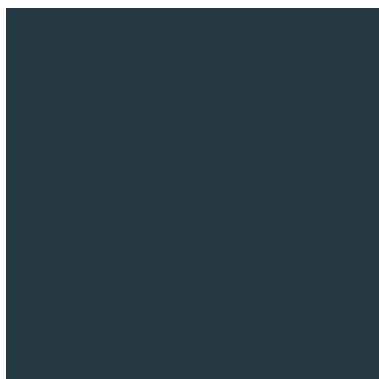


Crystallography 2017



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Accepted Abstracts

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Evaluation of ZnGeP₂ and DAST crystals for optical rectification based THz generation using Femtoseconds amplifier

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The paper reports the evaluation of ZGP and DAST, two different types of nonlinear crystals for the generation of efficient THz generation using 1.3 μm wavelength obtained from 60 fs Ti: sapphire amplifiers at 1 kHz repetition rate. DAST is a positive biaxial organic crystal with very high deff. values whereas ZGP is a positive uniaxial semiconductor crystal with moderate deff. value. It has been observed that figure of merit (FOM) of these crystals along with the coherence length (l_c) provide complete information about their utility as a potential source of THz generation. The FOM of DAST and ZGP in THz domain are theoretically calculated and correlated to their experimental values of conversion efficiency. The FOM of DAST is almost 372.12 times higher than the ZGP but experimental THz conversion efficiency in both the case are similar and $\ll 1\%$. Theoretical and experimental data of DAST and ZGP crystals are comprised in Table 1. We investigated the role of refractive indices of these crystals in optical and THz domain and corresponding coherence length (l_c) to understand the THz conversion efficiency.

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Precipitant-less crystallization of protein molecules induced by substrate with heterogeneous topography and surface potential gradient

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Surfaces having heterogeneous topography are known to facilitate protein crystallization by diminishing the energy barrier for nucleation. A precipitant is, nevertheless, required for shielding the charges on protein molecules, so that they can overcome electrostatic repulsion and self-assemble into crystalline structure. For yet-to-be crystallized proteins, zeroing on the right precipitant is a non-trivial problem and therefore, despite existence of several heterogeneous nucleant surfaces, number of proteins that are yet to be crystallized continues to be large. In this talk, we will present a novel surface which is decorated with nanoscopic patterns and also surface charges, the combined effect of which show the remarkable ability to induce crystallization without use of any precipitant. This effect is demonstrated by crystallizing several protein molecules with molecular weight ranging from 14-450 kDa. These surfaces are shown to induce also directed crystallization of a specific protein from a mixture of two or more protein species and even simultaneous crystallization from a mixture of proteins. In essence, these surfaces consist of nanoscopic wrinkles with spatially varying curvature and surface charges. Kelvin probe force microscopy (KPFM) measurements show that surface potential gradient as high as 140 V/ μm are generated on these surfaces which can drive largescale molecular ordering in the liquid at the vicinity of the surface. As a result, the surface itself acts both as a precipitant also as a nucleant. Heterogeneity allows it to crystallize protein molecules having large range of radius of gyration, that too at low to moderate concentration of the protein in respective solutions. The prospect of precipitant-less crystallization of protein is expected to open up several possibilities in the areas of disease diagnosis, drug discovery, drug delivery and protein engineering.

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Spin-layer locking in globally centrosymmetric but locally non-centrosymmetric two dimensional materials

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In this talk, I will discuss a novel phenomenon called spin-layer locking and its physical consequence in a new class of two dimensional materials with the crystal structure that is globally centrosymmetric but locally non-centrosymmetric. I will give three examples: Mono-layer PtSe₂ film, a tri-layer (LaO)₂(SbSe₂)₂ film and a bi-layer NbSe₂ superconductors. Firstly, I will discuss a theoretical analysis of the recent surprising experimental observation of helical spin texture in a centrosymmetric mono-layer PtSe₂ film by the angle-resolved photoemission spectroscopy. This observation can be explained by dipole induced Rashba effect with spin-layer locking: Opposite spins are degenerate in energy, while spatially separated in the top and bottom Se layers. In my next example of a tri-layer (LaO)₂(SbSe₂)₂ film with a similar dipole induced Rashba effect and spin-layer locking, I will discuss a direct physical consequence, electrically tunable multiple Dirac cones, due to the narrow band gap in this system. Finally, I will discuss a two dimensional superconducting material, bilayer NbSe₂, and show that a finite momentum pairing (known as Fulde-Ferrell-Larkin-Ovchinnikov pairing) can be induced by in-plane magnetic fields due to the spin-layer locking.

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Crystal structures of a polypeptide processing and secretion transporter

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Bacteria secrete peptides and proteins to communicate, to poison competitors, and to manipulate host cells. In Gram-positive bacteria, peptidase-containing ABC transporters (PCATs) function both as maturation proteases and as exporters for quorum-sensing or antimicrobial polypeptides. In Gram-negative bacteria, PCATs interact with two other membrane proteins to form the type 1 secretion system. We showed here the first crystal structures of PCAT1 from *Clostridium thermocellum* in two different conformations. These structures, accompanied by biochemical data, show that the translocation pathway is a large α -helical barrel sufficient to accommodate small folded proteins. ATP binding alternates access to the transmembrane pathway and regulates the protease activity, thereby coupling substrate processing to translocation.

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Structural diversity and similarity among Clp chaperones from plants and mycobacteria

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Unfolded or damaged proteins in a cell usually get targeted for degradation before they start accumulating and reach toxic levels. In bacteria as well as plants, chaperones and proteases perform a major role in this important protective and restorative function. Caseinolytic protease-associated chaperone C1 (ClpC1) is one such protein that performs the function of cellular protein quality control, primarily through its association with ClpP1P2 protease core in mycobacteria, wherein the chaperone aids in ATP-dependent unfolding of protein substrates to be degraded by the protease machinery. In case of plants, they have the Clp chaperones ClpC1 and ClpC2 which associate with a similar protease core - ClpPR, all within the chloroplast stroma. In addition, plants have an additional stromal chaperone called ClpD which also associates with Clp protease. ClpC and ClpD proteins belong to the family of AAA+ HSP100 proteins. Both are functional as hexamers and have a 3-domain organization wherein the N-terminal domain is mostly involved in substrate recognition and the middle and C-terminal domains are with ATPase activity, aiding substrate unfolding. Crystal structures reveal the N-terminal domain of ClpC1 from *M. tuberculosis* and *A. thaliana* to be very similar in organization; however, the plant specific AtClpD has a structural organization quite different from any known Clp chaperones that have been characterized so far. Herein, we discuss the findings from our structural studies on Clp chaperone proteins from *Mycobacterium* and *Arabidopsis*.

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Self-catalyzed growth of InAs nanowires on graphite for flexible optoelectronic device applications

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The advent^{1, 2} of the two-dimensional (2D) graphene, has sparked enormous research interest owing to its extraordinary electronic and optical properties including ultra-high carrier mobility^{3, 4}, exceptionally high thermal conductivity, flexibility and high optical transparency^{5, 6} which offers huge potential for applications in transparent, stretchable and flexible electronics. The monolithic integration of semiconductor nanowire (NWs) on graphene/graphitic substrates (GS) has stimulated enormous research interest over the recent years as it would enable the exploitation of the exceptional qualities of the former with the intriguing properties of the latter and provide a unique platform for the development of high performance, sophisticated, flexible and cost-effective optoelectronic nanodevices. The growth of InAs nanowires on graphite holds enormous promise for the development of flexible and functional hybrid devices such as solar cells and light emitting diodes. InAs NWs were grown on GS by solid-source MBE. Mechanically exfoliated graphite films from highly oriented pyrolytic graphite (HOPG) were transferred onto Si (111) substrates and subsequently loaded into the system and thermally outgassed. Indium (In) droplets were pre-deposited on the films prior to growth initiation at pre-optimised conditions. The InAs NWs were then grown at a temperature of 450°C to 500°C by the spontaneous opening of In and As for NWs growth. The surface morphology of the NWs was investigated using a FEI XL30 SFEG scanning electron microscope (SEM) while Transmission electron microscope (TEM) images were taken with a JEOL-JEM 2100 microscope working at 200 kV. Figure 1a shows the 45° tilted SEM image of InAs NWs grown on graphite while the selective area electron diffraction pattern and typical HRTEM image of as-grown NWs are shown in Figures b and c respectively. The nanowires are vertically well aligned with no observable tapering. Compared to InAs NWs grown on Silicon, it will be shown that the NWs presents a relatively low density of defects. InAs-NWs/graphite heterojunction devices exhibiting rectifying behaviour was observed. A Room temperature photovoltaic response with a cut-off wavelength of 3.4 μm was realized. This unravels a promising technique for the monolithic integration of InAs NWs with graphite for applications in flexible Infrared Optoelectronic Devices.

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Local structure of ion pair interaction in Lapatinib amorphous dispersions characterized by synchrotron X-ray diffraction and pair distribution function analysis

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For many years, the idea of analyzing atom-atom contacts in amorphous drug-polymer systems has been of major interest, because this method has always had the potential to differentiate between amorphous systems with domains and amorphous systems which are molecular mixtures. In this study, local structure of ionic and non-ionic interactions was studied by High-Energy X-ray Diffraction and Pair Distribution Function (PDF) analysis in amorphous solid dispersions of Lapatinib in Hypromellose Phthalate (HPMCP) and hypromellose (HPMC-E3). The strategy of extracting Lapatinib intermolecular drug interactions from the total PDF X-ray pattern was successfully applied allowing the detection of distinct nearest neighbor contacts for the HPMC-E3 rich preparations showing that Lapatinib molecules do not cluster in the same way as observed in HPMC-P, where ionic interactions are present. Orientational correlations up to nearest neighbor molecules at about 4.3 Å were observed for polymer rich samples; both observations showed strong correlation to the stability of the systems. Finally, the superior physical stability of 1:3 LP:HPMCP was consistent with the absence of significant intermolecular interactions in (Δ) in the range of 3.0 to 6.0 Å, which are attributed to C-C, C-N and C-O nearest neighbor contacts present in drug-drug interactions.

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Thermally induced phase transitions in *breathing crystals*: Structural peculiarities

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A family of heterospin complexes based on copper (II) hexafluoroacetylacetonate $\text{Cu}(\text{hfac})_2$ with persistent nitronyl nitroxides L^{R} was named as *breathing crystals* due to their ability to undergo reversible 'Single-Crystal-to-Single-Crystal' phase transformations. Studying of these processes facilitates a detail investigation and understanding of solid dynamics. Phase exchange clusters 'Cu-O•-N' or 'N•-O-Cu-O•-N'. This reorganization causes an appearance of magnetic anomalies on the dependence of the effective magnetic moment vs temperature (or pressure) [1-5]. Our studies of more than one hundred complexes showed a wide variety of magnetic anomalies caused by structural transformations and provide valuable information on the spin state in a heterospin solid.

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A novel concept in membrane protein crystallization: Conjugated engineered-micelles

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We present a general strategy for producing crystals of integral membrane proteins which is conceptually different from crystallization procedures commonly employed. Our working hypothesis has been based on the idea that high quality crystals of membrane proteins can be produced via conjugating mechanisms which are capable of bringing detergent-solubilized membrane proteins into proximity and which, at the same time are: (1) Highly specific, mild and non-covalent; (2) capable of exerting control over both the optimal distance and binding affinity between detergent-protein complexes; (3) suitable for use with diverse membrane proteins, regardless of biological origin or size of the hydrophilic domains; and (4) simple to implement. These criteria are satisfied by a novel type of detergent micelles that we call engineered-micelles. Embedded in the engineered-micelles are specially synthesized hydrophobic molecules which may be conjugated to one another via specific interactions. Two examples of such molecules are hydrophobic [metal:chelator] complexes and complementary hydrophobic nucleoside base-pairs. These interactions lead to micellar aggregates with a variety of different architectures as determined by cryo-TEM imaging and which have been shown to provide necessary and sufficient conditions for the successful growth of membrane protein crystals.

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Elucidation of crystal and electronic structures within highly strained BiFeO₃ by transmission electron microscopy and first-principles simulation

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Crystal and electronic structures of ~380 nm BiFeO₃ film grown on LaAlO₃ substrate are comprehensively studied using advanced transmission electron microscopy (TEM) technique combined with first-principles theory. Cross-sectional TEM images reveal the BiFeO₃ film consists of two zones with different crystal structures. While zone II turns out to have rhombohedral BiFeO₃, the crystal structure of zone I matches none of BiFeO₃ phases reported experimentally or predicted theoretically. Detailed electron diffraction analysis combined with first-principles calculation allows us to determine that zone I displays an orthorhombic-like monoclinic structure with space group of Cm (=8). The growth mechanism and electronic structure in zone I are further discussed in comparison with those of zone II. This study is the first to provide an experimentally validated complete crystallographic detail of a highly strained BiFeO₃ that includes the lattice parameter as well as the basis atom locations in the unit cell.

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Proton dynamics in ZnO nanorods: An NMR study

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The rotating-frame spin-lattice relaxation of two types of the hydrogen donors was well distinguished in the ^1H nuclear magnetic resonance (NMR) measurements, providing a unique opportunity to study the distinct proton dynamics in ZnO nanorods. NMR relaxometry is a powerful technique of atomic-scale access to probe ion hopping motion in solids. The laboratory-frame relaxation rate is effective for probing nuclear spin processing in radio frequency range, i.e., fast diffusing spins. The rotating-frame relaxation rate, on the other hand, effectively probes motions occurring at ultralow-frequencies. While spin-lattice relaxation in the laboratory-frame showed a single-exponential form presumably due to spin mixing by spin diffusion, the spin-lattice relaxation in the rotating-frame showed a well-resolved double-exponential form, allowing us to distinguish the dynamics of the two distinct proton species in ZnO synthesized at relatively low-temperature of 573 K. Here, we demonstrate that the conversion from interstitial H (Hi) to oxygen-substitution H (HO) in ZnO dynamically takes place at elevated temperatures by means of the ^1H NMR. The activation barriers for migration of Hi and for binding of Hi with an oxygen vacancy to form HO are revealed to be 0.27 eV and 0.51 eV, supporting those obtained by ab initio calculations. In proton-implanted ZnO, we identify comprehensive hydrogen species and investigate their dynamical properties. Unlike in unirradiated sample, after irradiation mobile protons at the interstitial site were observed in the systems synthesized at relatively high-temperature of 773 K. The activation energy obtained was 0.46 eV by the Arrhenius relation, corresponding to that of long-range hopping motion. Multiple NMR lines at ~ 1 ppm, assigned to the hydroxyl group were observed and their diffusion properties have been investigated before and after irradiation. Our work gives manifest evidence for the first time from a microscopic point of view that implanted protons become mobile in the lattice.

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Crystal genes in metallic liquids and glasses

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It has been widely speculated that dominant motifs such as short-range icosahedral order can influence glass formation. Less understood is how these motifs (crystal genes) in the liquid can influence phase selection upon devitrification. These crystal genes are the underlying structural order that transcends liquid, glass and crystalline states. By comparing the amorphous states of the same alloy compositions formed by sputtering and rapid solidification and their devitrification pathways, we can quantify the distribution of the common packing motifs in the liquid or glass and in stable and metastable phases which form. We will discuss how this approach brings new insight into the origin of vitrification and mesoscopic order-disorder transitions in condensed matter. A genetic algorithm is applied to search for the energetically favorable stable and metastable crystal structures of complex metallic compounds and a cluster alignment method reveals the most common packing motifs in crystalline and non-crystalline structures.

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Boron suboxide properties and low pressure growth

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Boron Suboxide (B_6O) is a compound semiconductor possessing α -rhombohedral Boron type structure (R3m) and is the second most studied material of the Boron-Rich solids after B_4C . The allowed phase width of B_6O is expressed as $B_{12}(O_2-xB_x)$ where $0 \leq x \leq 1$. In the stoichiometric unit cell of B_6O , two oxygen atoms are positioned along the hexagonal $\langle 111 \rangle$ (c-axis) at the boron-icosahedral interstitial sites 2c, with the single 1b central position left unoccupied. The oxygen atoms donate one electron each to the boron icosahedra and compensate for the electron deficiency of pure α -B. The resulting short interatomic bond lengths and strong covalent bonding establish the bulk properties of B_6O , which possess the smallest unit cell volume of the α -boron derivatives. This structure is different from the semi-metallic structure of B_4C , where the 1b site is occupied and three interstitial atoms form a chain along the c-axis. When stoichiometric ($x=0$) B_6O is intrinsic high-resistivity semiconductor with an expected hole mobility at 300K approaching $100 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$ and an optical band gap of about 2.5 eV and a melting point of 2075 °C. It is also a Super-Hard class material with bulk modulus of 314 GPa and a Vickers hardness exceeding 45 GPa. Sub-stoichiometric crystals of B_6O contain boron atoms replacing interstitial oxygen atoms and possess diminished properties. We will present a low pressure method for producing stoichiometrically correct B_6O macroscopic crystals, contrasting this method with alternate approaches in the literature and discuss applications for B_6O which include nuclear detectors and cutting technologies.

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Optically active phonons in titanil crystals and their effects on the operation of nonlinear optical laser sources

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Birefringent optical crystals have enabled operation of nonlinear optical laser sources since the 1960's. The effectiveness and robustness of various nonlinear optical (NLO) processes in these crystals, such as second harmonic generation (SHG), sum-frequency generation (SFG), and optical parametric amplification (OPA), relies on the lack of interaction between the laser beams and the resonant modes in the NLO crystals. In this way, the NLO polarization driven in the birefringent NLO-active crystals is only driven by the instantaneous oscillations of electrons. In this work, we report on a different type of light-matter interaction in NLO laser sources in which the optically-active phonon modes present in certain NLO crystals of titanil family (e.g. KTiOPO₄, KTiOAsO₄) couple to the interacting laser beams. These interactions lead to the effects such as wavelength shifts in the output beams. These effects are explained by the impulsive excitation optically active phonons in these crystals which effectively leads to ultrafast modulation of the crystal's optical nonlinearity. We will discuss the general principles behind the application of birefringent crystals in NLO laser sources, and introduce the effects of intrinsic resonances, such as lattice phonons present in certain NLO materials, on the operation of NLO devices. We also discuss the implications of these photon-phonon interactions in the terahertz (THz) wave generation.

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Dielectric and magnetic study of gel grown iron-manganese-nickel ternary levo-tartrate crystals

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Various metallic tartrate crystals find different applications in science and technology. Iron-manganese-nickel ternary levo-tartrate crystals of different compositions have been grown by single-diffusion gel growth technique in silica hydrogel medium. The metallic composition in the crystals was estimated by EDAX. The coloration of the crystals changed with composition of metallic content. The powder XRD study suggested the crystalline nature and indicated the presence of some extra phases. The grown crystals were characterized by dielectric and magnetic studies. The dielectric constant, conductivity and imaginary part of permittivity and dissipation factor decreases with increasing frequency. Resistivity of the sample increases with increasing frequency. Magnetic susceptibility is calculated. Samples were found paramagnetic in nature, i.e., the magnetic field is strengthened by the presence of the material.

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A size dependent phase map and phase transformation kinetics for iron(III) oxide nanomaterials ($\gamma \rightarrow \epsilon \rightarrow \alpha$ pathway)Seungyeol Lee and Huifang Xu
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Nanometric iron(III)-oxide has been of great interest in a wide range of fields due to magnetic properties, eminent biochemical characteristics and potential for technological applications. To date, five crystalline polymorphs of Fe_2O_3 are known: (1) $\alpha\text{-Fe}_2\text{O}_3$ (i.e., hematite), (2) $\beta\text{-Fe}_2\text{O}_3$, (3) $\gamma\text{-Fe}_2\text{O}_3$ (i.e., maghemite), (4) $\epsilon\text{-Fe}_2\text{O}_3$ (i.e., luogufengite), and (5) $\zeta\text{-Fe}_2\text{O}_3$, all of which have different morphologies, various size and magnetic properties. Among the iron-oxides, $\epsilon\text{-Fe}_2\text{O}_3$ is considered as a remarkable phase due to its giant coercive field at room temperature and ferromagnetic resonance capability. The natural $\epsilon\text{-Fe}_2\text{O}_3$ (luogufengite) is discovered from vesicles' surfaces of basaltic scoria. Here we present the first size-dependent phase map for $\epsilon\text{-Fe}_2\text{O}_3$ via a $\gamma \rightarrow \epsilon \rightarrow \alpha$ pathway together with the activation energies for the phase transformations based on X-ray powder diffraction (XRD) and high-resolution transmission electron microscopy (HRTEM). HRTEM images of $\epsilon\text{-Fe}_2\text{O}_3$ nanocrystals show the inversion and pseudo-hexagonal twins, which are fundamentally important for understanding the correlation between its nanostructure and magnetic properties. Two activation energies for $\gamma\text{-Fe}_2\text{O}_3 \rightarrow \alpha\text{-Fe}_2\text{O}_3$ phase transformations are $186.37 \pm 9.89 \text{ kJ mol}^{-1}$ and $174.58 \pm 2.24 \text{ kJ mol}^{-1}$, respectively. The results provide useful information about the size, crystal structure and transformation of the nanometric iron-oxide polymorphs for applications in areas such as designing engineered materials. Combining the phase map with their kinetic properties predicts that stability regime of the nanosized Fe_2O_3 polymorphs as the function of crystal size, temperature and annealing times. The proposed size-dependent phase map will help to improve controlled synthesis of $\epsilon\text{-Fe}_2\text{O}_3$ nanocrystal, a promising material for many future applications.

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Structure-based design of IL-17 antagonists

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Statement of the Problem: IL-17A is a pro-inflammatory cytokine that is implicated in many autoimmune and inflammatory diseases. Disruption of interactions between IL-17A and its main receptor, IL-17RA may be effective in treating these diseases. Monoclonal antibodies targeting pathway of IL-17A have shown significant efficacies in treating psoriasis and psoriatic arthritis over existing therapies. To develop non-antibody IL-17A antagonists, structure information of IL-17A, its complex with IL-17RA and inhibitors are valuable. To develop non-antibody based IL-17A antagonists, we identify peptides, small molecules and fragment leads through various techniques. We designed and produced well behaved IL-17A and IL-17RA, and obtained crystal structures of IL-17A and IL-17RA. These structures provide the structural basis for IL-17A signaling through IL-17RA. We then move on to determine the structures of IL-17A in complex with peptide and small molecule antagonists. Since both peptide and small molecules disrupt the native structure of IL-17A and hinder crystallization, to achieve these structures we used FAB of an IL-17A targeting antibody as a crystallization chaperon to stabilize IL-17A/peptide and IL-17A small molecule complexes. Furthermore, we conducted fragment screen using large numbers of high diffracting apo IL-17A crystals, and identified two binders. These structures enabled us to understand the structural basis of IL-17A signaling, identify lead materials and design IL-17A antagonists with much improved potencies.

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Unusual molecular movements in the solid state

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Crystallization is a kinetic process and the experimental conditions like solvents, concentration, pH, temperature and time have greater control on the nature of products in the synthesis of coordination network structures. During crystallization, the ligands bind to the metal ions reversibly and hence, the least soluble polymer will crystallize first, independent of the metal-ligand ratio used in the crystallization. In the kinetic products, quite often the solvents are bonded to the metal ions. The removal of these coordinated solvents is likely to transform the kinetically formed coordination polymers (CPs) into thermodynamically stable products. Such structural transformations have been demonstrated in many coordination polymeric network structures, if the solid state structure of the products can be determined unequivocally. If the structural transformation to thermodynamic product is accompanied by the parallel alignment of double bonds, then the photochemical reactivity could be tested through the formation of cyclobutane rings from [2+2] cycloaddition reactions. Such techniques have been successfully used to predict the structural transformation of linear CPs to photoreactive ladder structures due to desolvation. In his laboratory the speaker has encountered a number of such molecular movements in the solid state which will be highlighted in this talk.

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Fe-excess ions as the electronic charge suppliers in $\text{Fe}_{1+x}\text{Te}_{1-y}\text{Se}_y$ for development of a ferromagnetic component in the superconducting state and a zero thermal expansion in the normal state

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Superconductivity in α -FeSe has received special attention due to its simple crystalline structure. It is known that the wavy layered α -FeSe structure can accommodate a significant amount of extra Fe ions. These non-stoichiometric Fe ions occupy the interstitial sites that are slightly below the center positions of the Se square sublattice. The general picture established so far for the links between superconductivity and magnetic ordering in iron chalcogenide $\text{Fe}_{1+y}(\text{Te}_{1-x}\text{Se}_x)$ is that the substitution of Se for Te directly drives the system from the antiferromagnetic end into the superconducting regime. Here, we report on the observation of a ferromagnetic component that developed together with the superconducting transition and a zero thermal expansion of the crystalline lattice in the normal state in Fe-excess crystals, using neutron and X-ray diffractions, resistivity, magnetic susceptibility and magnetization measurements. The superconducting transition is accompanied by a negative thermal expansion of the crystalline unit cell and an electronic charge redistribution, where a small portion of the electronic charge flows from around the Fe sites toward the Te/Se sites. Two magnetic phases are identified. The low-temperature magnetic phase, which coexists with superconductivity, involves the ordering of the lattice Fe and interstitial Fe ions. An extremely large thermal expansion of the lattice is observed in the superconducting state. Thermal expansion coefficients of the lattice are quenched upon loss of superconductivity. Zero thermal expansion is retained over a very broad temperature range from 20 to 200 K. These behaviors are understood as being due to the electronic charge redistribution, in which the excess Fe ions on the interstitial sites act as electronic charge suppliers that strengthen the electronic connections between the Te/Se and Fe ions on the lattice sites once the temperature is raised.

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