# Oral Session

-Oral Session-

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*Graduate School of Frontier Biosciences, The University of Osaka, Japan*

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*Institute for Solid State Physics, The University of Tokyo, Japan*

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Shin-ichiro Ideta[a], M. Arita[a], Y. Kumar[a], Y. Miyai[a,b], S. Kumar[c], K. Shimada[a,d,e]

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# The Use of Non-Canonical Amino Acids to Study Protein Function. Green Fluorescent Protein and Rob Protein

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Several strategies now exist for the ribosomal synthesis of proteins containing non-proteinogenic amino acids. These enable the incorporation of one or more modified amino acids into predetermined positions in a protein. While a wide variety of amino acid side chains not found in natural proteins can be incorporated, bacterial ribosomes do not readily incorporate amino acid analogues such as D-amino acids or beta-amino acids.

Over the past several years, we have also developed a strategy for modifying the 23S ribosomal RNA in *E. coli* ribosomes; this is the ribosomal constituent that mediates the peptide bond formation. By the use of structurally modified puromycin analogues, libraries of clones harboring plasmids with modified 23S rRNAs can be screened to identify clones capable of incorporating modified amino acids not normally incorporated by bacterial ribosomes.

Green Fluorescent Protein (GFP) is a naturally occurring protein that has been the source of inspiration for many recent studies. GFP utilizes a cluster of three canonical amino acids to cyclize and oxidize, forming a novel fluorophore within a beta barrel protein conformation. The initial finding has prompted numerous studies of GFP analogues that produce a broad spectrum of colors, with altered amino acid chemistry and facility of amino acid cyclization with concomitant oxidation. Presently, we describe a novel set of synthetic dipeptidomimetic structures that exhibit weak fluorescence in aqueous solution, but whose fluorescence is strongly enhanced in more hydrophobic environments such as beta barrels. They have structures reminiscent of the formed fluorophore in GFP, but are significantly brighter than GFP or any of its synthetic analogues.

In addition, we have studied altered DNA transcription in *E. coli* involving the interaction of Rob protein with RNA stress response gene *micF*, the latter of which encodes a 93-nucleotide antisense RNA that post-transcriptionally controls the expression of the outer membrane porin gene *ompF* by binding to its target ompF mRNA, thus diminishing porin expression. Altered Rob protein interaction with *micF* is increased slightly by altering Arg40 or Arg90 in each of two helix-turn-helix motifs in Rob that are responsible for *micF* binding. Their increased binding produces an increase in the cellular antisense RNA transcript, which diminishes cellular ompF porin and alters cell phenotype, reducing the uptake of some macrocyclic antibiotics and toxic metal cations.

# An SRCD Journey from Brazil involving the CEDRO Beamline

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The dissemination of Synchrotron Radiation Circular Dichroism (SRCD) spectroscopy has significantly expanded the repertoire of structural biophysical methodologies available to the biomolecular community in South America. By overcoming key limitations of the conventional CD method, offering enhanced signal-to-noise ratios, providing access to the vacuum ultraviolet region, and improving the characterization of complex and low-structured systems, SRCD has become a powerful technique for probing protein secondary and tertiary structures.

In Brazil, activities in the SRCD field have mainly started in 2012 [1], following specialized training and a strong scientific collaboration with Prof. Bonnie Wallace (Birkbeck College, University of London), a leading figure in the field. This partnership enabled the transfer of expertise and laid the foundation for synchrotron-based structural spectroscopy in the country. Since then, SRCD studies in Brazil have addressed fundamental questions in protein folding, conformational stability, mechanisms of antimicrobial peptides, protein–ligand interactions, and protein incorporation into nanostructured systems, thereby strengthening national research in structural biology and biophysics. The consolidation of this expertise fostered new collaborations and helped establish a national community focused on advanced synchrotron-based spectroscopic methods. These efforts culminated in the proposal and development of a SRCD beamline at the Sirius synchrotron in Brazil. Designed to deliver high-brilliance measurements in the ultraviolet and vacuum ultraviolet regions, CEDRO enables experiments with improved spectral quality and expanded experimental capabilities. Its implementation represents a strategic milestone for structural biology in Brazil and Latin America, integrating international expertise, national scientific demand, and state-of-the-art synchrotron technology to expand research capacity and drive innovation in biomolecular science.

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# Time-resolved ARPES and XRD study of charge-density-wave materials

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Collective excitations ubiquitously emerge as a consequence of spontaneous symmetry breaking. A prototypical example in solid-state systems is the charge density wave (CDW), in which the formation of a periodically modulated electronic state gives rise to characteristic amplitude and phase modes across the CDW phase transition. These collective modes, reflecting fluctuations of the order parameter, provide direct insight into the underlying symmetry and many-body interactions. Owing to their fundamental importance and rich dynamics, CDW amplitude and phase excitations have attracted sustained and widespread interest for several decades.

In this presentation, I will report on our recent investigations of the ultrafast dynamics in CDW materials using time-resolved X-ray diffraction (tr-XRD) and angle-resolved photoemission spectroscopy (tr-ARPES). We focus first on $VTe_2$, which exhibits a CDW phase below 480 K accompanied by a structural transition from the trimerized 1*T* phase to a monoclinic 1*T''* phase. Figure 1 shows the fluence-dependent tr-XRD results for 2/3 0 11/3 superlattice reflection. At low excitation fluence (0.4 mJ/cm²), coherent oscillations at 1.5 THz are clearly observed, which we identify as the CDW amplitude mode. In contrast, at high fluence (4.9 mJ/cm²), the oscillatory component is strongly suppressed and accompanied by a relatively slow recovery, indicative of photoinduced CDW melting dynamics. Furthermore, I will present complementary results on $TaTe_2$ and 4Hb-$TaS_2$, which exhibit distinct nonequilibrium behaviors, underscoring the material-dependent pathways of ultrafast CDW dynamics.

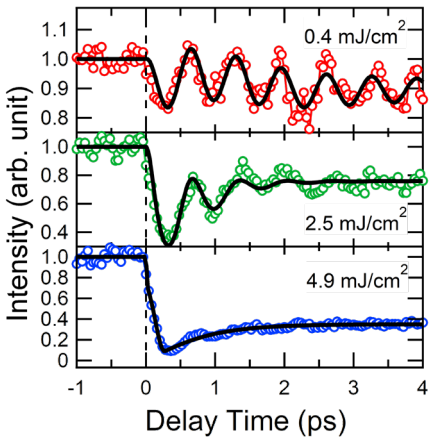


**FIGURE 1.** Summary of the fluence-dependent dynamics of the 2/3 0 11/3 superlattice reflection.

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# Spin- and angle-resolved photoemission studies on magnetic topological insulators

Xue Han[a,b], Jason Qu[a,b], Hengxin Tan[c], Zicheng Tao[d], Noah M. Meyer[a,b], Patrick S. Kirchmann[a], Yanfeng Guo[d,e], Binghai Yan[c], Zhi-Xun Shen[a,b] and Jonathan A. Sobota[a]

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$MnBi_{2n}Te_{3n+1}$ (MBT) compounds have been intensively studied in recent years as they constitute the first intrinsic bulk magnetic topological insulator family that has been synthesized. When time-reversal symmetry (TRS) is spontaneously broken, MBT has been shown to host exotic quantum phenomena such as the quantum anomalous Hall effect. However, despite the clear evidence of broken TRS, angle-resolved photoemission spectroscopy (ARPES) studies predominantly report a surface state exhibiting no gap in the magnetic phase, in contradiction to theory. Furthermore, the electronic structure of MBT remains poorly understood, which hinders research to exploit applications of its unique magnetic topological properties.

Here, we present an experimental methodology to tackle these problems by reconstructing the wavefunction of the $MnBi_2Te_4$ and $MnBi_4Te_7$ surface states using spin-resolved ARPES. We will first show the intricate spin-orbital texture of the surface states by systematically tracking the spin-polarization and orbital characters as a function of momentum. Then, we will introduce a wavefunction model that quantitatively describes the experimental data. Our results demonstrate that the surface states are well-described by a single-band picture dominated by *p* orbitals, solidifying the microscopic understanding of MBT. Most importantly, based on the methodology, we will present a novel intrinsic mechanism for reducing the magnetic gap of topological surface states, providing crucial insight into the long-standing puzzle of the gapless Dirac cone in the MBT material family.

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# Understanding Ion Matter Interactions Using Synchrotron-Based X-ray Spectroscopic Techniques

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Ion beams play a crucial role in nanoscience and nanotechnology by enabling precise synthesis, modification, and characterization. Ion beam processing is an effective technique for fabricating and tailoring materials through ion–matter interactions, enabling controlled modification of physical properties [1]. When energetic ions interact with solids, they transfer energy through nuclear ($S_n$) and electronic ($S_e$) energy loss mechanisms, generating defects such as vacancies, dislocations, clusters, and amorphous regions. At low energy, nuclear energy loss dominates, producing lattice defects, while at higher energies (~1 MeV/nucleon), electronic energy loss prevails through excitation and ionization processes. It enables patterning of nanomaterials and nanostructures. It is suitable for fabricating devices and materials by tailoring optical, magnetic, and electrical properties through processes: ion implantation and ion irradiation. This talk will provide basic information on ion beam interactions and how synchrotron-based X-ray spectroscopic studies, mainly XRD, XAS, XMCD, and PL, unveil the modifications in the structural, optical, magnetic, and electronic properties of materials. This will cover selected experimental results related to energy and magnetic materials [2-5]. The synchrotron-based facilities at KEK, Photon Factory (Japan), Elettra (Italy), and NSRRC (Taiwan) were used for these studies.

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# Ion-Irradiation-Driven Defect Engineering and Metallization in $VO_2$ Thin Films

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Strongly correlated transition metal oxides exhibit a wide range of intriguing physical phenomena, including high-temperature superconductivity, colossal magnetoresistance (CMR), and metal–insulator transitions (MIT) [1–3]. Among these, the MIT is one of the most fascinating and extensively studied phenomena due to its sensitivity to external stimuli such as temperature, strain, defects, and carrier concentration. Morin first observed a reversible, temperature-driven MIT in several titanium- and vanadium-based oxides, highlighting the role of electron correlation and lattice distortion in these systems [4]. Among the transition metal oxides exhibiting MIT, vanadium dioxide ($VO_2$) has attracted considerable attention owing to its transition temperature ($T_n \approx 340$ K), which lies close to room temperature, and its dramatic change in electrical resistivity spanning approximately three to five orders of magnitude across the transition. These unique properties make $VO_2$ a promising candidate for both fundamental studies and technological applications, particularly in electronic and optoelectronic devices.

Ion irradiation has emerged as an effective and controllable approach for tailoring the physical properties of materials in a reproducible manner. During ion irradiation, materials may undergo a variety of modifications, including defect generation, phase transformation, atomic displacement, deep ion implantation, amorphization, surface modification, and macroscopic deformation [5-6]. The density of irradiation-induced defects generally increases with ion fluence, leading to pronounced changes in the structural, optical, electrical, and magnetic properties, as well as in the surface morphology of thin films [7]. Consequently, understanding the influence of ion-induced defects on the MIT and electrical transport properties of $VO_2$ thin films is of significant importance for device-oriented applications. Several studies have reported ion-irradiation-induced modifications in $VO_2$ thin films. For instance, thermoelectric properties of ion-irradiated $VO_2$ have been investigated [8,9], while Gupta *et al.* demonstrated controlled tuning of the semiconductor-to-metal transition in Au-ion-irradiated $VO_2$ thin films [10]. Similarly, Khan *et al.* reported enhanced electrical conductivity in the insulating phase of $VO_2$ thin films following $Ag^{9+}$ ion irradiation [11].

In this work, we systematically investigate the effect of 150 keV Fe and Ni ion irradiation on the structural, electronic, and transport properties of $VO_2$ thin films. The films were deposited by pulsed laser deposition on r-cut sapphire ($1\bar{1}02$) substrates. Ion irradiation was performed over a fluence range of $1 \times 10^{14}$ to $1 \times 10^{16}$ ions/cm$^2$. Structural characterization using grazing-incidence X-ray diffraction (GIXRD) and Raman spectroscopy confirms the retention of the monoclinic phase of $VO_2$ after irradiation. However, temperature-dependent resistivity (R–T) and Hall effect measurements reveal a systematic reduction in the MIT temperature along with a significant enhancement in electrical conductivity with increasing ion fluence. Analysis of the carrier concentration supports the observed transport behavior. Furthermore, synchrotron-based X-ray photoemission spectroscopy (XPS) and X-ray absorption spectroscopy (XAS) measurements reveal the

presence of mixed vanadium oxidation states ($V^{4+}$ and $V^{5+}$) induced by ion irradiation. Photoelectron spectroscopy (PES) measurements provide direct evidence of irradiation-induced metallization in $VO_2$, which is fully consistent with the transport results obtained from R–T measurements.

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# Soft X-ray Emission Spectroscopy of Water in Confined and Interfacial Conditions

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Water in nanoconfinement and at interfaces governs ion selectivity, charge generation, and electrochemical reactivity, yet its hydrogen-bond network is hard to probe under realistic conditions. O *K*-edge X-ray emission spectroscopy (XES) provides a direct fingerprint of water's valence electronic states, including $1b_1$-derived states sensitive to hydrogen-bond motifs. Here I present XES studies enabled by the BL07U HORNET-II station at NanoTerasu. A vacuum-isolation silicon nitride membrane allows measurements of wet interfaces while maintaining ultrahigh vacuum, with precise temperature/humidity control for well-defined adsorbed and confined water layers. Humidity-dependent XES tracks the evolution from molecular adsorption to water-cluster formation at polymer interfaces [1]. For liquid-crystalline polymer membranes showing strongly different rejection for mono- and divalent salts, XES identifies distinct stable water structures in nanopores that correlate with transport beyond pore size and fixed-charge effects [2–4]. I also discuss interfacial charge generation by ultrafine water clusters on self-assembled monolayers, where hydroxide-related signatures appear at both hydrophobic and hydrophilic interfaces [5]. These results highlight operando soft X-ray spectroscopy as a route to design rules for membranes and energy materials [6].

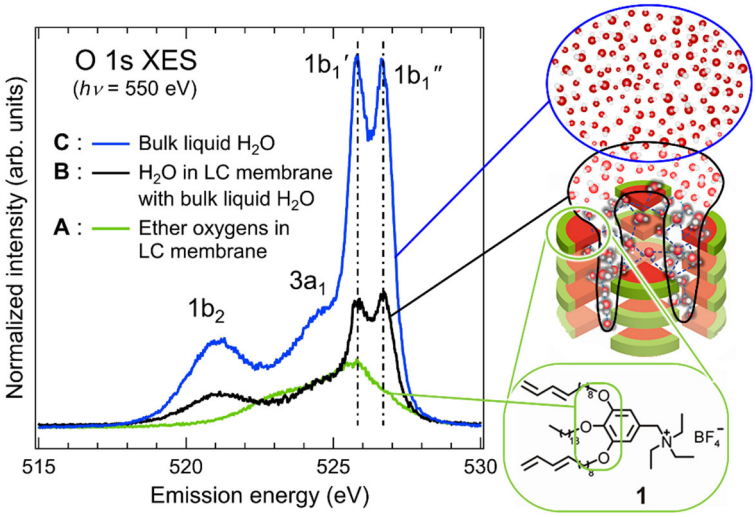


**FIGURE 1.** O 1s soft X-ray emission spectra indicate distinct water structures confined in nanopores of a liquid-crystalline polymer membrane, correlating with different salt rejection rates. Adapted from Ref. [4].

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# Recent Research and Development of ARPES Beamlines at HiSOR and Future Plan for Upgrade

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**Keywords:** Synchrotron radiation, Angle-resolved photoemission spectroscopy

The Research Institute for Synchrotron Radiation Science is a synchrotron radiation facility established at Hiroshima University. A compact 700 MeV electron storage ring provides synchrotron radiation in the vacuum ultraviolet (VUV) and soft x ray regions. Tunable photon energies in this range are indispensable for studying the fine electronic structures of novel materials such as superconductors, topological insulators, and Weyl semimetals using high resolution angle resolved photoemission spectroscopy (ARPES).

Our facility hosts several undulator beamlines dedicated to high-resolution ARPES (BL-1 and BL-9A), enabling measurements with an energy resolution better than 5 meV. At BL-1 (high-resolution ARPES beamline, $h\nu = 23 - 350$ eV), the beam size has recently been reduced by an order of magnitude (to ~70-80 μm in the vertical direction), and a new electron analyzer (A-1, MBS) equipped with a deflector mode has been installed to facilitate detailed measurements. In addition, we have introduced the three-axis goniometer of the focusing mirror for optimization of the focused beam more precisely. A laser source has also been introduced at the endstation to conduct the experiment with synchrotron radiation. These developments allow BL-1 to flexibly switch between synchrotron radiation and laser light depending on the experimental requirements, enabling highly efficient ARPES measurements. A spin-detection system will be introduced in 2026, along with new experimental apparatuses to support a wide range of research fields.

BL-9A provides low-energy-photon ARPES capabilities for solids and thin films, using synchrotron radiation in the ultraviolet region ($h\nu = 6.5$ - 40 eV). This beamline delivers high-brightness radiation with excellent energy resolution. Since October 2022, a hemispherical analyzer (ASTRAIOS 190, SPECS; acquisition angle ±20° to ±30°) and a six-axis manipulator (operational temperature range: ~10 - 300 K) have been installed at the endstation. Operando measurements are also possible.

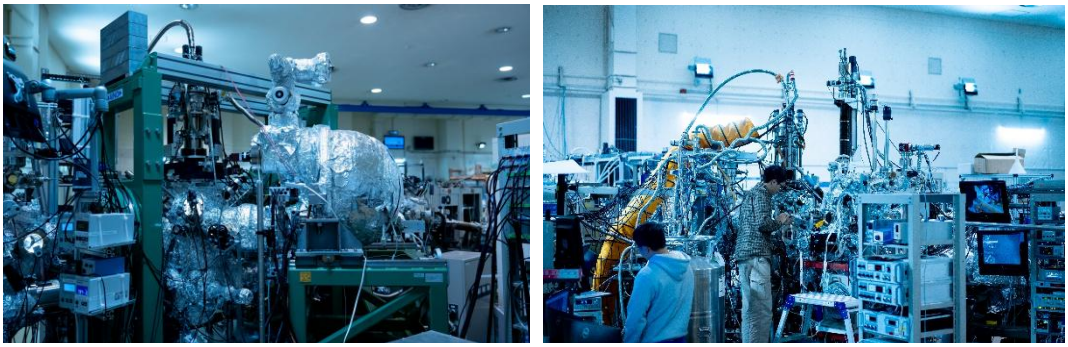

**FIGURE 1.** Endstations for the high-resolution angle-resolved photoemission spectroscopy. Left and right is BL-1 and BL-9A, respectively.

# Study on phonon properties and atomic arrangement of SiGe alloy using synchrotron radiation techniques

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**Keywords:** Phonon, Silicon-germanium, Synchrotron radiation

Silicon-germanium (SiGe) alloy has a low thermal conductivity due to a significant reduction of the phonon mean free path compared to those of bulk Si and Ge crystals and is one of the promising candidates as a next-generation material for thermoelectric devices. SiGe is also used in nanosheet transistor fabrication processes and attracting attention as a next-generation p-type channel material. As miniaturization progresses toward higher device performance, precise understanding of its thermal transport at nanoscale (phonon properties) and atomic configuration are important from the viewpoint of device design. In particular, the atomic arrangement of SiGe determines its phonon and electronic band structure. Inelastic x-ray scattering (IXS) with synchrotron radiation is a powerful technique to evaluate phonon energy and dispersion nondestructively, but there are no reports of applying this method to epitaxial SiGe thin films, which are commonly used in devices, because the penetration depth of hard x-ray into SiGe. In this study, I demonstrated phonon spectra and dispersion of high-quality bulk SiGe using IXS. Moreover, I tried to observe the atomic arrangement from three-dimensional large-area reciprocal lattice maps of bulk SiGe using synchrotron x-ray diffraction (XRD) with synchrotron radiation.

The single-crystalline SiGe samples for IXS and XRD were prepared by two different growth methods: the Czochralski [1] and traveling liquidus zone methods [2]. The IXS measurements were performed on the BL35XU and BL43LXU beamlines at the SPring-8 synchrotron facility [3]. The incident x-ray energy was set to 17.8 or 21.7 keV, which corresponds to Si (9 9 9) or Si (11 11 11) reflection, respectively. The three-dimensional large-area reciprocal lattice maps of bulk SiGe were obtained using the diffractometer through XRD measurements at the BL02B1 beamline in SPring-8 synchrotron facility. In addition, the reciprocal space was simulated using the free software DISCUS [4].

Figure 1(a) shows the phonon dispersion curves of bulk $Si_{1-x}Ge_x$ with the $x$ value of 0.45 obtained by IXS. The phonon dispersion of bulk SiGe were observed to consist of four phonons in the Γ–X ([00$q$]) direction: longitudinal optical (LO), transverse optical (TO), longitudinal acoustic (LA), and transverse acoustic (TA) phonon modes. I found that the LO and TO modes are split into three modes (Ge–Ge, Si–Ge, and Si–Si modes). Moreover, an anomalous phonon dispersion on the low-energy side (approximately 13meV), which is different from the optical and acoustic phonon dispersions, was observed [5]. Figure 1(b) shows the phonon dispersion curves obtained by the molecular dynamics (MD) simulation of bulk $Si_{1-x}Ge_x$ with the $x$ value of 0.45. In Fig. 2(b), the intensity of blue, magenta, and red colors shows the density of states (DOS) of the Si–Si, Si–Ge, and Ge–Ge vibration mode, respectively. The results of the optical and acoustic phonon modes in the simulation are in good agreement with the experimental results. Figures 2(a) and 2(b) also show that the experimental anomalous mode including the momentum dependence is well reproduced with the MD simulation. This mode did not appear in the MD simulation with the SiGe compound model (Si–Ge–Si–Ge only configuration). I found that the anomalous mode had no Ge fraction dependence experimentally, indicating that the mode originated from the Ge localized vibration without propagation properties [6-8].

Figure 2(a) shows the reciprocal lattice map of bulk $Si_{1-x}Ge_x$ with the $x$ value of 0.32 (center: 0, 0.5, 0). As a result, the checkerboard-like pattern derived from diffuse scattering due to the atomic arrangement was observed. Figure 2(b) shows the result of the reciprocal lattice space simulation based on the most stable structure obtained from density functional theory (DFT) and genetic algorithm [9]. The reciprocal lattice space based on the most stable structure reproduces checkerboard-like pattern and this profile is generally consistent with the XRD result (see Fig. 2(a)). Figures 2(c) and 2(d) show the simulation results for pure Si and SiGe with random atom position, respectively. In contrast to Fig. 2(b), diffuse scattering intensity was

weak in pure Si and scattered diffuse scattering in SiGe with random atom position. From the above, these results suggest that the atomic arrangement of bulk SiGe is not completely random, but rather that there is a tendency for atoms of the same type to bond over a wide area, i.e., percolation.

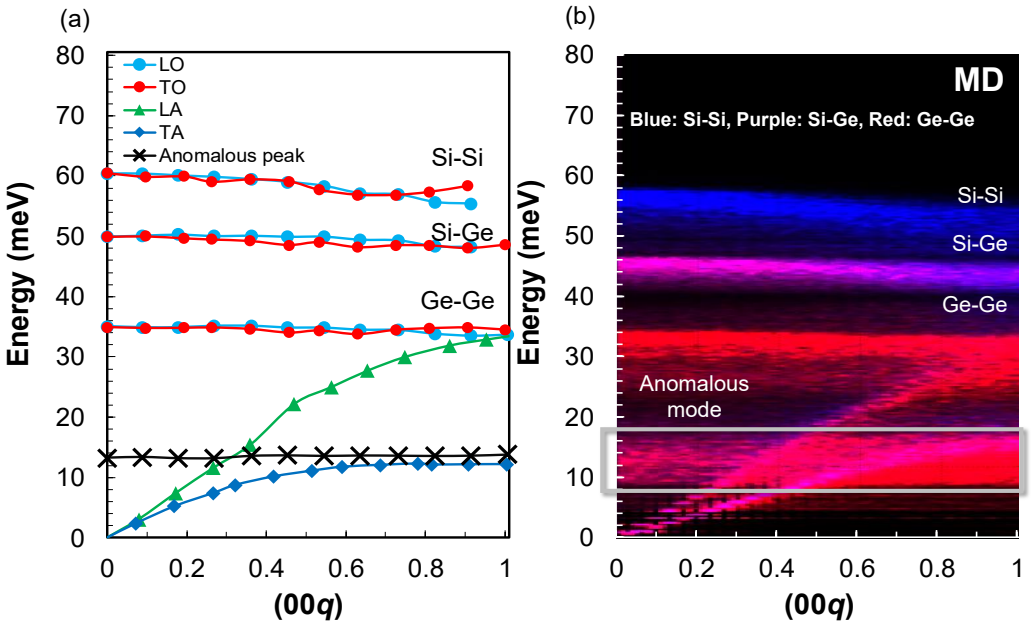


**FIGURE 1.** Phonon dispersion relations of bulk $Si_{1-x}Ge_x$ with the $x$ value of 0.45 [6]. (a) Phonon dispersion curves including the anomalous peaks obtained by peak positions of IXS spectra. (b) Corresponding phonon dispersion curves simulated by the MD calculations. The blue, magenta, and red colors show the Si–Si, Si–Ge, and Ge–Ge vibration modes, respectively. The phonon dispersion of the anomalous mode is marked with a gray rectangle.

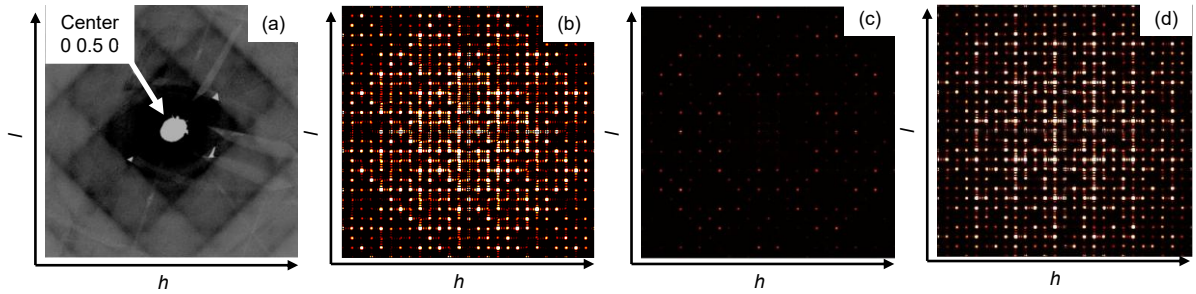


**FIGURE 2.** (a) Reciprocal space mapping of bulk SiGe bulk $Si_{1-x}Ge_x$ with the $x$ value of 0.32 (center: 0 0.5 0). Reciprocal space simulation results of (b) most stable SiGe (Ge: 30%) using DFT and genetic algorithm, (c) Si, and (d) SiGe with random atom position (Ge: 30%).

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# Time-resolved studies on Biomolecules with X-ray Free Electron lasers and development of compact X-ray Free Electron Lasers at Arizona State University

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In the Biodesign Center for Applied Structural Discovery at Arizona State University we aim to develop new revolutionary techniques that reveal the structure and dynamics of biomolecules towards new visionary discoveries in Medicine and Energy Conversion. Serial Femtosecond crystallography (SFX) provides a novel concept for structure determination, where X-ray diffraction “snapshots” are collected from a fully hydrated stream of nanocrystals, using femtosecond pulses at high energy X-ray free-electron lasers. As femtosecond pulses are shorter than the time-scale of most damage processes, femtosecond crystallography overcomes the problem of X-ray damage in crystallography. The proof of principle for time resolved serial femtosecond crystallography pave the way for the determination of molecular movies of the dynamics of proteins "at work". In my talk I will give an overview of highlights of recent structural discoveries with X-ray Free Electron lasers and report on the new development of compact X-ray Free Electron Lasers at Arizona State University.

# Structural Basis for the Assembly of Virus-Like Particles, Encapsulin

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Encapsulins are protein-based organelles in prokaryotes that form icosahedral shells capable of packaging specific cargo proteins. Here we focus on the *Pyrococcus furiosus* encapsulin (PfV), a highly thermostable icosahedral particle whose exceptional stability and versatility have enabled applications in bioengineering and nanomaterial design [1,2]. However, cargo proteins inside encapsulins adopt random orientations, which complicates structural analysis by averaging-based methods such as X-ray crystallography [3] and cryo-EM analysis. To address this challenge, we used vacuum ultraviolet circular dichroism (VUVCD) spectroscopy to estimate the secondary structure content of the internal cargo proteins [4]. In parallel, we aim to elucidate the assembly mechanism of encapsulin particles by combining these structural biology methods. This combined approach provides a practical framework for characterizing disordered cargo proteins within icosahedral particles and supports the future development of encapsulin-based nanocapsules.

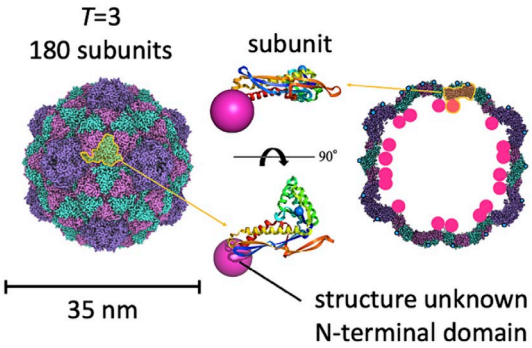


**FIGURE 1.** Overwiew of the *Pyrococcus furiosus* encapsulin [1].

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