimental method is developed under the collaboration with research scientist Wu Xiang’s group from Peking University, demonstrating stability and uniqueness of the focusing system using capillary lens. The home-made multilayer monochromator has almost being on site; in 2012, the monochromator can be tested and is expected to open to user program, conducting μ-XRF analysis with higher photon flux. For user support, the beamline staffs improve and maintain a hand by hand instruction over the sample preparation process, experiment designing, data analysis. The relevant information regarding the sample preparation and measurements has been posted on webpage to facilitate users’ experiments.

(3) Research Highlights

The users of XRF endstation keep innovative progresses; therefore, plenty of brilliant works have popped out. In the following several works are listed for instance. Dr. Qiaoguo Tan from Professor Wenxiong Wang’s group at HongKong University of Science and Technology has employed the μ-XRF mapping to study the hyperaccumulation of elements in the copper-poisoned oysters from Xiamen shore (Fig.1). Professor Zhaojun Li’s group at the Chinese Academy of agricultural sciences, has investigated the microscopic distribution of heavy metals in wheat. (Fig.2) With the help from beamline staff at XRF station, Professor Chengbao Jiang’s group at Beijing University of Aeronautics and Astronautics, has acquired microscopic elemental distribution of magnetic alloy NiMnGa.(Fig.3)

A. Hyperaccumulation of copper in oyster

Fig.1 Hyperaccumulation of elements in the copper-poisoned oysters from Xiamen shore (Professor Wenxiong
2011 Project of BSRF

Wang’s group at HongKong University of Science and Technology)

B. Microscopic distribution of heavy metals in wheat

![μ-XRF mapping of heavy metals in wheat](image)

Fig.2 μ-XRF mapping of heavy metals in wheat (Professor Zhaojun Li’s group at the Chinese Academy of agricultural sciences)

C. Microscopic elemental distribution in alloy

![Elemental distribution in austenite magnetic alloy NiMnGa](image)

Fig.3 Elemental distribution in austenite magnetic alloy NiMnGa (Professor Chengbao Jiang’s group at Beijing University of Aeronautics and Astronautics)

4W2-High Pressure Research Station

1. Operation

Totally 41 research projects and 1492.1 hours beam time were arranged, and 208 samples were tested during the two runs of dedicated synchrotron radiation mode in 2011. Most experiments used
ADXD method under room temperature, and the highest pressure achieved was 256GPa. In the high temperature ADXD experiments, 13 samples were tested and the highest pressure with high temperature using laser heating was $86GPa + 1600K$. 7 samples were tested using RXD method and the highest pressure was $125GPa$ in the $Mg_{0.75}Fe_{0.25}O$ RXD experiment.

22 research papers by users or high pressure station research group have been published or accepted using the experimental set up of HP station in 2011.

(2) Improvement of beamline and station

- **The improvement of gas loading system**

  The gas loading system has been developed successfully and opened to the users. Ne and He, etc, can be compressed into the sample hole in DAC as the pressure transmitting medium, the Ne also can be used as insulator in the laser heating experiments. In the high pressure XRD experiment of PbS with Ne as the transmission medium, according to the ruby fluorescence peak, the sample is still under a well hydrostatic pressure environment when the pressure reaches 50.4 GPa (Fig.1).

![Fig.1](image)  
**Fig.1** In the high pressure XRD experiment of PbS, the ruby fluorescence peak comparison when the pressure are 3.3GPa and 50.4GPa (Ne as the transmission medium).

- **X-ray Diffraction for Single-crystal**

  X-ray Diffraction for Single-crystal method has been established initially (Fig.2). In the Nov run of synchrotron mode, Si and LaB$_6$ single-crystal sample were tested separately without DAC. After linear velocity correcting (without absorption correcting), the intensity error of equivalent point system of LaB$_6$ was less than 30%. A Ge single-crystal sample was tested up to 11.2GPa in DAC (Fig.3).
Fig.2 Control procedure for the experiments of X-ray diffraction of single-crystal under high pressure

Fig.3 X-ray diffraction data of Ge single-crystal under high pressure

- **Change of beamline and station**

  To adjust the size of laser focus point, two convex lenses with same focus length were installed in the laser heating system.

  A new step motor was installed to upgrade the pitch angle control of the monochromator.

4B7-Mid-energy and Soft X-ray Optics Stations

(1) **The improvement and upgrade of mid-energy station**

  The experiment station of beamline 4B7A Mid-energy station was finished and tested
2011 Project of BSRF

2011 Project of BSRF successfully by experts on Nov.13, 2011. This project was checked and accepted on Dec.30, 2011. This new station (shown in Fig) constructed for X-ray absorption spectroscopy measurement mainly include a UHV chamber, load lock chamber, a multi-exit specimen distribution chamber, sample anneal equipment, MBE equipment and a He-filled chamber. The UHV chamber is equipped with a 13-element Si (Li) array detector system and the He-filled chamber is equipped with a single-element SDD detector system for XAFS measurement using PFY (partial fluorescence yield) mode respectively. The sample of solid, wet and liquid is able to be measured in this station, at detection levels down to 200ppm for element S. The energy range of emitted X-ray from beamline 4B7A is from 1750eV to 6000eV, so the XANES and EXAFS of element Si, P, S, Cl, K, Ca, Sc, Ti, V and so on can be obtained.

Fig.1 The new experiment station of beamline 4B7A. 1: UHV chamber; 2: multi-exit specimen distribution chamber; 3: MBE equipment; 4: load lock chamber; 5: anneal equipment; 6: The He-filled chamber.

Fig.1 The XANES of Silicon. The red arrow shows the characteristic peak due to SiO$_2$. 

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Fig.3 The XANES of Silicon. Before measurement, the silicon is dipped in hydrofluoric acid aqueous solution with concentration of 5% about 10 minutes for getting rid of oxidized layer on surface.

There are few reports and articles about the measurement and research of XANES of silicon in specimen not only in foreign but also in domestic. In order to satisfy the user’s requirement for obtaining XANES of element silicon, our team changed the Si(111) crystals of monochromator to InSb(111) crystals on Nov. 4 until Nov.10 2011, when the energy range of emitted X-ray from beamline 4B7A is from 1750eV to 3700eV, which covers the K absorption edge of element Si, P, S, Cl. Fig.2 shows the XANES spectrum of silicon, and the characteristic peak (at 1848.2eV) of SiO₂ pointed by red arrow indicates the surface of silicon is partially oxidized. In order to eliminate the effect of SO₂ on surface, the silicon is dipped in hydrofluoric acid aqueous solution with concentration of 5% about 10 minutes before measurement. The XANES spectrum of silicon without oxidization is shown in Fig.3 where the peak at 1848.2keV is disappearing. In addition, the XANES spectrums of standard specimens such as silicon dioxide and sodium silicate were also obtained in that time.
Fig.4 Sample holder for solution.

At present the He-filled chamber is equipped with simple sample holder (shown in Fig) for solution. The solution under test is enveloped in the hole of the sample holder by special tape suitable to XRF. The frame in the chamber is able to mount three sample holders. The PFY mode is adopted for data acquirement. Fig. shows the XANES spectrum of element K. The black solid line denotes the results of KCl aqueous solution at the upper part of the figure, and the red one denotes the results of KCl powder at the lower part of the figure. In addition, some users used thin ziplock bag loading solution for XANE measurement successfully. If the transmission mode is needed for measurement, user should make special sample holder which can control the thickness of the solution is within 100 microns, according to the transmission of water in this energy region.

Fig.5 the XANES spectrum of element K. the black spectrum denotes the results of KCl aqueous solution (5% wt. for K) and the red one denotes the KCl solid (5% wt. for K diluted by graphite powder).

The MBE equipment connected to the multi-exit specimen distribution chamber is used to grow
film on kinds of crystal substrate such as Si (111). The thickness of the growing film is monitored Real-time by the thickness monitor (SQM-160). After growing, the film can be transferred to the UHV chamber for X-ray absorption spectrum measurement via multi-exit specimen distribution vessel. For verifying the MBE equipment, we grow Ti film with 20 angstrom thickness on Si (111) substrate, then the XANES spectrum of the film is measured quasi-situ with TEY mode (or PFY mode). The result is shown in Fig.6.

![Fig.6 XANES spectrum of Ti film on Si(111) substrate](image)

**4B8-VUV Station**

4B8 beamline is optimized for VUV spectroscopy measurement, especially for steady-state and dynamic circular dichroism (CD) and fluorescence detections. It is operational under both the dedicated SR mode and the coupling mode. Remote access is available for the fluorescence measurement.

(1) **Beamline and Running**

Beamline parameters:

- Wavelength range: 125-360 nm
- Bandwidth: 0.8 nm
- Intensity: $10^{10}$-$10^{11}$ photons/s/

In 2011, besides the dedicated operations in summer and autumn, 4B8 beamline provided 1260 hour beamtime in the coupling mode. 53 users come from biological and materials field.

(2) **Fluorescence spectroscopy**

Fluorescence lifetime detection is essential to fluorescence study. Synchrotron radiation has
been the favorable excitation source for fluorescence lifetime measurement owing to its merits of short pulse, high repetition frequency and wide tunable wavelength range. We have developed the fluorescence lifetime detection based on the excitation of the light pulse from a designated single-bunch in 2010. It has been utilized for characterization of Ag nanoparticle inserted n-ZnO/AlN/p-GaN LED (Fig.2).

Remote access has been available to users for VUV excited fluorescence spectroscopy measurement at 4B8 since 2009. It has brought a tremendous improvement in experimental efficiency for VUV fluorescence users, most of them geographically dispersed around China. The remote system was previously based on commercial remote desktop software. However, the desktop access is very limited by connection bandwidth and sometimes rejected by user network gateway. Also it causes the concerns in internet safety, as the station computer is not under intranet control in remote desktop. To address these problems, we develop a Client/Server remote access based on TCP/IP communication application in Labview. Users, as a client end, now only control the fluorescence acquisition software instead of the station computer before, so the cyber safety is improved significantly. It only needs < 1K bandwidth in data collection, as only the command and data, instead of the desktop previously, are transmitted. Data can be now stored in client local position. The new software can detect the network disconnection and rebuild communication automatically as soon as the network connection is restored. This new access mode was firstly applied in this autumn operation for a user in Yunan province.

To meet the requirement for transmission measurement, we developed a multiple sample holder installed in fluorescence vacuum sample chamber. It is open to users in this autumn operation (Fig.3).
CD is a powerful tool for protein folding research. Besides the steady-state CD application (Fig.4), we emphasized on the dynamic CD measurement development.

We develop a rapid probe for protein solution reaction study using continuous flow (CF) method. This CF method combines synchrotron radiation circular dichroism (SRCD) with microfluidic mixing chip. Time-resolved studies by SRCD is a under-exploited area, as they have great potential for elucidation of protein folding/unfolding, the kinetics and mechanisms of enzyme activity, the binding and insertion of proteins into membranes. We set up instrumentation (Fig.5), including beam focusing, beam and chip alignment, CD calibration (Fig.6). A preliminary result was obtained on Cytochrome c folding (Fig.6).
Fig. 5  Left, microfluidic mixing chip; Right, dynamic SRCD instrumentation

Fig. 6 Left, CD calibration results using standard CSA at different position of observational channel; Right, Preliminary data of Cytochrome C folding measurement in GdmCl solution (red, unfolding state; green, folding state; black, folding intermediate)

(3) Femtosecond XRD development

Fig. 7 Schematic of laser-driven plasma fs X-ray source and pump-probe XRD detection

We initiated the development of femtosecond XRD instrumentation in 2011. Based on laser-driven plasma X-ray source, the fs X-ray pulse is generated as a probe for ultrafast XRD detection. Part of the laser will be used for sample excitation (Fig. 7). The X-ray energy is 8Kev, the Kα line of copper. It is expected that this new method will be available to users in 2012.
4B9A -XRD station

In 2011, XRD experimental station was opened to users for two opening periods in dedicated-mode. In the first opening period (from June 8th to July 15th), XRD station provided users with 674h of beam time to 19 research projects. In the second opening period (from Nov. 1st to 30st), total 537h of beam time were provided to 16 research projects. The experimental modes included XRD/SAXS/XAFS and so on.

In March 2011, new supporting platforms for XRD station have been equipped. This set of supporting system includes a 4-freedom platform for SAXS camera, a 2-freedom platform for image plate, a 3-freedom platform for CCD detector, and 1-freedom platform for holding samples. All motions can be driven by stepping motors or manually, providing an independent control or adjustment, respectively, for samples, SAXS camera and detectors.

In 2011, the equipment improvement was also included: A small CCD was used to monitor the beam spot during beamline adjustment. A multipath switch power-supply was developed. An overage photon shutter was renewed. A 1D detector (MYTHEN 24K) for XRD covering 120° was being built and will be equipped in 2012.

Fig.1 A 4-freedom platform for supporting the SAXS camera, providing the adjustment for the attitude (elevation, translation, tilt, and swing) of SAXS camera.

4B9B-Photoemission Spectroscopy Station

1) Progresses in the comprehensive PES endstation upgrading

Since the Jan. 2011 through early May 2011, main chambers and most components contracted with different supplier during the 2010 have been shipped to the lab. Detaching of the old system and installing the new sets have begun after have been delivering the June 8th to July 15th round of dedicated beamtime to users. Main vacuum chambers and core components
Fig.1 (upper) left is analysis chamber, right is radial sample distribution chamber sample storage chamber plus sample fast entrance chamber attached on it; (lower) left is sample preparation chamber, right is laser MBE chamber and STM chamber.

have been set up before the end of Oct. 2011 and their vacuum condition preliminarily reached at close indexes of design. The pictures above shown in the upper left to right are analysis chamber, radial sample distribution chamber sample storage chamber plus sample fast entrance chamber attached on it, correspondingly. The pictures at lower left to right are sample preparation chamber, laser MBE chamber and STM chamber, respectively. Acceptance tests have been performed for the analyzer on ground and after attached to the analysis chamber, the result of angle resolution ability measurement is given in the below pictures’ upper left panel; the low temperature measurement on the five dimensional manipulator sample holder is shown in the upper right penal, where 4.36K is at the cooling head and the 14.93K is at the sample position. The acceptance test results carried out on the STM are shown below. The left picture shows atomic surface pattern of Si (111)-7×7 in 15nm×15nm area with positive bias 0.9V, the right side picture with negative bias -0.9V, both measurement with a resolution of ~0.09nm.
low temperature measurement on the five dimensional manipulator sample holder; (lower) the left side picture is atomic surface pattern of Si (111)-7×7 in 15nm×15nm area with positive bias 0.9V, the right side picture with negative bias -0.9V, both measurement with a resolution of ~0.09nm.

(2) Operation

Photoemission station opened to users in the coupling mode from the beginning of 2011 to May, 2011, and also supplied beamtime to users in the first round of dedicated SR running in 2011 (8th, June to 15th, July). And then this station started to upgrade and stopped open to users.
# 2011 Publications

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<th>No.</th>
<th>Title</th>
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<td>12.</td>
<td>Interface engineering of high-Mg-content MgZnO/BeO/Si for</td>
<td>APPL. PHYS. LETT., 98, 471-474, 2011.</td>
<td>H. L., Liang</td>
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<td>Local structure of Se nanotube investigated by X-ray absorption fine structure spectroscopy</td>
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<td>55.</td>
<td>聚乙稀醇修饰Fe3O4纳米颗粒的制备表征及同步辐射X射线光电子能谱研究</td>
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<td>66</td>
<td>Bright green-emitting, energy transfer and quantum cutting of Ba$_3$Ln(PO$_4$)$_3$: Tb$_3$ (Ln = La, Gd) under VUV-UV excitation</td>
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<td>Luminescence and microstructures of Eu$^{3+}$-doped Ca$<em>9$LiGd$</em>{3/3}$(PO$_4$)$_7$</td>
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<td>Photoluminescence of Tb$^{3+}$ and Mn$^{2+}$ activated Ca$_9$MgGd(PO$_4$)$_7$ under vacuum ultraviolet excitation</td>
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<td>Single-Phase White-Emitting Ca$_9$MgGd(PO$_4$)$_7$:Ln$^{3+}$, Mn$^{2+}$ (Ln$^{3+}$=Ce$^{3+}$, Tb$^{3+}$, and Dy$^{3+}$) for Mercury-Free Lamps</td>
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<td>Vacuum ultraviolet and near-infrared excited luminescence properties of Ca$_9$(PO$_4$)$_2$:RE$^{3+}$, Na$^+$(RE Tb, Yb, Er, Tm, and Ho)</td>
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<td>Photoluminescence properties of RE$^{3+}$-activated Na$_5$GdP$_2$O$_8$ (RE$^{3+}$= Tb$^{3+}$, Dy$^{3+}$,Eu$^{3+}$, Sm$^{3+}$) under VUV excitation</td>
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<td>Photoluminescence Characteristics of Ca$_9$Ln (PO$_4$)$_7$:Tb$^{3+}$ (Ln$^{3+}$= Y$^{3+}$,La$^{3+}$,Gd$^{3+}$) under VUV Excitation</td>
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<td>Energy transfer processes in Ce$^{3+}$ and Tb$^{3+}$ co-doped Ln$_2$Si$_2$O$_7$ (Ln = Y, Gd)</td>
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<td>159</td>
<td>硼掺杂中孔炭的制备及其电化学性能</td>
<td>New Carbon Mater, 26</td>
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<td>Phys Chem Miner., 38, 639–646, 2011.</td>
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2011 Major events

Structural and Biophysical Methods for Biological Macromolecules in Solution

EMBO Lecture Course was held in IHEP in 2011

![EMBO Lecture Course](Image1)

Beijing China, 28 April-5 May, 2011

Workshop of EXAFS analysis was held by BSRF in 2011

![Workshop of EXAFS analysis](Image2)
## 2011 Seminar

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<td>THE ESRF UPGRADE PROGRAMME, Some Technical CHALLENGES</td>
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<td>Jiyong Zhao</td>
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<td>The University of Texas</td>
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<td>ANL</td>
<td>(1) Nuclear resonant x-ray scattering; (2) Inelastic x-ray scattering</td>
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Beamline Specs

4B9B- Photoemission Spectroscopy

【Beamline Specs】
Energy Range: 15 - 1000 eV
Resolution (ΔE/E): ~1500
Flux (photons/s): > 1×10^{10}
Beam Size (H×V): < 2×0.8 mm²

4B9A-XRD

【Beamline Specs】
Energy Range: 4 - 15 keV
Resolution (ΔE/E): 3×10^{-4} @ 9 keV
Flux (photons/s): 1×10^{10} @ 8 keV
Beam Size (H×V): 2×1 mm²
Angular resolution: 0.9 arc-second

4B8- Vacuum Ultraviolet

【Beamline Specs】
Energy Range: 125-360 nm
Band width: 0.8 nm
Flux (photons/s): 2.0×10^{10} @ 180 nm
Beam Size (H×V): 2×1 mm²
**4B7B- Soft X-ray Optics**

**【Beamline Specs】**

Energy Range: 50eV-1700 eV
Resolution (E/\(\Delta E\)): \(~1000\)
Flux (photons/s): \(~1\times10^{12}\) @ Fe L edge
Beam Size (H×V): conducting sample: 1×0.1mm\(^2\)
nonconducting sample: 4×2 mm\(^2\)

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**4B7A- Mid-energy Spectroscopy**

**【Beamline Specs】**

Energy Range: Si (111): 2050 eV-5700 eV
InSb (111): 1750 eV-3400 eV
Flux (photons/s): \(~10^{10}\) @ S K edge
Resolution (E/\(\Delta E\)): \(~7000\) @ S K edge
Beam Size (H×V): 3×1mm\(^2\)

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**4W2- High Pressure Structure**

**【Beamline Specs】**

Energy Range: 10-25 keV (Monochromatic light)
5-35 keV (White light)
Resolution (\(\Delta E/E\)): \(7\times10^{-4}\) @20 keV
Flux (photons/s): \(~1.2\times10^{8}\)@20 keV
Beam Size (H×V): 26×8 \(\mu m^2\)
**4W1B- X-ray Fluorescence Microanalysis**

**[Beamline Specs]**

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<td>Energy Range</td>
<td>8 - 15 keV</td>
<td>5 - 18.5 keV</td>
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<tr>
<td>Resolution ($\Delta E/E$)</td>
<td>$&lt; 7 \times 10^{-2}$</td>
<td>$&lt; 5.5 \times 10^{-4}$</td>
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<td>Flux (photons/s)</td>
<td>$&gt; 1 \times 10^8$ @ 15 keV</td>
<td>$&gt; 1 \times 10^{10}$ @ 15 keV</td>
</tr>
<tr>
<td>Beam Size (H×V)</td>
<td>10 µm</td>
<td>30, 50, 100 µm</td>
</tr>
<tr>
<td>XRF Detectability</td>
<td>Dozens of ppm</td>
<td>1 ppm</td>
</tr>
</tbody>
</table>

**4W1A- X-ray Imaging**

**[Beamline Specs]**

<table>
<thead>
<tr>
<th>Imaging Mode</th>
<th>Energy Range</th>
<th>Flux (photons/s)</th>
<th>Spatial Resolution</th>
<th>Beam Size (H×V)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Phase contrast imaging</td>
<td>6~22 keV</td>
<td>$\sim 10^{10}$ @ 8 keV</td>
<td>$\sim 10$ µm</td>
<td>20×10 mm²</td>
</tr>
<tr>
<td>nano-resolution Imaging</td>
<td>5~12 keV</td>
<td>$\sim 10^8$ @ 8 keV</td>
<td>30 nm, 50 nm, 100 nm</td>
<td>10×10 µm², 15×15 µm², 60×60 µm²</td>
</tr>
</tbody>
</table>
3B1A, 3B1B- LIGA and Lithography

【Beamline Specs】

3B1A-LIGA: White light
3B1B-Lithography: 0.5-2 nm

3W1A-Macromolecular crystallography

【Beamline Specs】

Energy Range: 6 - 16 keV
Resolution (ΔE/E): $4 \times 10^{-4}$
Flux (photons/sec): $10^{11}$
Beam Size (HxV): 0.8× 0.6 mm$^2$

1W2B-Macromolecular crystallography

【Beamline Specs】

Energy Range: 5 - 18 keV
Resolution (ΔE/E): Better than $4 \times 10^{-4}$
Flux (photons/sec): $10^{12}$
Beam Size (HxV): 1× 0.6 mm$^2$
1W2A-SAXS

【Beamline Specs】
Angular resolution: 0.5 mrad  
Energy Range: 0.154 nm  
Resolution ($\Delta E/E$): $\sim 10^{-3}$  
Flux (photons/sec): $\geq 1 \times 10^{11}$  
Beam Size (HxV): 1.2 × 0.3 mm$^2$

1W1B-XAFS

【Beamline Specs】
Energy Range: 4 - 25 keV  
Resolution ($\Delta E/E$): $< 3 \times 10^{-4}$ @ 9 keV  
Flux (photons/sec): $> 3 \times 10^{11}$ @ 10 keV  
Beam Size (HxV): 0.9 × 0.3 mm$^2$

1W1A- Diffuse X-ray Scattering

【Beamline Specs】
Energy Range: 8.05 keV, 13.9 keV  
Resolution ($\Delta E/E$): $4.4 \times 10^{-4}$ @ 8.05 keV  
Flux (photons/sec): $> 1 \times 10^{11}$ @ 8.05 keV  
Beam Size (HxV): 0.7 × 0.4 mm$^2$