Summer School on Mathematical Crystallography
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Abstracts of Poster Presentations
A lattice $\Gamma$ (of rank and dimension $d$) is a discrete subset of $\mathbb{R}^d$ that is the $\mathbb{Z}$-span of $d$ linearly independent vectors of $\mathbb{R}^d$ over $\mathbb{R}$. A linear isometry $R$ of $\mathbb{R}^d$ is called a similarity isometry of a lattice $\Gamma$ if there exists a positive real number $\beta$ such that $\beta R \Gamma$ is a sublattice of finite index in $\Gamma$. The set $\beta R \Gamma$ is referred to as a similar sublattice of $\Gamma$.

A (crystallographic) point packing generated by a lattice $\Gamma$ is a finite union of $\Gamma$ with distinct shifted copies of $\Gamma$. Point packings serve as models of ideal crystals, that is, crystals having multiple atoms per primitive unit cell. Examples of point packings include the honeycomb lattice, diamond lattice (crystal structure of diamond, tin, silicon, and germanium), and hexagonal closed packing (crystal structure of quartz). In this study, we extend the notion of similarity isometries to point packings. In particular, we identify the similarity isometries of point packings and the corresponding (similar) subpackings. Moreover, we investigate the properties of the set of similarity isometries of point packings, and compare them with known results on the group of similarity isometries of lattices.
Symmetry and topological features of uranium-based fullerene-like materials

Stephanie A. Mackley (Department of Chemistry, University of Notre Dame, 301 Stinson-Remick Hall, Notre Dame, IN 46556), Sergey M. Aksenov (Department of Civil and Environmental Engineering and Earth Sciences, University of Notre Dame, 301 Stinson-Remick Hall, Notre Dame, IN 46556), Nico Van Cleemput (Department of Applied Mathematics, Computer Science, and Statistics, Gent University, Krijgslaan 281 - S9 - WE02, 9000 Ghent, Belgium.), Peter C. Burns (Department of Chemistry, Department of Civil and Environmental Engineering and Earth Sciences, University of Notre Dame, 301 Stinson-Remick Hall, Notre Dame, IN 46556) smackley@nd.edu

An extensive family of uranium peroxide nanoclusters (UPCs) has been developed over the past decade, and the study of these clusters sheds light on the behavior and properties of the actinides at the nanoscale level. These nanoclusters are a new family of polyoxometalates (POMs), which are metal-oxide clusters containing multiply bonded O atoms that need a truncating surface feature to form.

UPCs were found to self-assemble in water under alkaline conditions in 2005, and the first clusters discovered were U24, U28, and U32, where U represents a uranyl ion and the number refers to the number of uranyl polyhedra that construct the cluster. According to density functional theory (DFT), bonding interactions in dimers of peroxide-bridged uranyl ions, in which the peroxide is bidentate to both uranyl ions, favor a bent configuration, encouraging structures with curved features, as expressed in UPCs.

Previously the program CaGe was used to analyze the potential 3-connected vertex isomers of graphs that contained the following: 28 vertices, 3 squares, any number of pentagons and hexagons; 30 vertices, 2 squares, any number of pentagons and hexagons; and 36 vertices, 4 squares, any number of pentagons. It was shown that the UPCs adopted the highest symmetry possible for a graph having the corresponding number of nodes and connectivity. However, not all vertices in UPCs are 3-connected, and they require a more complex approach. Here using CaGe, the 3D net topology is read into the program in order to generate the exact 2D graph. Here we report the point groups and graphical representations of UPCs to systematically study their topologies and compare clusters with similar topologies but different ligands, the same number of vertices but different configurations, and to explore the topological possibilities of UPC formation.

Probabilistic classifications of the symmetries of more or less periodic or quasiperiodic 2D images

Peter Moeck, Department of Physics, Portland State University, Portland, OR 97207-0751, pmoeck@pdx.edu

An information theory based approach [1,2] allows for objective classifications of the crystallographic (or non-crystallographic) symmetries of noisy images that are deemed to be periodic (or quasiperiodic) in two dimensions (2D) [3-5]. These classifications are objective because they are based solely on the fulfillment of certain numerically derived inequalities [1,3], whereby confidence levels of the classifications [5] are also provided. The prevailing common practice is, by contrast, to make crystallographic symmetry classifications on the basis of somewhat subjective judgments that do not take supergroup-subgroup relations into account. Those classifications are bound to be misleading or false on occasions, especially when the images feature a comparatively large amount of generalized noise, metric specializations [6], and/or pseudo-symmetries of the Fedorov type [7]. Generalized noise includes all effects of (unavoidably) imperfect recordings of images, all kinds of rounding effects and numerical approximations by all kinds of image processing algorithms and heuristics, and all structural defects in crystalline or aperiodic real-world samples. When there are many sources of this kind of noise and the effects of none of these sources dominate, the resulting generalized noise is approximately Gaussian distributed. This distribution is the precondition for the application of geometric Akaike Information Criteria (g-AICs) from the robotics and computer vision communities [1], which are in essence geometric bias corrected sums of least squares residuals. Conditional symmetry model probabilities within user-selected model sets [2] can also be calculated on the basis of g-AICs and are particularly useful in cases of high levels of generalized noise in conjunction with Fedorov-type pseudo-symmetries so that it becomes visually impossible to distinguish between real symmetries and pseudo-symmetries. The information theory based approach delivers only probabilistic crystallographic (or non-crystallographic) symmetry classifications as it is fundamentally unsound to assign abstract mathematical concepts such as a single 2D Bravais lattice type, a crystallographic (or non-crystallographic) 2D Laue class, and plane symmetry group with 100 % certainty to a real-
world image of a crystal (or quasicrystals). It makes, on the other hand, a lot of sense to report as result of a real-world measurement of a symmetry in an image not only the probability of the identification of the highest symmetric group/class present, but also to provide the corresponding probabilities of several of its subgroups/subclasses.


Extract Domain wall vibration modes from symmetry adapted Landau model

Peng Chen¹, Louis Ponet¹², Keji Lai³, and Sergey Artyukhin¹

¹Quantum Materials Theory, Istituto Italiano di Tecnologia,16163 Genova, Italy.
²Scuola Normale Superiore di Pisa, 56126 Pisa, Italy
³Department of Physics, University of Texas at Austin, Austin, TX 78712, USA.
peng.chen@iit.it

Scanning microwave impedance microscopy (SMIM) is emerging as a powerful probe of vibrations at the nanoscale. The radio-frequency dielectric loss due to the vibration of ferroelectric domain walls (DWs) has recently been discovered. Domain wall sliding modes were understood to be activated when the external AC field during a half-cycle favors one domain over the other. A recent observation of a signal from nominally silent 71° domain walls in BiFeO₃ (BFO) challenges this picture, emphasizing the need for better understanding of SMIM signal, even when the field of the tip favors neither domain across the wall. SIM signal in the puzzling case of BFO domain walls is simulated using symmetry adapted Ginzburg-Landau theory and finite element method. The domain wall-localized modes hidden among the bulk phonons are brought to light, seen as a handle-like branch, connecting the acoustic phonons to the optical modes. This approach shows how realistic SMIM signal can be obtained from phase field-like simulation and how DW-localized modes may be identified and excited in possible domain wall-based devices.

Figure 1. (a,b) The phonon spectral function for polar modes in BFO with R71 DW. The intense bands are the polar modes. The faint stripe at low energy, merging with the phonon band away from the zone center corresponds to the DW sliding modes. The spectral weight extends to k~2λ in the direction, perpendicular to the wall, as seen in panel (b). (c) The simulated SIM loss signal across R71 DW I(r,ω). Peak at the DW and a signature from the long-range strain profile are seen at the sliding mode frequency. The notable asymmetry in the polarization δP₃ profile for the DW sliding mode, that leads to the excitation of this mode by the vertical electric field is shown below; (d) The Spectral function for both polar and acoustic phonons along k|| direction (a cross section plot of (a) and (b) through Γ point). (e,f,g) Real-space polarization profile δP₂ of the low frequency DW sliding modes extracted from Landau model in the upper panels, along with schematic illustrations of corresponding DW vibrations in the lower panels. The initial position of the DW is marked with white dashed lines. (h,i) The same plots as (e,f,g) but presenting DW breathing modes. The labels 1~5 in (e,f,g,h,i) are used to indicate the DW localised modes in the spectral function.
Elaboration and a comparative spectroscopic and structural study of two new polymorphs of Schiff bases compounds
Soumeya MAZA1, Aouatef CHEROUANA1, Slimane DAHAOUI2, El-Eulmi BENDEIF2, Sébastien Pillet2, Pierrick Durand2, Dominik Schaniel2
1Université des frères Mentouri, URCHEMS, Constantine1, Algérie, 2 Université de Lorraine, CRM2, CNRS, Nancy, France
email: maza.soumeya@gmail.com

Abstract. A polymorph according to McCrone [1] “is a solid crystalline phase of a given compound resulting from the possibility of at least two different arrangements of the molecules of that compound in the solid state.” Although polymorphic compounds have the same chemical composition, they present different structures, leading to considerable variation in their physicochemical (density, hardness, solubility, colour, etc) [2], optical and electrical properties, such as diamond and graphite. Latterly, it has been proved that there are many conventional methods for controlling polymorphism based on a systematic exploration of all possible crystallization conditions, such as solvent or temperature variation in Schiff bases compounds [3]. The compounds we were interested in were derivatives imines from 3-amino 1,2,4-triazole and 4-bromobenzaldehyde.

We will present in this contribution, a comparative study of two polymorphs of Schiff bases compounds. The condensation reaction of 3-amino-1,2,4-triazole with 4-bromobenzaldehyde in ethanol in a small variation condition of synthesis, led to two polymorphs crystallizing in two different space groups: \( P_{na21} \) for polymorph (I) with volume \( 931.09(3) \) Å\(^3\) and \( P_{2_1}/n \) for polymorph (II) with volume \( 921.41(4) \) Å\(^3\). The two polymorphs were characterised by infrared and UV-Vis spectroscopy as well as by single crystal X-ray diffraction studies. The structural analysis shows that the main difference between the two polymorphs was observed at the angle between the phenyl and triazole rings that is 3.86° for the first one and 21.08° for the second polymorph. Furthermore, the molecular packing of the orthorhombic polymorph contains more interesting interactions, which seems to be a favourable factor for more efficient charge transfer within the crystal.

Fig1. Intermolecular hydrogen bonds occurring in compounds: (a) Polymorph I (b) Polymorph II

Synthesis, Crystal Structure, Characterisation, TD-DFT Calculation, Hirshfeld Surface Analysis and Biological Properties of New Coordination Polymer Catena-[(μ2-4,4'-sulfonyldianiline k2N:N')-aqua-(μ2-nitrato-k2O,O') (di nitrato-k2O,O') cadmium]

Amani Hind Benahsene1, Rokaya Henchiri2,3, Samia Zaou4, Nasreddine Ennaceur2,3, Lamia Bendjeddou1

amani.benahsene@hotmail.com

1Unité de Recherche Chimie de l’Environnement et Moléculaire, Structurale ‘CHEMS’, Faculté des Sciences Exactes, Campus Chaabet Ersas, Université Frères Mentouri Constantine 1, 25000 Constantine, Algeria.
2 Laboratory of Materials, Energy and Environment UR 14/ES 26 University of Gafsa, 2100 Gafsa, Tunisia.
3 Laboratory of Quantum and Molecular Photonics, Institut d’Alembert, École normale supérieure Paris-Saclay, 94230 Cachan, France.
4Laboratoire d’Electrochimie des Matériaux Moléculaires et des Complexes Université Sétif 1, Algérie

The coordination chemistry of cadmium in both biological and non-biological areas and specially, has attracted the interest of many researchers [1]. Polymeric coordination networks of Cd are known for their unique chemical physical and biological properties and their potential applications. Inspired by the above-mentioned points, we synthesized a new coordination polymer: Catena-[(μ2-4,4'-sulfonyldianiline k2N:N')-aqua-(μ2-nitrato-k2O,O') (dinitrato-k2O,O') cadmium](I) that crystallises in the monoclinic system. Compound (1) is a 2D polymer, asymmetric unit is constituted by a Cd ion coordinated to, two DDS ligand, two nitrate anion and one water molecule, the Cd center is located in a distorted pentagonal bipyramid. Biological properties of compound (1) and DDS ligand was investigated, the compounds were screened for Gram-positive bacteria and Gram-negative bacteria by the disk diffusion method. DMSO was used as a negative control. The disk diffusion method allowed us to highlight the antibacterial power of the products tested on six bacteria; negative gram: Escherichia coli, salmonella.typhi and positive gram: s. areus and Bacillus.ser (Table.1). TD-DFT calculation was performed in aim to corroborate the result of the biological properties.

![Figure 1. Molecular structure of compound (I)](image)

<table>
<thead>
<tr>
<th>Gram negative</th>
<th>Gram positive</th>
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<tbody>
<tr>
<td></td>
<td>Escherichia coli</td>
</tr>
<tr>
<td>Concentration (mg/ml)</td>
<td>40</td>
</tr>
<tr>
<td>DDS</td>
<td>-</td>
</tr>
<tr>
<td>Compound (1)</td>
<td>16</td>
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</tbody>
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Table 1: Diameters of the inhibition area (mm) of DDS and compound (1)

Abstract for summer school on Mathematical Crystallography

Limitations for fitting pseudo-Voigt function with an experimentally observed profile

Prabal Dasgupta and Worku Godano

School of Material Science & Engineering

Jimma University

Ethiopia

Sample related X-ray diffraction profiles are often fitted with a pseudo-Voigt function, which is a linear combination of Cauchy and Gaussian function, particularly in case of size-strain analysis. This work theoretically proves that the Cauchy content $\eta$ must be greater than 0.328 else no meaningful result in terms of crystallite size could be extracted from such a pseudo-Voigt profile. Cauchy content values ($\eta$) published by several authors were studied. It was found that their reported $\eta$ values agree with the present theory.
Lanthanide-transition metals molecular materials: Synthesis and Crystal structure.

Mamoudou Diallo†‡*, Nicolas Claiser‡, Claude Lecomte‡, Magatte Camara†, Mohamed Souhassou‡.

† LCPM—Groupe ‘Matériaux Inorganiques: Chimie Douce et Cristalloigraphie’, Université Assane Seck de Ziguinchor, BP 523 Ziguinchor, Sénégal
‡ Laboratoire Cristallographie, Résonance Magnétique et Modélisations, CRM2, UMR 7036, Institut Jean Barriol, Université de Lorraine et CNRS, BP70239, F54506 Vandœuvre-lès-Nancy France

*Correspondence author: mamoudou777@hotmail.com

The knowledge of the molecular materials structures combined with chemical crystallography concepts has always helped the chemist to understand the solid formation from different entities and consequently stirred his imagination for the construction of new varying combinations. However, the growth of a pure, well-shaped and sufficient size single crystal remains a challenge. The study of materials with structures consisting of metal centers that are linked into extended networks by bridging organic ligands is an important and growing area of modern chemistry \[1\]. Our work consists in synthesizing through slow diffusion in gel media \[2\] new tridimensional heterometallic molecular materials difficult, if not impossible, to obtain by conventional methods. A new family of isostructural compounds crystallizing in the triclinic system (space group P-1) has been obtained. The structure is composed of dinuclear chains link together by oxalate ligands. The three-dimensional network is ensured by hydrogen bonds O-H---O of water molecules assisted by π-π stacking interactions \[3\]. A concern underlying the chemical interest of these coordination complexes will be the search for interesting physical properties, especially magnetic, that could lead to potential applications.

Keywords: Lanthanides; Crystal growth; Characterization; Neodymium – Copper mixed compound molecular materials.

Figure1: ladder-like structure of the Nd-Cu complex in the (\(\tilde{b}, \tilde{c}\)) plane (100K)

[1] Chem. Rev., 2012, 112(2) is dedicated to this type of compound.
X-ray diffraction characterization of an intermetallic metastable phase 
Al₄Cu₉ phase in a hybrid joining of friction stir weld.

Neetesh Soni¹, Prof. Ambrish Singh¹, and Prof. Lin Yuanhua²
ntsoni7@gmail.com; +86 18380322160
School of Materials Science and Engineering, Southwest Petroleum University, Chengdu, Sichuan 610500, China.

Abstract
The intermetallic phases identification and confirmation of formation during the fabrication of hybrid joint from friction stir welding process. The X-ray diffraction analysis and generation of peaks indication the formation of intermetallic by the reference of the XRD data. The phases analysis confirmation from the using the software of HighScoreplus for XRD data analysis. It is also found that the relevant other intermetallic phase such as Al₂Cu, Al₅Cu₀-θ, ε₁-Al₅Cu₃, and Al₄Cu₉ formed during the fabrication time. The results concluded the γ₁- Al₄Cu₉ phase in the space group of P43m with cubic structure the lattice parameters a= 0.87068nm formed in brittle in nature the hardest phase of the hybrid joint of Al-Cu.

Key Words : XRD; Hybrid joint; Intermetallic; space group