

# POSTERS

Abstracts



3<sup>rd</sup> Edition of International Conference on

## **Advanced Spectroscopy, Crystallography and Applications in Modern Chemistry**

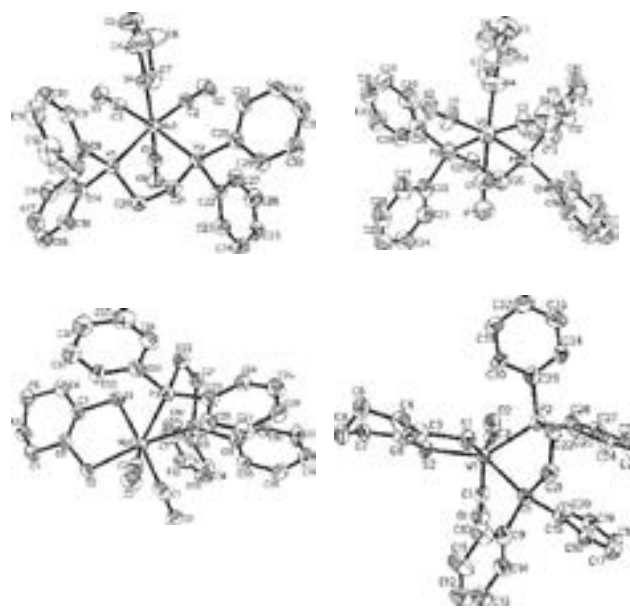
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## CRYSTALLOGRAPHY OF NOVEL MONODITHIOLENE MOLYBDENUM AND TUNGSTEN COMPLEXES AND THEIR PRECUSORS

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Monodithiolene complexes of molybdenum and tungsten have always attracted significant scientific interest as firstly they can potentially be adapted as artificial molybdopterin/tungstopterin cofactors and secondly their crystal structures can provide powerful information about the coordination sphere in the natural Mo/W cofactor. With this information a better comprehension of the reaction mechanisms as well as the physicochemical properties of the natural enzyme can be achieved. So far the most accurate structural analogue of native molybdoenzymes' first coordination sphere was designed by Holm et al in 2001 [1]. Today's many challenges remain regarding the synthetic efficiency, structural accuracy and catalytic activity. In our lab, we developed a novel synthetic strategy for establishing Mo and W monodithiolene complexes. The synthetic success was supported by some notable crystal structures of those complexes and their metalprecursors [2]. Pre activated compounds 1 and 2 are isomorphous and crystalize in the P21/c space groups with clearly octahedral geometry and trans angles of 172.22(12)° to 176.38(14)° in 1 and 171.9(4)° to 176.8(4)° in 2. The Bailar twist angle in 1 ranges between 54.95° and 60.43° and in 2 between 55.34° and 59.88°. The focal molecules 3 and 4, which were synthesized from 1 and 2, respectively, by replacing the labile thf and one of the basal CO ligands, crystallize in the orthorhombic space group P212121. The geometry of the final compounds changes from clearly octahedral to decidedly trigonal prismatic, which is strongly associated with dithiolene complexes as evidenced by several related crystal structures [3-8], even though such complexes are extremely rare. It has to be pointed out that in the case of 3 and 4 the nearly perfect trigonal prismatic geometry is confirmed by the Bailar twist angle. Most surprisingly in 3 and 4 the torsion angles of the P-C-C-P moiety of dppe is close to 0 with only 7.3°. This indicates an almost planar arrangement which is extraordinary for dppe complexes.



**Figure 1:** [Mo(CO)<sub>3</sub>(dppe)(THF)] (1), [Mo(CO)<sub>3</sub>(dppe)(THF)] (2) top and [Mo(CO)<sub>2</sub>(cydt)(dppe)] (3), [Mo(CO)<sub>2</sub>(cydt)(dppe)] (4) bottom. Thermal ellipsoids are shown at the 50% probability level. H atoms are not shown for clarity reasons.[2]

### Recent Publications

1. Lim B., Willer M., Miao M., Holm R. J. Am. Chem. Soc., 2001, 123, 8343-8349
2. Elvers B., Nowack R., Schulzke C., Fischer C. in preparation.
3. Yan Y., Keating C., Chandrasekaran P., Jayarathne U., Mague J., DeBeer S., Lancaster K., Sproules S., Rubtsov I., Donahue J. Inorg. Chem. 2013, 52, 6743-6751.
4. Tsukada S., Abe N., Gunji T., Polyhedron 2016, 117, 73-79
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- M., Mague T., Donahue P., *Inorg. Chem.*, 2009, 48, 2103-2112
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  8. Barnard K., Wedd A., Tiekin E., *Inorg. Chem.* 1990, 29, 891-892.

**Biography**

Nicolas Chrysochos received his Master degree of science in biochemistry from University of Greifswald. Since 2015 is PhD-student under supervision of Prof. Dr. Carola Schulzke at Bioinorganig Chemistry, Institute of Biochemistry, University of Greifswald. His PhD research concentrate on the development of new models for the molybdopterin and tungstopterin cofactors with focus on coordination sphere, physicochemical properties and catalytic activity of the model compounds. During his PhD is paying particular attention on the crystallography of the target models.

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# E-POSTER

Abstracts



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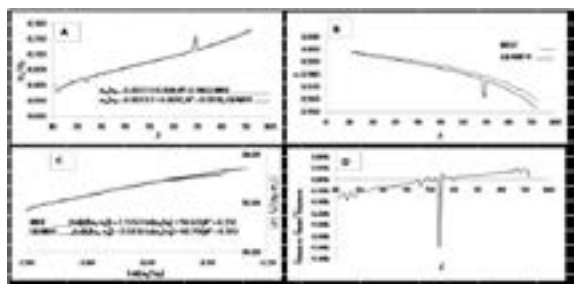
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# THE X-RAY FEMTOSCOPE ALLOWS US TO MEASURE THE INTERACTION BETWEEN DARK MATTER AND THE ATOMIC NUCLEI OF CR, XU AND TM

**Edward Jimenez**

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The x-ray femtoscope measures dimensions and interactions in the range of femtometers. In this way it detects interactions at the boundary of the nuclear surface, and has even allowed measuring the radii of protons on the nuclear surface and the electrons of the K layer [1], [2]. To measure dimensions of the order of the femtometers, it uses resonance and interference of the x-rays with the nuclear surface, using only the K edge data, for each of the elements of the periodic table  $11 < Z < 92$ . Because of the non-invasive nature of low energy x-rays, we can measure a minimal abnormality of the cross section or energy (k edge) on the nuclear surface. For this reason, we can detect dark matter or WIMPs, which interact and hide on the nuclear surface [3]. Fortunately, after studying these interactions with all the elements of the periodic table, only three elements: Cr, Xe and Tm present resonances. Dark matter ( $< (100 \pm 2) \text{ eV}/c^2$ ) acts directly and resonantly with the excess mass, energy and cross section of the atomic nuclei of xenon, thulium and chromium, through the weak force, which is represented by the solution of the Navier Stokes equations [4]. The dark matter is hidden in the vicinity of the nuclear surface ( $10^{-1} \text{ m}$ ), it interacts modifying the effective sections and the K edge energy [5]. We studied the total absorption of low energy x-rays ( $< 1.16 \text{ MeV}$ ) for the elements of the periodic table  $11 \leq Z \leq 90$ , with a precision of the order of the Rydberg constant, and the radius of the neutron ( $0.842(3) \text{ fm}$ ) using experimental NIST data and GEANT4 simulation for  $(0.993(9) < R^2 < 0.999(6))$  [6]. Finally, it was proved theoretically and experimentally that the weak force controls the circular trajectories of the nucleon layers in the atomic nucleus, the interaction with dark matter and the nuclear stability  $P(x, y, z)$ .



**Figure 1. A:** Cross section excess measure presence of dark matter for  $^{24}\text{Cr}$  and  $^{69}\text{Tm}$ . B.-Evolution of nuclear stability  $P$ , depending on the ratio of the cross sections. We obtained the probability  $P(x, y, z, t)$  which is the fundamental solution of the Navier Stokes equations, measures the Nuclear stability and represents both the behavior of the atomic nucleus in equilibrium and out of equilibrium such as gamma or beta decay C.- Calculation of the Rydberg constant using Navier Stokes model. D.- Energy excess. For  $^{54}\text{Xe}$ , we can see the resonance in energy.

## Recent Publications

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2. Pohl, R et al. (2010). The size of the proton. Nature 2010, 466, 213--216.
3. M. Markevitch, A. H. Gonzalez, D. Clowe et al (2004) : DIRECT CONSTRAINTS ON THE DARK MATTER SELF-INTERACTION CROSS SECTION FROM THE. MERGING GALAXY CLUSTER 1E 0657 56. The Astrophysical Journal, 606:819--824, (2004).
4. David Harvey F. Courbin J. P. Kneib et al. (2017) : A detection of wobbling brightest cluster galaxies within massive galaxy clusters. Monthly Notices of the Royal Astronomical Society, Volume 472, Issue 2, 1 December 2017.
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6. E. Aprile et al. (2017) : Search for bosonic super-WIMP interactions with the XENON100 experiment,. (XENON Collaboration), Phys. Rev. D 96, 122002, (2017).

**Biography**

Edward Jimenez, has experience in low-energy x-ray diffraction, in oil refining applications and especially in allophanes, which is a nano clay that contains silicon and aluminum and exists in the form of powder and one of the largest reserves of allophane is in Ecuador. His main research focuses on the structure of the nuclear surface and the measurement of nuclear stability parameters, with the aim of implementing the x-ray femtoscope. Currently, he is the research director of the Faculty of Chemical Engineering of the Central University of Ecuador. In addition, he was director of research of the Petroleum Company, PETROECUADOR, 2008-2015.

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## Cu(I) COMPLEXES WITH BULKY BIPODAL SCORPIONATE LIGANDS

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Cu(I) complexes possess a broad range of applications in catalysis, photo-luminescent materials and in biological sciences. In this regard, the development of proper ligands systems that can stabilize Cu(I) metal will contribute to the coordination chemistry and applications of this metal. The salt metathesis reaction of CuI with two sodium precursors (NaBb and NaBb-1) of bipodal scorpionate type ligands [Bb = dihydrobis(2-mercapto-benzimidazolyl)borate, (Bb-1 = dihydrobis(2-mercapto-benzothiazolyl)borate)], has been explored in the presence of selected phosphine ligands (PPh<sub>3</sub>, PCy<sub>3</sub>, PPh<sub>2</sub>Me, PPh<sub>2</sub>Py),

Figure 1. All of the resulting Cu(I) complexes were formed as predominantly a single monomeric isomer and were characterized using a combination of <sup>1</sup>H, <sup>13</sup>C{<sup>1</sup>H}, <sup>31</sup>P{<sup>1</sup>H} NMR spectroscopy, and in two cases by X-ray crystallography. In the X-ray crystal structure of complex 1 and 6, the Cu(I) center adopts a distorted tetrahedral geometry. The complexes 1 and 6 exhibit a (B)H Cu distances of 2.008 Å and 1.866 Å length, respectively. Based on IR spectroscopy and X-ray crystallography data, 1 and 6 adopt a k<sup>3</sup>-S,S,H coordination mode in solid state.

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## EXPLORING THE EVOLUTION OF THE ORBITAL AND MAGNETIC ORDERING IN $\text{Ca}_2\text{RuO}_4$ UNDER AN APPLIED FIELD

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Despite researchers developed a very good understanding of metallic and insulating states in condensed matter systems, the situation changes dramatically in the proximity of a metalinsulator (MI) transition [1]. In fact, difficult to model electronic correlations are very often at the origin of such abrupt change that the whole model to describe the system properties and excitations need to be adapted to the different electronic behavior. MI transitions are also peculiar as it is not straightforward to identify a primary order parameter. Recently a lot of interest arose around 4d based materials, where the occupancy of the 4d shell is a critical element in establishing the electronic correlations [2]. Ru based materials are often in a metallic state, however a notable exception is represented by  $\text{Ca}_2\text{RuO}_4$  (fig.1), this distorted Ruddlesden Popper system, is in an insulating state at room temperature, however the transport

properties can be easily modified increasing the temperature [3] or the pressure [4], or as more recently demonstrated applying an unprecedentedly low voltage to the system [5]. Resonant X-ray scattering (RXS) offers a unique opportunity to monitor the structural, magnetic and electronic properties of this fascinating material by following the evolution of the diffraction peaks related to the orbital, magnetic and structural properties of the system as function of the temperature and of an applied field. In this talk, after a brief introduction to the RXS technique, we will review the current understanding of the system behavior and present our new insight about the evolution of the electronic properties of the system [6]. The most exciting result being the fully reversible suppression of the orbital ordered before the destructive IM transition is completed.

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# PRECIPITANT-LESS CRYSTALLIZATION OF PROTEIN MOLECULES INDUCED BY SUBSTRATE WITH HETEROGENEOUS TOPOGRAPHY AND SURFACE POTENTIAL GRADIENT

**Animangsu Ghatak** and **Anindita Sengupta Ghatak**

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**S**urfaces with heterogeneous structures facilitate protein crystallization by diminishing the energy barrier for nucleation. Nevertheless, a precipitant remains necessary for shielding the charges on protein molecules, which then overcomes electrostatic repulsion and self-assemble into crystalline structure. For yet-to-be crystallized proteins, identifying the right precipitant is non-trivial and therefore, despite existence of several heterogeneous surfaces, number of such yet-to-be crystallized proteins continues to be large. In this talk, we will describe a novel surface decorated with both nanoscopic patterns and surface charges, the combined effect of which show the remarkable ability to induce crystallization without use of any precipitant. In fact, several protein molecules with molecular weight ranging from 14-450 kDa could be crystallized in this process. These surfaces can induce also crystallization of a specific protein from a

mixture of two or more protein species and even simultaneous crystallization from a mixture of proteins. Kelvin probe force microscopy (KPFM) measurements of these surfaces show that surface potential gradient as high as 140 V/ $\mu\text{m}$  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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## NON-EUCLIDEAN CRYSTALLOGRAPHY

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**N**on-Euclidean crystallography seems to be a new direction in modelling new phenomena as fullerenes, nanotubes, quasi crystals. The existence of such materials gives us the feeling [1], [2] that our experience space in small size can be non-Euclidean, for instance hyperbolic (H3) in the sense of János Bolyai and Nikolai I. Lobachevsky. Polyhedral models as for nanotube in Figure, and the unified projective metric geometry with the newer linear algebraic description provide us with these methods. The mathematical tools have also been overviewed in our conference papers [3], [4] with my colleagues, we are working on this topic. Author's hyperbolic football manifolds on some Archimedean solids are described in [1], in particular the classical football on {5, 6, 6} had already been published in 1988 (in a Dubrovnik Proceedings) without any fullerene reference. Extremal ball packing (with density 0.77147) and covering (with density 1.36893), realized at the football tiling, are better than those of

the Euclidean cases. These are our recent results in [5]. These latter investigations led us also to a polyhedral scheme in Figure from [6], as fundamental domain (asymmetric unit under a symmetry group) for so-called cobweb (or tube) manifold  $Cw(6, 6, 6)$ , where identifying (as with topological glue) the base faces  $s-1$  and  $s$  by  $1/3$  screw motion  $s$ , and repeating this process, we get a tube structure. At some vertices four polyhedra  $Cw$  can meet, imitating carbon (C) atoms with four bonds. We can extend this construction for polyhedra  $Cw(2z, 2z, 2z)$  ( $3 \leq z$  odd natural number). So we get an infinite series of compact hyperbolic manifolds (i.e. every point has a ball-like neighborhood) as new topological structures. With these we also get new models for possible nanotube structures realized in the hyperbolic space (H3), maybe also in our experience space (Euclidean, E3) in small size (?).

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DOI: 10.21767/2470-9905-C1-006**SYNTHESIS AND CRYSTAL STRUCTURE OF NEW POLY(ORGANIC-  
INORGANIC) POLYMERS POLY[Cu(NO<sub>2</sub>-ACAC)<sub>2</sub>]<sub>n</sub>****Hadi Salman Al-Lami**

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Coordination polymers are a class of polymers whose repeated units are coordination complexes. A subclass of these is the metal organic frameworks that are coordinated with organic ligands containing potential voids. Coordination polymers are relevant to many fields such as organic, inorganic, bio, electro chemistry; material science and pharmacology. Many potential applications led to extensive studies in the past few decades. Coordination polymers have many applications such as dyes, molecular storages, catalysts, ion exchange, electrical conductors, bioactive molecules, sensors, and single molecule magnet. Also, they can be used in the fields of molecular electronics, medicine, luminescence and optics. Herein, we report the synthesis of the poly{bis (3 nitro 2,4 pentanediono) copper(II)} linked via nitro group as bridging agent. Thus, we believe that this moiety can be functioned as a channel for energy and electron transference, presenting the X ray single crystal structure of [Cu {Cu(NO<sub>2</sub> acac)<sub>2</sub>}<sub>3</sub> Cu]<sub>n</sub>. The organo inorganic polymer, poly{bis (3 nitro 2,4 pentanediono) copper(II)}, [Cu(NO<sub>2</sub> acac)<sub>2</sub>]<sub>n</sub>, has been prepared and its crystal structure was determined. The structure consists of a trimeric unit in which,

acetylacetonate ligated symmetrically to copper atoms that pose in the center of octahedrons. The three octahedral fragments of the trimer are linked to each other through nitro group. Crystal Data: C<sub>10</sub>H<sub>12</sub>CuN<sub>2</sub>O<sub>8</sub>, Mr = 351.76, triclinic, P 1 (No. 2), a = 5.8237(2) Å, b = 7.7963(3) Å, c = 7.8847(3) Å, α = 81.988(2)°, β = 75.294(2)°, γ = 72.217(2)°, V = 328.98(2) Å<sup>3</sup>, T = 143(2) K, Z = 1, Z' = 0.5, μ(Mo Kα) = 1.703, 3021 reflections measured, 1421 unique (Rint = 0.0156) which were used in all calculations. The final wR2 was 0.0686 (all data) and R1 was 0.0217 (I > 2σ(I)). The three repeating units are linked via the nitro group as bridged moiety attached to a position of the acetylacetonate ligand. The base plane of each monomeric unit being formed with the four oxygen atoms, namely O1, Oi1, O2 and Oi2 belongs to the acac ligand coordinated to the central Cu atom. Cu atom is bonded axially to Oii3 and Oiii3 of the nitro groups whose belong to the prepared monomers adopting distorted octahedral geometry in each monomer. Thus, it seems that the axial Cu Oii3 and Cu Oiii3 are longer than the equatorial Cu1 O11.9233(13) Å and Cu1 O2 (1.9195(13) Å) led to distorted octahedral geometry, in which the Cu atom is located at its center.

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# INVESTIGATING CRYSTAL GROWTH IN AMBROXOL HYDROCHLORIDE SOLUTIONS WITH THE HELP OF FBRM TECHNIQUE IN CASE OF NON-TYPICAL SPHERICAL CRYSTALLIZATION METHODS

**Orsolya Gyulai** and **Zoltan Aigner**

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**S**pherical crystallization is usually the last technological step in the production of solid form drugs. Not only purification can be achieved with it, but we can manufacture the optimal morphology of the crystals. Spherical morphology with suitable mean particle size is advantageous when direct tablet making technique is used. This way the amount of the additives can be reduced and smaller tablets can be produced. In our previous research [1] it was found that the spherical crystallization of ambroxol hydrochloride can be achieved by the non-typical methods, such as spherical agglomeration and cooling crystallization. Because of the spherical morphology, flowing and compaction properties of the powder have improved. In the present work the parameter optimization was further investigated with the help of an FBRM

probe, continuously observing the crystal growth in the non-typical crystallization systems. With this on line technique, it was possible to control the mean particle size and the optimal mixing time, and solvent-antisolvent ratio could also be determined. In case of the cooling crystallization, we applied an alternating temperature profile around the metastable zone in order to standardize the particle size. It was a heating-cooling cycle, so the smaller particles could dissolve when heating happened, then crystallize onto the surface of the larger crystals. With the FBRM probe, this process could be investigated and the exact, optimal length of the heating-cooling periods could be determined.

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## THE FABRICATION OF ITO NANOWIRES BY RF-SPUTTERING

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**T**in-doped indium oxide (ITO) is considered as one of the most important transparent conducting oxide (TCO) materials used in the fabrication of optoelectronic devices such as light-emitting diodes (LED), solar cells, flat panel displays, sensors, etc. Diverse routes to produce highly conductive and transparent ITO thin films have been developed to date. ITO film is still dominant in the market because of its mature technology, though other materials have been researched to replace it on some flexible devices. Recently, the nanoscale structures (e.g., nanorods, nanowires, nanotetrapods, and nanobelts) of semiconducting metal oxides have attracted much attention due to the high surface-volume ratio, excellent photoelectric properties and various potential applications. In our previous study, high conductivity and transparency of the ITO nanowires improved light extraction

efficiency in blue and green LEDs, and bipolar resistive switching behavior of the ITO nanowire networks was observed. There are many different methods to growth ITO nanowires, such as chemical vapor deposition, chemical synthesis, oblique incidence electron-beam (e-beam) deposition, sputtering, and thermal treatment. But the most stable and economical techniques are e-beam deposition and sputtering. Sputtering deposition is one of the most favorable and facile techniques in terms of the scale-up and mass production. However, synthesis of high quality ITO nanowires by sputtering has not been demonstrated. The direct current (DC) sputtering resulted in relatively low density of ITO whiskers and the growth rate was slow, so the radio-frequency (RF) sputtering is needed to study for wide application.

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## REAL SPACE MODELING OF SOLUTION-STATE SAXS USING INFORMATION THEORY

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Small angle X-ray scattering measurements of dilute, homogenous particles in solution are resolution limited measurements of the thermodynamic ensemble. Similar to X-ray crystallography and electron microscopy, SAXS observations made at higher resolutions imply a greater detail in the structural measurement. Here, I present a new approach to understanding bioSAXS data using two fundamental properties of Information Theory (namely, the Shannon Sampling and Noisy-Coding Channel theorems). These theorems allow for the error-free recovery of the SAXS signal, in the form of a real-space, cross-validated pair-distance,  $P(r)$ , distribution function. The  $P(r)$ -distribution contains the structural assessment of the thermodynamic ensemble. I will show that the Information theory framework can be used to develop structural modeling algorithms for shape determination and docking. Specifically, I will demonstrate an adaptive

simulated-annealing, density modeling algorithm that targets the  $P(r)$ -distribution using the Kullback-Liebler divergence, an Information Theory difference metric. The algorithm scales with resolution. Using a SAXS dataset of a 25 base-pair, double-stranded DNA, the volumetric model illustrates features of the major and minor groove as the resolution of the SAXS dataset increases. Further tests on SAXS of the P4-P6 group I intron RNA domain reveal the large solvent channels observed in the X-ray crystal structure. Furthermore, I will show the Information Theory approach can be used in antibody-antigen studies to uniquely determine the structure of the complex in the solution state. Our approach shows that modeling can be made more reliable by exploiting theorems from Information Theory.

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## DIELECTRIC AND MAGNETIC STUDY OF IRON- NICKEL- MANGANESE TERNARY LEVO TARTRATE CRYSTALS

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<sup>2</sup>Saurashtra University, India

Several metallic tartrates deserve special attention due to their various applications. In the present investigation, mixed tartrate crystals of three different metals are reported. Using single diffusion gel growth technique, iron–nickel–manganese (Fe–Ni–Mn) ternary levo-tartrate compound crystals were grown with different concentrations. Spherulitic crystals with different coloration were obtained for various concentrations of metals. The concentrations of metals were determined by EDAX. The presence of functional groups was confirmed using Fourier

transform infrared (FT-IR) spectroscopy. The powder XRD study suggested that the crystals belong to the orthorhombic system. Paramagnetic nature of the crystals was revealed from VSM study. The dielectric study suggested that the dielectric constant, conductivity, imaginary part of permittivity and dissipation factor decreases with increasing frequency. Resistivity of the sample increases with increasing frequency.

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## CO-CRYSTALLIZATION- TOWARDS ENHANCED BIOLOGICAL ACTIVITIES EXAMPLES OF CRYSTAL ENGINEERING APPROACH

**Sammer Yousuf and M. Iqbal Choudhary**

University of Karachi, Pakistan

**L**eishmaniasis is caused by protozoa parasites of the genus *Leishmania*, a biologically diverse group of flagellate parasites. Leishmaniasis is endemic in tropical and subtropical regions, particularly Afghanistan, Iran, China, Nepal, Bangladesh, etc. Based on the high prevalence of Leishmaniasis in Pakistan and associated morbidity, our research group has started to work on this disease by using different strategies. Present lecture will cover the results of structural modification of antileishmanial natural product and a commercially available drug by using a crystal engineering approach co-crystallization. Co-crystals are crystalline structures made up of two or more components in a definite stoichiometric ratio linked through non-covalent interactions in same crystal lattice. They differ in their biological and physiochemical properties from their components. They

have wide applications in drug designing and in analysis of active pharmaceutical ingredients (APIs). The co-crystals of anti-leishmanial natural product, sesselin (1) and an anti-cancer drug exemestane (2) with thiourea were synthesized by using neat grinding followed by liquid assisted grinding and solution methods. Both the pure sesseline, exemestane and their co-crystallized form with thiourea, (1 and 2, respectively) were evaluated for their anti-leishmanial activity in vitro against *L. major* promastigotes. The co-crystal (1) exhibited improved leishmanicidal activity ( $IC_{50} = 13.2 \pm 1.2 \mu\text{g/mL}$ ) in comparison to that of sesseline ( $IC_{50} = 29.4 \pm 1.0 \mu\text{g/mL}$ ). However, the co-crystal of exemestane with thiourea (2) found to be inactive.

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## CONTEMPORARY DIFFRACTION METHODS IN STUDY OF POLYCRYSTALS

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**D**iffraction in the polycrystal/crystalline powder is one of the most powerful techniques in study of microstructure and crystal structure of solids. This technique, in synergy with microscopic, spectroscopic and other physical techniques, enables a complete analysis of one- and multi-phase substances that are important in scientific and technological fields. Information on microstructure and crystal structure of a substance is stored in its diffraction pattern; in order to reveal this information, the diffraction pattern should be decoded by application of adequate mathematical and physical procedures which may often be rather complex. During the last decades, diffraction techniques in the polycrystal are developing rapidly due to the introduction of sophisticated instrumentation, powerful computers and by application of synchrotron radiation. This enables the collection and interpretation of diffraction data in a short real time, revealing: qualitative and quantitative phase analysis; 3D distribution of electron density (e.g. in metallic glasses); accurate measurement of periodicity in the crystalline substance; solubility

limits in solid solutions; precipitation processes in supersaturated solid solutions (e.g. metallic alloys); thermal expansion; phase transitions; phase diagrams; chemical stability, decomposition of chemical compounds; crystallite size, kinetics of crystallite growth, recrystallization, strains, annealing of defects; time-resolved dynamical processes; crystal structure, 3D positions of atoms, lengths and nature of chemical bonds, coordination, conformation; resolution of lattice planes and rows of atoms in the crystal; influence of crystal structure, microstructure and defects on physical and chemical properties and on biological activity of a substance, applications in a number of fields of human activities. [1] Possibilities of diffraction techniques in the polycrystal are illustrated by examples of authors' studies: phase transitions in TiO<sub>2</sub>, precipitation processes in Al-alloys, metastable and stable phase diagram of Ga<sub>2</sub>Se<sub>3</sub>-In<sub>2</sub>Se<sub>3</sub>, the graphitization of petroleum coke, biomineralization processes in bivalves, phase transitions in thermosolient crystals.[2-5].

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## THE VLASOV'S EQUATION FOR DESCRIPTION OF SOLIDS STRUCTURE

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One of the main tasks of theoretical physics is to obtain the basic equations for all aggregate states of matter (plasma, gas, liquid, solid). Aggregate states of matter are determined by the location, nature of the motion and interaction of particles. The predominant aggregative state of matter in the universe is plasma. At present, the Vlasov's kinetic equation is the basis of plasma physics. It is used to describe the universe, calculate plasma devices, tokamaks, etc. The Vlasov's equation describes the long-range interaction (or "action at a distance") and, depending on the type of interaction, distinguishes the Vlasov-Poisson, Vlasov-Maxwell, Vlasov-Einstein, and Vlasov-Yang-Mills equations. 70 years ago Vlasov suggested that in order to understand physical processes in systems consisting of many particles, it is necessary to use the equation proposed by him for describing the plasma [1]. In the basis of such approach, Vlasov put the introduction of a unified distribution function that depends on all the coordinates and their derivatives up to any order (non-local statistical mechanics). In modern crystallophysics the fact of the presence of a crystal structure with atoms localized near the lattice sites is not derived from the theory, but is postulated. From the Vlasov's viewpoint, "A crystal is not a postulated construction, but a certain state of motion of particles". As a result of the probabilistic approach, Vlasov obtained the main criterion for the existence of a crystalline state [2]. This criterion contains the condition for the beginning of the process of crystal formation from the homogeneous phase and makes it possible to determine the numerical value of the period.

This consideration was carried out by Vlasov for an ideal crystal. A theoretical description of the formation of a real (defective) crystal structure from the viewpoint of the classical approach is based on the model of high-temperature impurity precipitation. In accordance with this model, complexes "intrinsic point defect + impurity atom" are formed near the crystallization front. In the process of crystal cooling, the growth and coalescence of formed precipitates lead to the formation of a defective structure of the crystal. The formation of a defective crystal structure is controlled by its thermal growth conditions (growth rate, temperature gradients, cooling rate) [3]. We checked the positions of Vlasov's physics for real single crystals of semiconductor silicon. We confirmed the fact of complex formation near the crystallization front [4, 5]. The classical and probabilistic models for the formation of a defective crystal structure lead to identical results. The probabilistic approach allows give a new interpretation of the known results of studies of heat-treated crystals. The formation of thermal donors and thermal acceptors occurs as a result of the process of coalescence of impurity precipitates. Based on the solution obtained, three main conclusions can be drawn: (1) Vlasov's theory is a far-reaching and natural extension of classical mechanics. (2) Vlasov's equation can be used to describe any aggregate state of matter. (3) Vlasov's equation is a universal tool for describing the processes taking place in the physical world (both in the macrocosm and in the microcosm).

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## BRAGG PROJECTION PTYCHOGRAPHY ON LOW-DIMENSIONAL MATERIALS

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**X**-ray diffraction has long been used to investigate the properties of materials such as crystalline thin films. X-rays have the advantage over more surface-sensitive imaging modalities, such as atomic force microscopy, electron microscopy or photoemission electron microscopy because they can penetrate the entire sample. Bragg projection ptychography (BPP) is a coherent x-ray diffraction imaging technique which combines the advantages of scanning microscopy with the phase contrast of X-ray ptychography. Our research applies it for high resolution imaging of the phase-shifted crystalline domains associated with epitaxial growth. The distinct advantages of BPP are that the spatial extent of the sample is arbitrarily-defined, it is also non-destructive and it gives potentially diffraction limited spatial resolution at high brilliance 3rd generation synchrotron radiation facilities. Here we demonstrate the application of BPP

for revealing the domain structure caused by epitaxial misfit in a nanostructured metallic thin film. Experimental coherent diffraction data were collected from a niobium thin film, epitaxially grown on a sapphire substrate as the beam was scanned across the sample. The data were analysed by BPP using a carefully selected combination of refinement procedures. The resulting image shows a close packed array of epitaxial domains, shifted with respect to each other due to misfit between the film and its substrate. Bragg coherent imaging methods have the "dark field" advantage that they only consider signals from the parts of the sample that are contributing to the Bragg peak; all other sources of scattering and contributions from other components of the sample are suppressed.

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# CRYSTALLOGRAPHY AND THERMAL CONDUCTIVITY OF THERMOELECTRIC CLATHRATES

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Since their first discovery in 1965 [1] the intermetallic clathrates attracted attention of materials scientists, chemists and physicists in particular due to their fascinating crystal structures, especially the formation of large cavities within the three-dimensional framework which are usually occupied by filler species [2]. These cavities may be also un-occupied (empty clathrates [3]). From the point of view of chemical bonding, three types of atomic interactions are present in this family of inorganic materials: polar and non-polar covalent interactions in the framework, ionic forces and strongly polar covalent dative bonds between the filler atoms in the cavities and the framework [4]. The coexistence of the different bond kinds (inhomogeneity of the bonding) causes the reduced thermal conductivity and opens the possibility to tune the charge carrier concentration, which makes these materials interesting for thermoelectric applications. The combination of the electronic and phononic transport in clathrates suitable for thermoelectric application was

recognized and proven quite early [5,6]. One of the challenges on the way to an application is the preparation of large amounts of the material with reproducible properties, and its control by the up-scaling of the manufacture processes, due to the complexity of the phase diagrams [7]. Another challenge is the understanding of the low thermal conductivity of this family of materials. One possible mechanism is associated with the presence of low-energy non-dispersive optical phonons caused by vibrations ('rattling') of the filler atoms within the cage-like crystal structure [8,9]. Recently was shown, that these optic modes of the fillers hybridize with that of the framework, and there are no indications for the formation of isolated oscillators in the system. Moreover, the low thermal conductivity is characteristic also for the empty clathrates. A new phonon-filter mechanism was proven by the inelastic neutron scattering experiments [10,11].

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## CRYSTALLOGRAPHY OF DYNAMICS OF METAL NANOCCLUSERS DURING CHEMICAL REACTION AT THEIR SURFACE

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In heterogenous catalysis surface structure of metal catalyst may change what modifies surface interactions that in turn affect the structure. The process may generate dynamics of surface that can constitute true origin of chemical activity. One can consider concept of 'active processes' instead of 'active sites'. In our laboratory we have developed in situ powder diffraction technique that is able to register subtle changes of scattered intensities due to modifications of the nanocrystal surface and to interpret these changes via molecular simulations. Our results allowed quantitative distinction between surface relaxations and reconstructions [1]. The surface reconstruction in response to changing atmosphere appears to be quite common for metal nanocrystals. Sometimes it can lead to cyclic or turbulent phenomena if the reconstruction triggers change in the adsorbate coverage that in turn causes re-reconstruction (or cancels it out) [2]. Gold appears as the metal especially prone to reconstruction.

Our results point to gold surface reconstruction occurring on adsorption of many reactive gases. Interpreting precisely peak shape and position we could detect reversible size changes along given crystallographic direction pointing to reversible changes of the nanocrystal shape [3]. Gold surface appears to be mobile enough to quickly increase surface of crystal faces interacting more favorably with the adsorbate. Monitoring oxidation of CO we detected also appearance of a new form of nanocrystalline gold with deep reconstruction of crystal faces leading to a 200 and 220 peak split. The transition may deactivate gold as a catalyst. Precise monitoring of the metal peak position and shape during chemical reaction can provide insight into its structure and dynamics. Degree of the Bragg law violations for various peaks can indicate difference in the interaction with adsorbate on various crystal faces.

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