Oral Session

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From HiSOR to HiSOR-2

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Keywords: Synchrotron light source, Electron storage ring.

The HiSOR has been operational since 1996 [1]. It is a compact racetrack-type storage ring having 22 m circumference and 700 MeV electron energy. It has two 180-degree normal-conducting bending magnets which generate a strong magnetic field of 2.7 T. Due to this compact configuration, the natural emittance of the electron beam is 400 nm-rad, which is much larger than most of other operational synchrotron light sources. It has two straight sections, where two insertion devices, a planar undulator and an APPLE-II undulator, are operational, which cover the VUV spectral range. The high field bending magnets produce synchrotron radiation in a wide spectral range including tender X-rays. The injector of HiSOR is a microtron which provides 150 MeV electron beam. After accumulating about 300 mA beam, the beam energy is ramped up to 700 MeV. Beam injection is made twice a day, at 9:00 and 14:30.

For the future plan of HiSOR, we have been designing a compact storage ring which would achieve higher brightness, more undulators and more stable operation with top-up injection. Various lattice designs have been considered [2]. The target parameters are as follows; the beam energy around 600 MeV or less, the circumference smaller than 50 m, the numbers of insertion devices larger than 4. The latest version is based on a compact double-bend achromat cells with six straight sections. The beam energy would be 600 MeV and the circumference would be about 44 m. The ring would be equipped with a full energy injector to enable the top-up injection. The present injector, the microtron, would be used for a pre-injector. All the accelerator components would be constructed in the present building. The emittance of the new ring would be smaller than the present HiSOR by a factor of about 20, consequently, the brightness of the undulator radiation would be increased by two orders of magnitude. The top-up operation would enable stable and continuous experiments with a constant beam current.

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Introduction of Light Source Development in China

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Currently, there are three synchrotron radiation facilities in operation in China, Beijing Synchrotron Radiation Facility (BSRF: Energy 2.2GeV, circumference 200m), Hefei Light Source (HLS: 0.8GeV, 66m), and Shanghai Synchrotron Radiation Light Source (SSRF: 3.5GeV, 432m). There are also four free electron laser facilities (Shanghai, Hefei, Chengdu and Dalian) in operation in China.

FIGURE 1. Hefei Advanced Light Facility (HALF) under construction, in Hefei, Anhui.

In recent years, construction of fourth-generation light sources has been progressing, with the High Energy Synchrotron Radiation Light Source (HEPS, 6GeV, 1360m, Beijing) and Hefei Advanced Light Source (HALF: 2.2GeV, 480m, Fig. 1) being constructed. Test use has already been carried out at HEPS. In addition, plans for synchrotron radiation sources are underway in Wuhan, Jinhua, and Guangdong Province. In this presentation, I would like to give the latest information on the development of synchrotron radiation sources and free electron lasers in China, as far as I know, focusing on the HALF and Jinhua, in which I am currently involved.

O03

Development of Ultrafast Time-resolved Electron Diffraction Setups and Their Applications

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Methods have been developed to observe the light-driven atomic motions of molecules and materials on the ultrafast timescale of 10^{-14} to 10^{-12} (femto-to-picoseconds). This progress reveals the mechanisms of photoreactions and photoinduced phase transition phenomena in molecules and materials. [1,2]. Ultrafast time-resolved electron diffraction employs diffraction techniques to directly measure the photoinduced changes of atomic or molecular coordinates. In this presentation, I will discuss the progress of the developments of ultrafast time-resolved electron diffraction setups, *i.e.*, the conventional picosecond time-resolved electron diffraction setup, picosecond time-resolved electron diffraction setup with a high coherence electron probe, and femtosecond time-resolved electron diffraction setup with a synchronized radio frequency (RF) cavity [3]. **FIGURE 1** shows the photographs of the setups. The schematic illustration of the setup with an RF cavity is shown in **FIGURE 2**.

The presentation will also show the measurements of ultrafast structural dynamics of molecules and materials using ultrafast time-resolved electron diffraction setups. These measurements are combined investigation of ultrafast time-resolved electron diffraction measurements, ultrafast transient absorption measurements, and first-principles calculations. One of the topics is a recently published study about a one-dimensional van der Waals heterostructure [4]. The heterostructure contains carbon nanotubes (CNTs) as an inner core and boron nitride nanotubes (BNNTs) as an outer core. We found peculiar charge transfer channels between CNTs and BNNTs through the heterostructures. At the same time, I would like to introduce the photoinduced structural dynamics in a semiconducting solar cell material [5] and photo-responsive organic molecules [6].

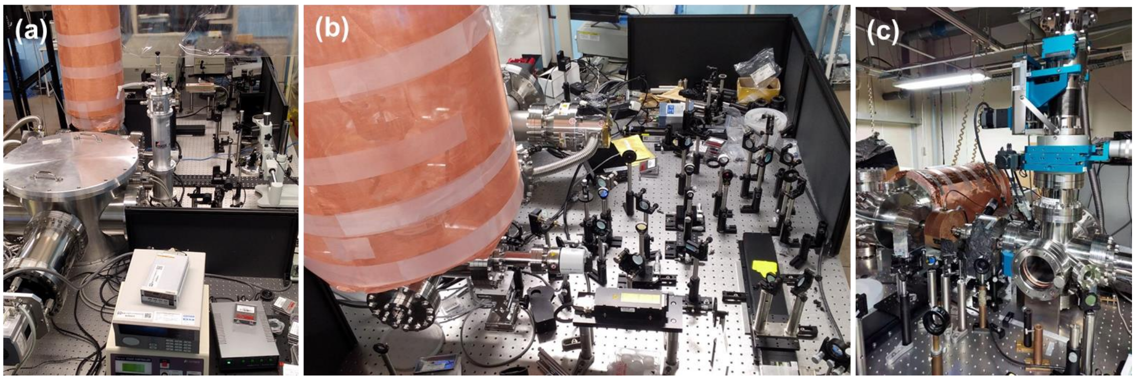

FIGURE 1. Photographs of the developed time-resolved electron diffraction setups. The conventional picosecond time-resolved electron diffraction setup (a), picosecond time-resolved electron diffraction setup with a high coherence electron probe (b), and femtosecond time-resolved electron diffraction setup with a synchronized radio frequency (RF) cavity (c).

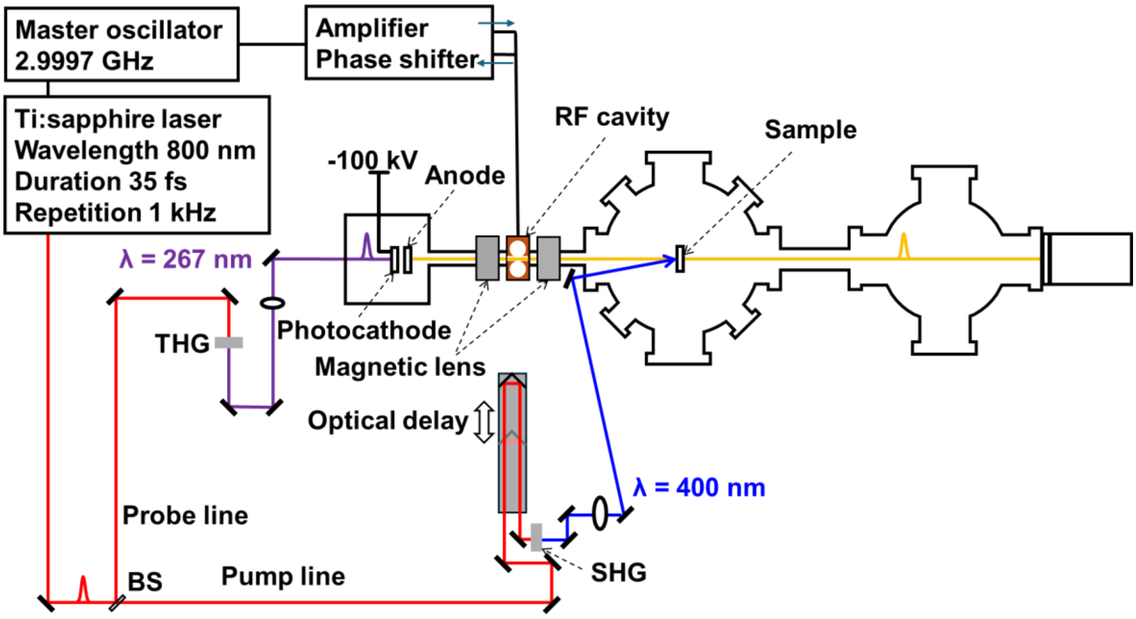

FIGURE 2. The schematics of the setup with an RF cavity

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Unraveling the Valley Depolarization dynamics in WS_2 with TR-ARPES

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In two-dimensional (2D) transition metal dichalcogenides (TMDCs), strong Coulomb interactions and their lack of inversion symmetry making them has led to tightly bound excitons which are ideal for valleytronics applications. However, the valley information encoded in bright excitons is rapidly lost due to the presence of many scattering channels such as intervalley exchange interactions as well as phonon-induced scattering. Additionally, the complexity of the exciton landscape, which hosts a variety of bright and dark excitons species, has further hindered any comprehensive understanding of valley depolarization dynamics.

Time- and angle-resolved photoemission spectroscopy (TR-ARPES) has emerged as a powerful tool for studying excitons in 2D semiconductors. By directly imaging excitons in energy and momentum space while simultaneously resolving their constituent electrons and holes, we could study different excitonic species within the material [1–4]. Here in this presentation, we will demonstrate how we can employ TR-ARPES to track the evolution of valley-polarized excitons in monolayer WS_2 across the entire Brillouin zone. By extracting exciton populations and key scattering timescales, we identify excitation conditions under which intervalley exchange scattering is suppressed. This suppression leads to the formation of a momentum-dark exciton that retains its valley selectivity for more than two orders of magnitude longer than its bright exciton counterpart. These findings offer new insights into controlling valley polarization, paving the way for future valleytronic applications.

(1)

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Unraveling the Strongly Entangled Spin-Dipole-Lattice Behavior: Phenomena Driven by Helical Magnetic Order

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The growing demand for advanced spintronic devices has created a strong impetus for research into multifunctional materials capable of responding dynamically to a variety of external stimuli. These innovative materials are distinguished by the intricate coupling of microscopic order parameters, including spin, orbital, lattice, dipole, and phonon, which result in a diverse array of interesting properties. Researchers have focused on the discovery and development of new multiferroic and magnetodielectric materials that have the potential for numerous real-world applications across technology sectors. However, these materials are relatively scarce; their scarcity can be attributed to the antagonistic nature of their magnetic and electric properties, which are often limited by low critical temperatures, typically below 40 K. The challenge of engineering materials to achieve higher critical temperatures remains a significant obstacle, with only a handful of compounds, such as CuO (T_N ~ 230 K) and certain hexaferrites, demonstrating coupled properties at significantly elevated temperatures.

An especially fascinating phenomenon within this context is Spin-Phonon Coupling (SPC), which occurs in strongly correlated systems. SPC is characterized by magnetic and structural phase transformations that are reflected in the phonon spectra of these materials. This coupling serves as a valuable gauge for monitoring a variety of exotic properties, which include magnetoelectric coupling, the spin Seebeck effect, magnetostriction, the phonon Hall effect, the spin-Peierls transition, and the thermal Hall effect, all of which are pivotal in the study of multiferroics.

In this report, we demonstrate a spectrum of simultaneously occurring and highly entangled phenomena induced by helical spin ordering within the polar and spin-frustrated magnetic system $Fe_3(PO_4)O_3$. Key phenomena observed in this unique system include magnetodielectric coupling in conjunction with weak ferroelectric ordering. Additionally, we note a distinct magnetostriction effect, which is evidenced by a dramatic reduction in the thermal variation of the lattice parameters. The system also exhibits pronounced spin-phonon coupling, characterized by unique and anomalous hardening and softening of various phonon modes at temperatures reaching $T_N = 163$ K.

To investigate these effects, we utilized high-resolution synchrotron X-ray diffraction (SXRD) to probe the structural changes that occur across the magnetic transition temperature. If the spontaneous lattice distortion resulting from magnetic ordering is sufficiently pronounced, the resultant magnetostriction effect can be quantitatively assessed using SXRD data. This approach offers notable advantages over more conventional techniques such as capacitive and strain-gauge measurements. Our findings revealed a clear downturn in the lattice parameters, including the unit-cell volume, indicating a significant volume magnetostriction effect. This effect plays a crucial role in contributing to the various phenomena we observed, including the magnetodielectric, multiferroic, and SPC properties.

Moreover, the dielectric peak we observed appears to be closely associated with the structural distortions driven by the strong magnetostriction effect. It is particularly noteworthy that the magnetostriction effect, which is often regarded as negligible in other SPC systems, plays a vital role in modulating phonons in this specific system, leading to an indirect form of spin-phonon coupling. Nevertheless, this system exemplifies a highly entangled interaction among spin, lattice phonons, and dipoles, which activates a diverse range of intriguing phenomena. As a result, this places it among the rare and exceptional materials in the field.

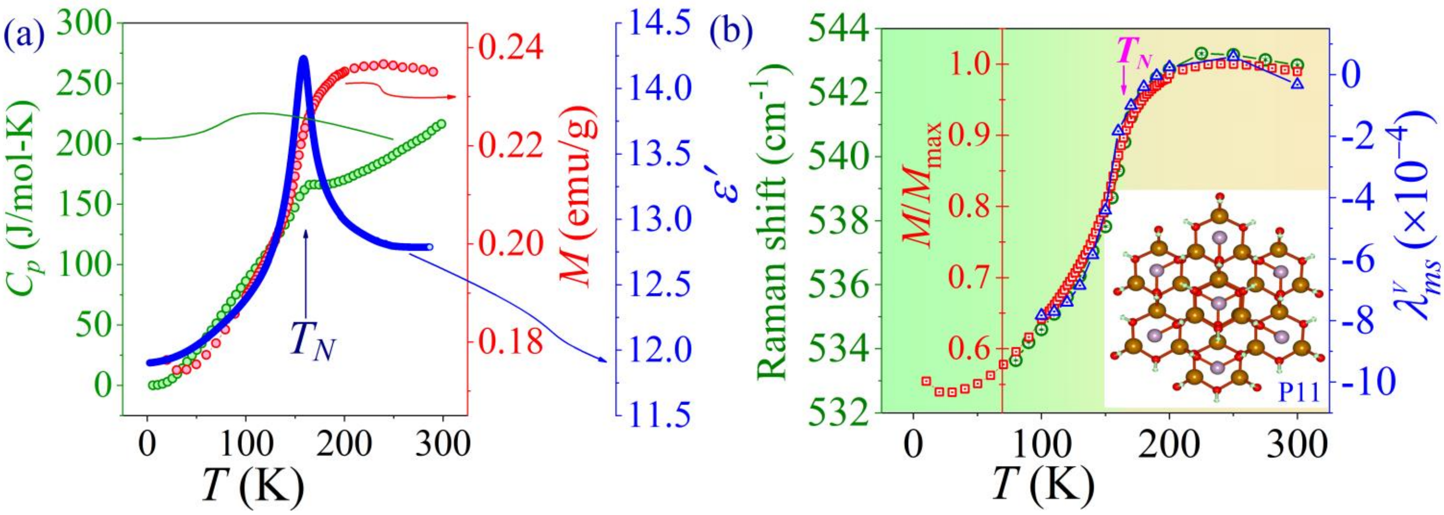

FIGURE 1. : (a): Specific heat (C_p), Magnetization (M), and Dielectric constant ($\mathcal{E}'$), variations as a function of temperature. (b): Raman shift, normalized magnetization, and volume magnetostriction coefficient variations as a function of temperature. All these curves unambiguously suggest the highly entangled behavior of spin, lattice, phonon, and dipolar degrees of freedom in this system.

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O06

Bayesian Hierarchical Analysis for Multi-dimensional Spectra

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In recent years, data-driven science has been attracting remarkable attention. The data-driven techniques such as Bayesian inference enable us to advance the synchrotron radiation X-ray data analysis. To develop innovative analysis methods and incorporate them into beamlines at SPring-8, Synchrotron Radiation Data-driven-science Group was established in January 2023. Our mission is to assist SPring-8 users in maximizing their experimental outcomes. Then, we developed Bayesian analysis methods for synchrotron radiation X-ray measurements, e.g., X-ray photoemission spectroscopy, X-ray absorption spectroscopy, X-ray diffraction, Compton scattering, Mössbauer spectroscopy, small-angle scattering, and so on. Currently, the developments have been completed for 14 beamlines, the majority of the 26 public beamlines at SPring-8.

In this talk, we introduce Bayesian hierarchical analysis for multi-dimensional spectra such as time-series and/or temperature-series spectra. Conventional least-squares fitting has to be the step-by-step analysis as shown in Fig.1. In this analysis, the information available at each step is very limited. The least-squares fitting has initial value dependence and the results are sometimes trapped by local minima. In addition, the least-squares fitting is a point estimation, which means that it is difficult to evaluate the estimation accuracy. Moreover, we have to determine the models such as fitting functions prior to the analysis by human judgement, leading to a human dependent analysis. However, Bayesian hierarchical analysis provides seamless analysis from multi-dimensional spectra as shown in Fig.2, enabling more precise estimation by using posterior probability distributions and quantitative model selection without human judgement. To discuss the effectiveness of Bayesian hierarchical analysis, we present two applications, e.g., the adsorption process of gas molecules on a metal-organic framework observed via time-resolved X-ray diffraction (shown in Fig.3) [1] and the reduction process of a catalyst for automobile exhaust gas observed via temperature-dependent hard X-ray photoemission spectroscopy [2].

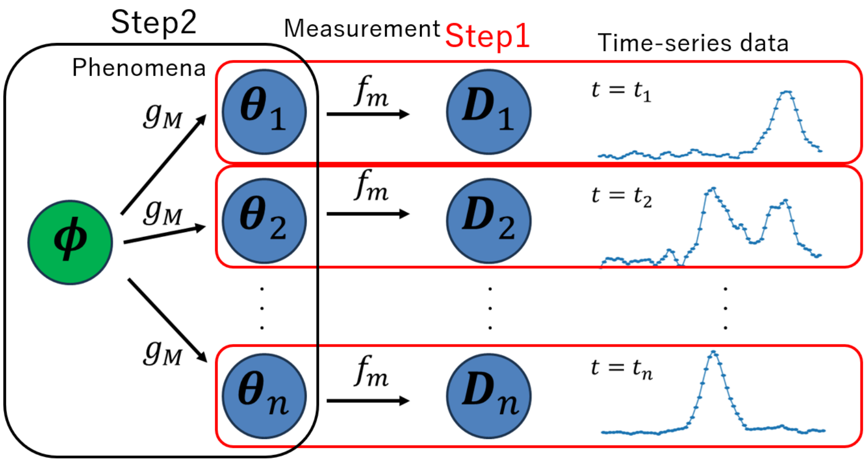

FIGURE 1. Conventional analysis framework for multi-dimensional spectra.

O06

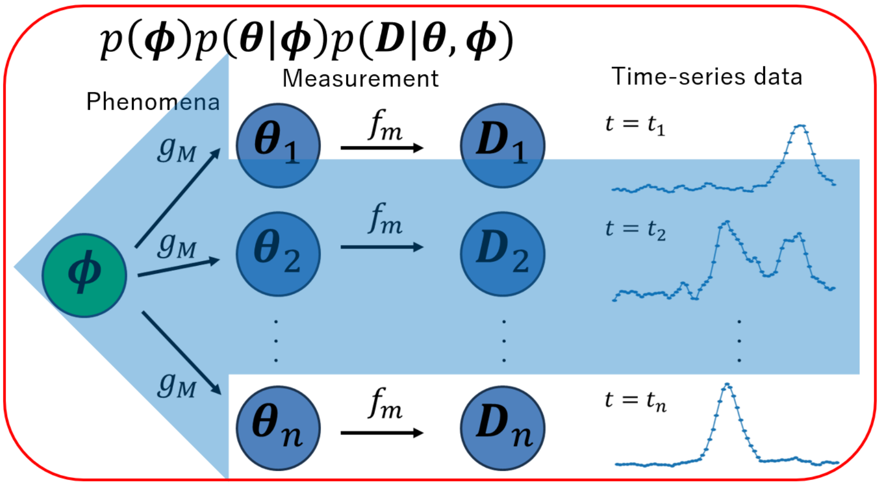

FIGURE 2. Bayesian hierarchical analysis framework for multi-dimensional spectra.

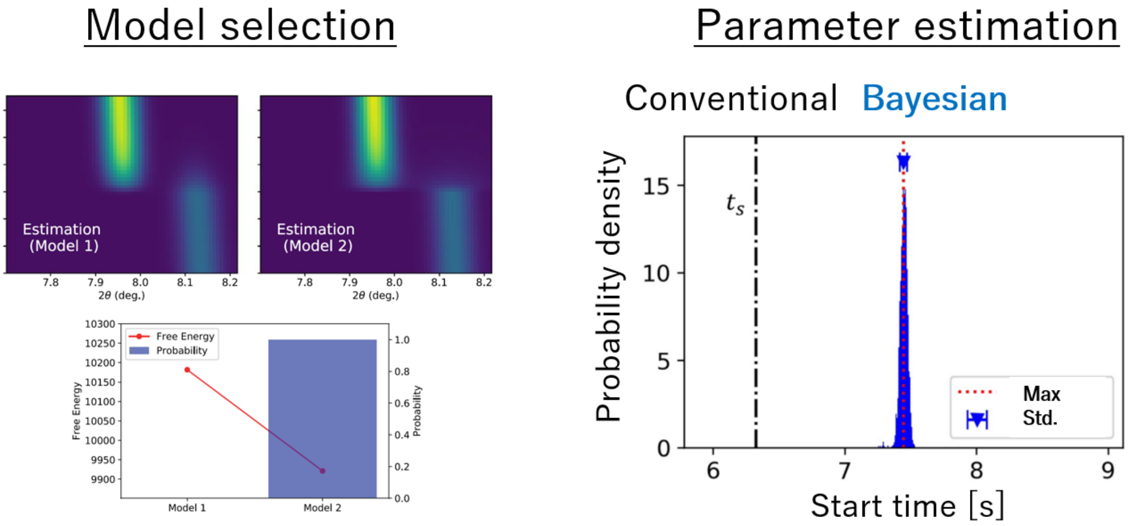

FIGURE 3. Bayesian model selection and parameter estimation based on posterior probability distribution.

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Potential in Vitro Anti-Tumor Effects of Novel Indole Derivatives

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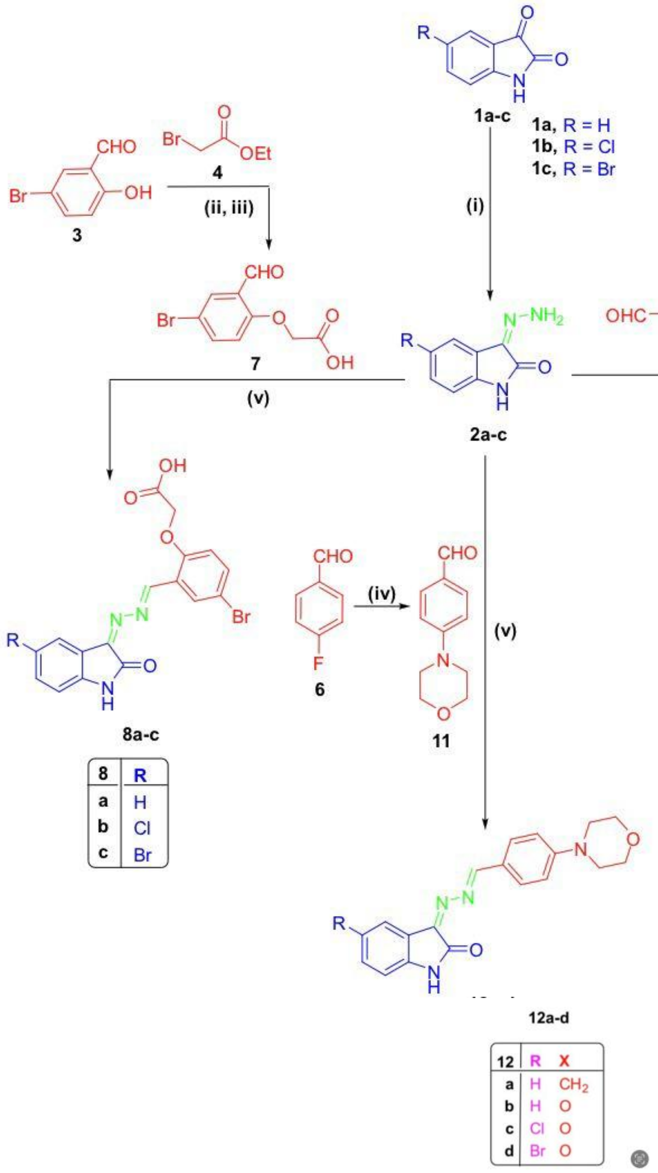
Indole alkaloids, such as isatin, are one of the most abundant and complex alkaloids, which ubiquitously exists in natural products. Isatin compound is derived from indole with formula $C_8H_5NO_2$. Isatin is a well-known natural product that can be found in plants of the genus Isatis in *Couroupita guianensis* and in humans, as a metabolic derivative of adrenaline. Isatin is widely recognized for its antibacterial, antiviral, anticonvulsant, anti-inflammatory, as and anti-cancer properties [1]. The current study continues searching for new biological activities for the active novels of isatin derivatives, highlighting its importance as potential anti-cancer compounds

In scheme 1, the key starting compound was 2a-c (hydrazones) prepared by the reaction of isatin 1a-c with hydrazine hydrate [2]. 4-Morpholinobenzaldehyde (11) was prepared by the reaction of 4-fluorobenzaldehyde (6) with the morpholine [3]. Hydrazones 2a-c reacted with the aldehydes 11 in ethanol, in the presence of acetic acid under reflux to afford the corresponding hydrazones 12a-d, respectively. The structures of the compounds were confirmed through their IR, ^{1}HNMR, ^{13}CNMR and CHN thermal analyses. The structure of the latter newly synthesized hydrazones was confirmed through their IR, ^{1}HNMR, ^{13}CNMR and CHN thermal analyses [4].

Out of 12 indole compounds synthesized, we studied, in this phase, the effect of 4 novel compounds on normal (Wi38, fibroblast cell line) and cancer cell lines (A549 lung cancer cell line) after 48 h as compared to no treatment and cells and after treatment with doxorubicin (DOX) as an anti-cancer reference drug. We tested four compounds, including compound 12a: 5-Chloro-3((4-morpholinobenzylidene)hydrazineylidene) indolin-2-one, compound 12b: 5-Bromo-3-((4-morpholinobenzylidene)hydrazineylidene) indolin-2-one, 12c: 5-Chloro-3-((4-morpholinobenzylidene)hydrazineylidene)indolin-2-one, and 12d: 5-Bromo-3-((4-morpholinobenzylidene)hydrazineylidene)indolin-2-one.

The IC_{50} measured after 24 h of treatment of Wi38 was 0.047 mM for DOX, 4.97 mM for compound 12a, 5.6 mM for compound 12b, 1.192 mM for compound 12c, and 0.019 mM for compound 12d. The IC_{50} after 24 h of treatment of A549 lung cancer cell line was 0.07 mM for DOX, 3.8 mM for compound 12a, 3.44 mM for compound 12b, 3.79 mM for compound 12c, and 9.218 mM for compound 12d.

By analyzing cell apoptosis (programed cell death) and cell cycle by flow cytometry, we found that the four-compound increased apoptosis and arrested the cel cycle of the tumor cells. Altogether, these data indicate that isatin compounds derivatives from indole have potential anti-tumor effects by increasing cell death and arresting cell division.



8	R
a	H
b	Cl
c	Br

10	R	R₁
a	H	H
b	H	OMe
c	Cl	H
d	Cl	OMe
e	Br	H
f	Br	OMe

12	R	X
a	H	CH_2
b	H	O
c	Cl	O
d	Br	O

Figure 1. Reagents and conditions: (i) $NH_2NH_2.H_2O$, MeOH, reflux 1 h; (ii) DMF/K_2CO_3, stirring 12 h; (iii) NaOH/MeOH, reflux 1 h; (iv) Morpholine, DMF/K_2CO_3, stirring 24 h; (v) EtOH/AcOH, reflux 8 h.

Further structural characterization of indoles is crucial for understanding their anti-tumor mechanisms and optimizing their applications. Spectroscopic techniques such as UV-visible spectroscopy, fluorescence spectroscopy, and NMR spectroscopy are pivotal in elucidating the absorption, fluorescence, and detailed molecular structure of indole derivatives, respectively.

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O08

Preferential Solvation and Thermal Stability of Proteins in Aqueous Solutions of Sugars and Polyols

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It is well known that the thermal stability of proteins is generally increased by the addition of sugars and polyols, but decreased by the addition of urea and guanidine hydrochloride. Such effects of cosolvents on the protein stability are related to the protein preferential solvation; that is, stabilizers such as sugars are excluded from proteins, while denaturants such as urea are adsorbed to proteins. The strength of the preferential interaction has been represented by a preferential interaction parameter, $\xi_3 = (\partial g_3/\partial g_1)_{T,\ \mu_1,\ \mu_3}$, where g_i, μ_i, and T is the concentration of component i, the chemical potential of component i, and temperature, respectively, and in a three-component system, water is designated as component 1, protein as component 2, and the cosolvent as component 3. The value of ξ_3 can be determined by densimetry, but the experimental data of ξ_3 have been limited.

Recently, we demonstrated that small-angle X-ray scattering (SAXS) was useful in quantifying the preferential solvation of proteins in aqueous solutions of sugars [1]. In addition to this, we can also provide a simple method for calculating ξ_3 on the basis of the SAXS data. For the validation of this method, we measured SAXS of lysozyme in aqueous solutions of glucose, sorbitol and glycerol, and calculated ξ_3 for these systems. The obtained values of ξ_3 were close to the literature values based on the densimetric experiments [2-4].

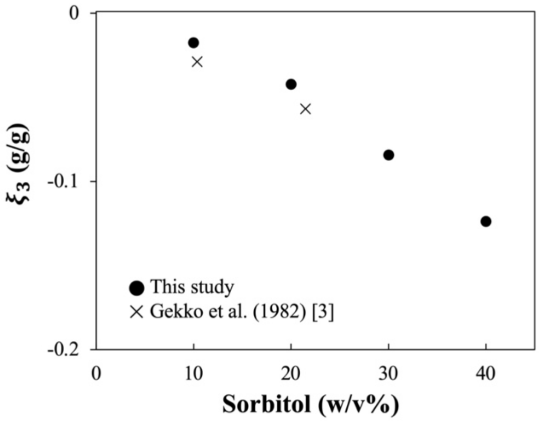

FIGURE 1. Preferential interaction parameter ξ_3 of lysozyme in sorbitol-water mixtures as a function of sorbitol concentration calculated from the SAXS data (this study, ●) and the densimetric data (Gekko et al. [3], ×).

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BL-9B, Laser-SARPES

Present Status and Future Prospect of Spin-Resolved ARPES at HiSOR

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Keywords: Spin- and angle-resolved photoemission spectroscopy, VLEED spin detector

Visualization of the electron behaviors in functional materials, such as semiconductors, magnets, and superconductors, is essential because it is closely connected to their numerous functionalities relevant to device applications. The fundamental properties of the electrons in solids are predominantly described by distinct quantum parameters including energy, momentum, and spin. In this context, spin- and angle-resolved photoemission spectroscopy (SARPES) is a very powerful experimental method that can reveal the "complete" electronic structure in energy-, momentum-, and spin-resolved manners [1,2].

Since the discovery of strongly spin-orbit coupled exotic quantum materials such as Rashba systems, topological insulators, and Weyl semimetals, the importance of SARPES experiments has rapidly increased. Nevertheless, SARPES measurements are time-consuming compared to the conventional spin-integrated measurements due to the extremely low efficiency of the spin detector. Thus, we typically sacrifice the energy and momentum resolution for practical experiments to obtain a sufficient signal-to-noise ratio.

To overcome this problem, we have developed a very low energy electron diffraction (VLEED) type high-efficiency spin detector using Fe(001)p(1x1)-O target [3,4]. At HiSOR, we constructed two SARPES instruments combined with photon-energy-tunable vacuum ultraviolet synchrotron radiation (16-300 eV) and ultraviolet laser (6 eV) light sources [4-6]. For both instruments, two VLEED spin detectors are installed orthogonally each other after a hemispherical electron analyzer. Since one VLEED spin detector can measure two spin components (P_x & P_z or P_y & P_z) by changing the magnetization direction of the Fe(001)p(1x1)-O target, we can perform three-dimensional spin vectorial analysis. In this talk, we will present the recent research highlights utilizing our aforementioned high-efficiency SARPES systems and future prospects, such as developing a multichannel spin polarimeter, time-resolved SARPES, and operand SARPES.

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Electronic dark states and Fermi arcs in cuprates

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In nature, there are many materials with more than one pair of sublattices in their primitive cell. These sublattices have been recognized as important in the study of graphene and other two-dimensional materials with the concept of pseudospin [1]. In strongly correlated systems, charge density waves or magnetism would naturally result in translational symmetry breaking, generating pairs of sublattices. However, the presence of these sublattices in the primitive cell has been ignored in theoretical models for the sake of brevity. In this talk, I will introduce our recent studies on the effect of quantum phases between sublattices (pseudospins) would affect angle-resolved photoemission spectroscopy (ARPES). We found the dark state of electrons in materials with two pairs of sublattices, where it means the dispersive band of electronic states is undetectable over the entire Brillouin zone at any experimental conditions including photon energy, polarization, and scattering geometry [2]. This dark-state model can be applied to Bi-based cuprates and used to explain their Fermi arcs. If time permits, I will also discuss on how the short-range order of dopants in a two-dimensional crystalline insulator affects their electronic structure in terms of pseudogap [3] and aperiodic (rotonic) dispersion [4].

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Strange story about liquid water using soft X-ray spectroscopy

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Keywords: soft x-ray spectroscopy, liquid water

Water is ubiquitous and one of the most important materials in our life. And it is known as the most abnormal material; many abnormal properties are shown such as extremely high boiling points compared with similar compounds, etc. Many researchers take on the challenge to understand the origin of that abnormality.

Soft X-ray emission spectroscopy (XES) is a powerful tool to measure the electronic states in material. Especially, XES is very sensitive the environment surrounding molecules. Using this spectroscopy, electronic states of liquid water were observed. Observed spectra showed double peaks assigned to the $1b_1$ state. However, different models, dynamics [1] or structure [2], are proposed to interpret these peaks, and a long debate is continuing for more than 15 years. This is a strange situation. We constructed model structure of liquid water and performed XES calculations within the framework of density functional theory [3]. Our new model can clearly reproduce experimental temperature and isotope dependence of XES of liquid water. Our conclusion is that both interpretations, dynamics and structure, are important to reproduce experimental spectra.

Next target is aqueous solutions. I introduce recent results such as ethanol aqueous solutions as an example of homogeneous solutions and water in liquid crystal membrane as an example of heterogeneous solutions.

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