International Union of Crystallography

Commission on Mathematical and Theoretical Crystallography

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Program and Abstracts

Abstracts and Outlines of Lectures

Geometry of Periodic Networks and Crystal Chemistry

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Outline

A. Introduction to graph theory
   1. cycles, sums, rings, strong rungs
   2. trees, cyclomatic number
   3. planar graphs
   4. polyhedra as graphs

B. Periodic graphs and nets
   1. crystal structures as nets
   2. embeddability and sphere packings
   3. quotient graphs
   4. minimal nets
   5. regular, semiregular nets
   6. point and vertex symbols

C. Periodic tilings and nets
   1. natural tilings of nets
   2. signatures
   3. duals
   4. self-dual tilings and their nets
   5. transitivity

D. The RCSR database
   1. symbols for nets
   2. searching the RCSR database

E. Deconstructing crystal structures
   1. MOFs, COFs, ZIFs and coordination polymers
   2. zeolites
   3. structure building units and points of extension

Coincidence Site Lattices

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Abstract

Given a lattice Γ, one may ask for which isometries R the subset $\Gamma \cap R\Gamma$ is a sublattice of full rank. If it is a sublattice of full rank, we call it a coincidence site lattice (CSL). In crystallography, CSLs are an important tool for the analysis of grain boundaries. Thus they have

been studied intensively for several decades, mainly in dimensions ≤ 3. More recently also CSLs in higher dimensions and more generally, coincidences of $\mathbb{Z}$-modules have been investigated.

We will start our talk with a detailed introduction into the basic mathematical notions of CSLs and CSMs. We present the most important techniques of number theory that have been used to solve the coincidence problem for lattices and modules in dimensions ≤ 4 and give an overview of what is known so far. Furthermore we will discuss connections to related topics, including similar sublattices and colourings. In addition, we will have a look on several generalizations of the standard theory, including multiple coincidences, coincidences of shifted lattices, and multilattices.

Color Symmetry

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Abstract

We give an informal introduction to the basic ideas in the study of colored symmetrical patterns and color symmetry. We start with colorings of some finite sets of points and explore the concepts further with colorings of some three-dimensional objects and some infinite periodic patterns. Throughout, we treat a coloring as a partition of the set of objects that are assigned colors.

Introduction to the Crystallography of Twins

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Abstract

A twin is an oriented association of crystals (individuals, domains) of the same phase. They can form when an oriented pressure is applied to a crystal (mechanical twins), following a phase transition (transformation twins), or during crystal growth. In the latter case, twinning can be considered the result of a fault during the growth.

The probability of the occurrence of a growth twin is related to the structural continuity across the interface. To date, there is no general theory capable of giving the *necessary and sufficient* conditions for the formation of a growth twin. The reticular theory, which exploits the existence of a common sublattice in terms of the twin index and obliquity, gives in most cases the *necessary* conditions. More complex cases are explained by the theory of *hybrid twins*, which is the latest extension of the reticular theory. Both the classical reticular theory and the theory of hybrid twins will be presented, with practicals to compute the twin index, the obliquity, and the unit cell of the twin lattice. The analysis of hybrid twins through the software *Geminography* will also be introduced.

A more general, structural theory, capable of finding both the necessary and the sufficient conditions, is currently under development. The general ideas of this project will also be presented, if time allows.

Construction of Self-Affine Tilings and their Spectral Properties

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Abstract

We shall review several known methods to construct self-affine tilings, whose dual Delone sets give models of quasi-crystal structure. When the Delone set has Meyer property, we can decide whether the tiling dynamics is pure discrete or not by an algorithm. (This is a joint work with J.Y. Lee.)

Surfaces and Nets

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Outline

A. Surface topology

1. Euler-(Poincaré) characteristic, χ
2. Euler's theorem for polyhedra
3. cap and pants construction of multi-handled polyhedra
4. holes in surfaces: χ reduced by 1 for each hole
5. surface genus: $\chi = 2(1-g)$, $\chi = 1-g$
6. Global Gauss-Bonnet Theorem and Gaussian curvature: $\iint K da = 2\pi\chi$
7. orientable (nice) vs. non-orientable (nasty) surfaces
8. simply vs. multiply-connected surfaces

B. Orbifolds and topology of symmetrical patterns

1. 2D isometries and *orbifolds*
   - *Conway symbols*
   - *Orbifold cost* = Ξ(orbifold)
2. orbifolds of planar tilings
   - 2D mirrors, rotations, glides, and translations
3. orbifolds of convex polyhedra via projection onto $\mathbb{S}^2$
   - $\Xi > 0$; point groups as elliptic orbifolds
4. orbifolds of various toroidal polyhedra: universal covers in $\mathbb{E}^2$
   - $\Xi = 0$; 2D wallpaper groups as euclidean orbifolds

C. From 2D to 3D structures via $\mathbb{H}^2$

1. models of $\mathbb{H}^2$
2. $\Xi < 0$; orbifolds in $\mathbb{H}^2$
3. orbifold classes: C H S P A M T K
4. Ξ and area of asymmetric domain in $\mathbb{H}^2$
5. ranking of hyperbolic isometries
6. "Sponge groups": hyperbolic orbifolds that are commensurate with $\mathbb{E}^3$

7. the covering map from $\mathbb{H}^2$ to TPMS
8. *PGD*-surfaces as quasi-homogeneous 2D embeddings
9. *PGD*-surface subgroups: from $*246$ to $\circ\circ\circ$
10. *H*, *CLP*-surface subgroups

D. Building 3D nets: `epinet.anu.edu.au`
1. "H tilings"
2. "h-nets"
3. "U tilings"
4. "s-nets" via barycentric embeddings
5. navigating `epinet`
6. future growth of `epinet`

Computing (with) Affine Crystallographic Groups

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Abstract

GAP (`www.gap-system.org`) is a computer algebra system for the computation in groups and various other algebraic structures. It provides a wealth of different group theoretic algorithms for all kinds of groups. Affine crystallographic groups are not supported out of the box, however. As these groups are not finite in general, they require special algorithms for most computations. Such algorithms have been implemented in extension packages, and shall be discussed in these lectures.

After giving an overview on the different types of crystallographic groups and their equivalence concepts, we describe in detail the algorithms which enable GAP to perform essentially the same computations as with any other (finite) group. In addition, a few further important algorithms for space groups are discussed, among them the computation of representatives of all space group types for a given point group, the computation of maximal subgroups of a space group with a given index, and the classification of points in Euclidean space according to their stabilizer in a space group (determination of Wyckoff positions). A number of applications of these algorithms are given as well.

Topological Crystallography

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Abstract

This is an expository lecture on modern crystallography based on *discrete geometric analysis*, a hybrid field of several traditional disciplines: graph theory, geometry, theory of discrete groups, and probability, which has been developed in the last decade. The mathematical part

relying on algebraic topology is fairly elementary, but may be still worthwhile for crystallographers who want to learn how mathematics is effectively used in the practical science. A brief history of crystallography is also explained.

Translational Tilings by a Polytope, with Multiplicity

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Abstract

We study the problem of covering $\mathbb{R}^d$ by overlapping translates of a convex body P, such that almost every point of $\mathbb{R}^d$ is covered exactly k times. Such a covering of Euclidean space by translations is called a k-tiling. The investigation of simple tilings by translations (which we call 1-tilings in this context) began with the work of Fedorov and Minkowski, and was later extended by Venkov and McMullen to give a complete characterization of all convex objects that 1-tile $\mathbb{R}^d$.

By contrast, for $k \geq 2$, the collection of convex objects that k-tile is much wider than the collection of objects that 1-tile, and there is currently no known analogous characterization for the convex objects that k-tile. Here we first give the necessary conditions for convex bodies that k-tile, by proving that if a convex body (necessarily a polytope) k-tiles $\mathbb{R}^d$ by translations, then it is centrally symmetric, and its facets are also centrally symmetric. These are the analogues of Minkowski's conditions for 1-tiling polytopes, but it turns out that very new methods are necessary for the development of the theory. In the case that P has rational vertices, we also prove that the converse is true; that is, if P is a rational polytope, is centrally symmetric, and has centrally symmetric facets, then P must k-tile $\mathbb{R}^d$ for some positive integer k.

Abstracts of Poster Presentations

Generating Views of Folded Crystallographic Flat Origami based on their Numerical Representations

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Abstract

Having numerical representations of various objects under study allows us to use computer technology to simulate various operations on the objects under study. This offers advantages when the operations on the actual objects are too difficult or take too long to do. In this poster presentation we show how the result of folding crystallographic flat origami can be predicted by software based on numerical representations of the crease pattern on the (unfolded) origami pattern. The prediction relies on the software having access to a database of small images showing how small portions of the pattern would look when folded. The numerical representation developed allows these images to be named systematically so that elements from the numerical representation of any crease pattern can be used to index into the database of images and create mosaics of these small images. This method eliminates the need to spend time to actually fold the crease pattern.

Constructible Polynomials, Crystal Structures and Graph Reconstruction

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Abstract

Given a simple graph structure G of order n, we define its discrete degree sequence polynomial representation as $f_G(v) = \sum_{i=1}^{k} a_i v^i$, where a_i is the number of vertices of G of degree i. Let p be a fixed prime number. A polynomial $f \in \mathbb{Z}_p[v]$ is said to be constructible if there exists a simple graph structure G such that $f(v) = f_G(v)$.

In this paper, we established some properties of the sequence $\langle a_i \rangle_{i=1}^{k}$ for the polynomial $f(v) = \sum_{i=1}^{n} a_i v^i$ to be constructible. In addition, for each $k \in \mathbb{N}$, we characterized those

polynomials in $\mathbb{Z}_p[v]$ of degree k which are constructible. More interestingly, we have shown that if $f, g \in \mathbb{Z}_p[v]$ are constructible and $\alpha, \beta \in \mathbb{Z}_p$ then $\alpha f + \beta g$ is also constructible.

On the other hand, suppose that $f_G \in \mathbb{Z}_p[v]$ is a polynomial representation of a graph structure G. Then the set of all valid reconstructions of f_G, denoted by $\mathcal{R}(f_G)$, is the set of all graphs H satisfying $f_H \equiv f_G$. Here, we established necessary and sufficient conditions such that we can fully recover the original graph structure G.

Finally, we applied the above results in studying crystal structures via polynomial representations.

Where are all the Vanadium MOFs?

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Abstract

Zinc and copper are favourite choices as metals in metal-organic frameworks (MOFs), however, often they are unstable in water. MOFs assembled from metals with higher valences (Cr^{3+}, Al^{3+}, Zr^{4+} etc.), on the other hand, tend to have greater chemical stability. The fact that vanadium can adopt a range of oxidation states, forms a variety of different clusters and is rarely used for MOF synthesis has led us to pursue the synthesis of new vanadium-containing MOFs. Here, we present two new vanadium MOFs that are isostructural to the frameworks of MIL-88 (or MOF-235) and MIL-101, which we call MIL-88(V) and MIL-101(V), respectively.

A Geometric and Numerical Analysis of Nanostructures during Chemical Synthesis in Experiments Conducted in the Research Center for the Natural and Applied Sciences

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Abstract

The fast emerging developments in nanoscience and nanotechnology had led to investigative studies of different aspects of nanocrystals. The crucial role for using nanocrystals as building blocks for various applications caught the attention of modern scientists and researchers. In this paper, we reviewed some recent studies related to nanoparticles conducted in the University of Santo Tomas. The characteristic features of crystal surfaces revealed in the observations during chemical synthesis were correlated to the structure symmetry of the medium under controlled conditions.

Sublattices of the Square Lattice and Coincidence Rotations

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Abstract

An algorithm is presented in finding the intersection of sublattices of the square lattice $\mathbb{Z}^2$ using a 2×2 matrix representation of the form

$$\begin{bmatrix} a & b \\ 0 & c \end{bmatrix} \quad a, b, c \in \mathbb{Z},\ 0 \leq b < a,\ 0 < c,$$

where $[a\ \ 0]^T$ and $[b\ \ c]^T$ are two linearly independent translations which generate a sublattice of $\mathbb{Z}^2$. By considering the restrictions on a, b, and c, we can identify two linearly independent translations which define the intersection.

Moreover, employing the same matrix representation in canonical form and by identifying the square lattice with the ring of Gaussian integers, we find the coincidence site lattice (CSL) corresponding to a coincidence rotation $R \in SO(2, \mathbb{Q})$. Using the well known relation between coincidence rotations and primitive Pythagorean triples, we derive a formula for finding the matrix representation of the resulting CSL.

Chirally Perfect Colorings of Regular Tilings with a Singular Center

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Abstract

In this research, we use perfect colorings of the Euclidean (4^4) tiling to obtain perfect colorings of a tiling with a singular center. The (4^4) tiling can be distorted into a tiling with a singular center using a conformal map. We use the conformal map to determine the conditions so that a chirally perfect coloring of the (4^4) tiling is also a chirally perfect coloring of the tiling with singularity after deformation.

Semi-Perfect Colorings of Hyperbolic Tilings

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Abstract

In this work we discuss conditions that facilitate the determination of semi-perfect colorings of tilings. These conditions are applicable to a class of tilings where the stabilizer of a tile in the symmetry group G of the uncolored tiling is non-trivial. We illustrate the results using colored tilings that emerge from the hyperbolic semi-regular tiling $8 \cdot 10 \cdot 16$.

A coloring of a tiling is semi-perfect if the group of symmetries that induce a permutation of the colors is a subgroup of index 2 in G.

Color Groups Arising From Index 5 And 6 Subgroups Of Symmetry Groups

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Abstract

Coloring a symmetric object reveals properties of the object which are not easily recognizable. In the study of color symmetry, one of the main goals is to classify colorings through their color groups, which is the subgroup of the symmetry group which induces a permutation of colors. In this paper, we look for methods of coloring a symmetric object which will give a color group of index 5 or 6 in the object's symmetry group. To get a color group of index 5, we take an index-5 subgroup H of the symmetry group G of the object, and proceed with a coloring which will give a color group H^* such that $H \leq H^* \leq G$. Since $[G : H] = 5$ which is prime, then H^* is either H or G. We then look for necessary and sufficient conditions for the equality of H^* and G. If these conditions are not satisfied, then $H^* = H$ and we have a coloring with color group of index 5 in G. On the other hand, to get a color group of index 6, we take an index-6 subgroup H of G, and similarly proceed with a coloring which will give a color group H^* such that $H \leq H^* \leq G$. Afterwards, we look for ways to determine whether H^* is G, H, or some intermediate subgroup between H and G.

Modeling Structural Analogues of Carbon Nanotubes Using Color Symmetry

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Abstract

Carbon nanotubes are allotropes of carbon obtained by wrapping up a graphene sheet with a hexagonal lattice along a given vector into an infinite monoperiodic cylindrical tube. This paper discusses the process to arrive at colorings of single wall carbon nanotubes that can be used to describe their structural analogues. To illustrate the applicability of the method, we derive the colorings which represent the rolled-up versions of the ten theoretically most stable carbon-boron nitride ternary graphite-like monolayers.

Production of Ceramics Nanopowder by a Sol-Gel Method

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Abstract

This project is focused on the production of ceramics nanopowder by a sol-gel method. Working on the area of nanopowder has now become the priority in most of advanced material laboratories world-wide. Nanopowders enable the production of new products and continue to replace conventional powders in many applications because of their unique properties, such as higher surface area and improved performance of the resulting end products. Base on the trends, this research has been carried out in order to gain further insight on the process of producing nanoparticles of ceramics powder. These nanoceramics will capture a significant marketplace that requires higher performance of materials as well as devices. For instance, ceramics based on zirconate or/and cerate are well known as ionics and/or electronics conductors in hydrogen and/or water vapor atmospheres at high temperatures. Their potential to be used as a solid electrolyte in advanced electrochemical devices such as fuel-cell, steam electrolyzer, and hydrogen sensor has been proven widely. The commonly used method to prepare the compound is via solid-state reaction (SSR). However, the milling and grinding processes introduce contaminates from abrasive materials. The mechanically-ground mixture also needs prolonged calcination steps to form a desired single-phase compound, thus, promote crystalline growth which is undesirable in the fabrication of dense fine-grained ceramics. Recently, a number of wet chemical methods (WCMs) such as sol-gel have been carried out in many scientific laboratories. Sol-gel method can produce powders with high degree of crystallinity and homogeneous nanopowder because its reaction forms metal-organics complexes networks that leads to atomic or molecular scale mixing. Thus, it allows for reduction in calcination temperature and time due to the low temperature ceramics processing.

Color Groups Associated with the Three-Dimensional Crystallographic Lattices and the Black and White Groups

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Abstract

The theory of color groups and color-fixing groups of colored lattices gives insight into the study of the black and white groups and in general to the study of spin groups.

In this work we characterize the colorings of a three-dimensional crystallographic lattice Λ arising from a sublattice L with respect to the color group H consisting of symmetries of the lattice that permute the colors and the color-fixing group K of the colored lattice. We consider the case of the primitive cubic, tetragonal, orthorhombic, and monoclinic lattices. We then relate these results to the study of black and white groups and spin translation groups.

An Application of Euclidean Designs to Structural Analysis for Rhodium Clusters

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Abstract

The notion of Euclidean design was introduced by Neumaier-Seidel (1989) as a good configuration of finite points in Euclidean space. In this poster, Euclidean design is applied to structural analysis for rhodium clusters and we show a hidden mechanism in the growth of cubic Rh clusters composed of 8 to 12 atoms, that is, from a cube to two connected cubes. In the usual first principles calculation, initial structures have been given rather ad-hoc way, but the method proposed in this poster is systematic and theoretical without limitation of atom numbers. This is the first application of Euclidean design to atomic cluster science. (This is a joint work with Yoshiyuki Kawazoe, Motoko Kotani, and Yunye Liang.)

Investigation of the Effects of Cu Vacancies on its Simulated X-ray Diffraction Pattern

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Abstract

X-ray Diffraction (XRD) has been a common analysis technique for identifying the crystallinity of a sample. The XRD patterns are affected when inconsistencies in the crystal, such as vacancies, appear. For this paper we chose, to investigate Cu because of its simple crystal structure, and it has also been thoroughly investigated. By modeling vacancies in a group of unit cells in the Cu crystal, we were able to simulate the XRD pattern with vacancies and we compared it to the ideal XRD pattern. From the comparison between the two patterns, we were able to conclude that by adding defects in the crystal, the intensities of the smaller peaks would increase, and slight peak broadening occurs using this model.