Soft Packings, Nested Clusters, and Condensed Matter
Packings mous, amas imbriqués et matière condensée
(Org: **Karoly Bezdek** (University of Calgary), **Nikolai Dolbilin** (Steklov Mathematical Institute), **Egon Schulte** (Northeastern Universit) and/et **Marjorie Senechal** (Smith College))

KAROLY BEZDEK, University of Calgary, Dept. of Math. and Stats., Calgary, Canada
On totally separable packings of soft balls

A packing of balls in Euclidean d-space is said to be totally separable if any two packing elements can be separated by a hyperplane disjoint from the interior of every packing element. This notion was introduced by G. Fejes Toth and L. Fejes Toth (1973) and has attracted significant attention. In this talk first, I prove that the convex hull of N unit balls forming a totally separable packing in Euclidean d-space for d=2, 3 is minimal if and only if the convex hull of the centers is a line segment of length 2(N-1). Second, I extend this result to totally separable packings of N congruent soft balls in Euclidean d-space for d=2, 3.

MIKHAIL BOUNIAEV, The University of Texas Rio Grande Valley
On the Concept of t-bonded Sets

One of the properties of the (r, R)-systems, or Delone sets, is that any two points of a Delone set can be connected by a broken line, with distances between two consecutive vertices bounded by 2R. This property plays an important role in proving theorems of the local theory for regular and multi-regular systems. We will show that similar results obtained for the local theory in the assumption that the set is a Delone set, could be proved for the sets we call t-bonded sets, i.e., for uniformly discrete subsets of Euclidian space, which hold a property that is a generalization of the property of the Delone sets mentioned above. Though similar results can be obtained for t-bonded sets, as far as the local theory is concerned, the class of t-bonded sets is a significant extension of the class of Delone sets as it includes all finite sets, t-bonded sets with bounded projections onto subspaces of initial Euclidian space, and other sets that are not Delone sets. The local theory for t-bonded sets deserves to be developed to describe various materials like zeolites whose atomic structure is a multi-regular "microporous" point set, or the structural type of Niobium Oxide. Results presented in the talk have been recently achieved through joint collaboration with Nikolay Dolbilin, who initially introduced the concept of the t-bonded sets in 1976 under the name of d-connected sets though it did not receive due consideration at that time.

EVAN DECORTE, McGill University
The Witsenhausen problem in dimension 3

The orthogonality graph is the graph whose vertex set is the unit sphere in $\mathbb{R}^3$, in which two vectors are joined with an edge when they are orthogonal. Witsenhausen in 1974 asked for the largest possible fraction of the sphere which can be occupied by a Lebesgue measurable independent set in the orthogonality graph, and he gave the upper bound of $1/3$. We improve this upper bound to 0.313 using an approach inspired by the Delsarte bounds for codes, combined with some combinatorial reasoning. This represents the first progress on the Witsenhausen problem in dimension 3 since the original statement of the problem. Joint work with Oleg Pikhurko.

JEAN-GUILLAUME EON, Institute of Chemistry, Federal University of Rio de Janeiro - Brazil
Topology and symmetry of modular compounds from the viewpoint of their labelled quotient graphs

The combinatorial or bond-topology of a crystal structure is defined as the respective underlying net, which can be represented by a labelled quotient graph with voltages in the translation group of the crystal structure. Thus, in principle, every topological property of crystal structures can be determined from an analysis of their labelled quotient graph. Due to the finiteness of the quotient graph, the substitution is expected to turn the analysis easier. Building-units of crystal structures can be finite or infinite, corresponding to one-, two- or even three-periodic subnets. Decomposing periodic nets into their building-units relies on graph-theoretical methods classified as surgery techniques. Instead, these operations can be performed on their labelled quotient graphs revealing directly topological relationships. Modular compounds constitute a large and important class of materials; in this case, the structure of two-periodic modules, their stacking direction and linking mode can be put into evidence on the labelled quotient graph. The maximum symmetry of a crystal structure is given by the group of automorphisms of the labelled quotient graph that are consistent with net voltages over the respective cycles. In modular compounds the maximum symmetry of the module, i.e. its layer group, can be determined directly from the quotient graph. Partial symmetry operations between non-equivalent modules are associated to automorphisms of the quotient graph that may not be consistent with net voltages over the respective cycles. These operations generate a groupoid structure. The example of the pyroxene family will be considered for illustration.

NIKOLAI EROKHOVETS, Steklov Mathematical Institute of Russian Academy of Sciences
Operations sufficient to obtain any Pogorelov polytope from barrels. Improvements for fullerenes.

A fullerene is a simple 3-polytope with all facets pentagons and hexagons. Any fullerene is a Pogorelov polytope, i.e. it can be realized in Lobachevski (hyperbolic) 3-space as a bounded right-angled polytope. A k-barrel is a simple 3-polytope with boundary glued from two patches consisting of a k-gon surrounded by pentagons. The 5-barrel is the dodecahedron. Results by T. Inoue (2008) imply that any Pogorelov polytope can be combinatorially obtained from k-barrels by a sequence of (s,k)-truncations (cutting off s consequent edges of a k-gon by a single plane), $2 \leq s \leq k-4$, and connected sums along k-gonal faces (combinatorial analog of glueing two polytopes along k-gons perpendicular to adjacent facets). We prove that any Pogorelov polytope except for k-barrels can be obtained from the 5- or 6-barrel by $(2,k)$-truncations, $k \geqslant 6$, and connected sums with 5-barrels along pentagons. In the case of fullerenes we prove a stronger result. Let $(2,k;m_1,m_2)$-truncation be a $(2,k)$-truncation that cuts off two edges intersecting an m_1-gon and an m_2-gon by vertices different from the common vertex. There is an infinite family of connected sums of 5-barrels along pentagons surrounded by pentagons called $(5,0)$-nanotubes. We prove that any fullerene except for the 5-barrel and the $(5,0)$-nanotubes can be obtained from the 6-barrel by a sequence of $(2,6;5,5)$-, $(2,6;5,6)$-, $(2,7;5,5)$-, $(2,7;5,6)$-truncations such that all intermediate polytopes are either fullerenes or Pogorelov polytopes with facets 5-, 6- and one 7-gon with the heptagon adjacent to some pentagon. This work is supported by the Russian Science Foundation under grant 14-11-00414.

ALEXEY GLAZYRIN, University of Texas Rio Grande Valley
Average degrees in sphere packings

The talk is devoted to the problem of determining the maximum possible average degree in a packing of spheres. This problem will be considered under various restrictions and, in each scenario, we will show the general approach of finding upper bounds on an average degree.

UNDINE LEOPOLD, Northeastern University
Euclidean Symmetry of Closed Surfaces Immersed in 3-Space

(Joint work with Thomas W. Tucker.) Given a finite group G of orientation-preserving Euclidean isometries and a closed surface S, an immersion $f : S \to E^3$ is in G-general position if $f(S)$ is invariant under G, points of S have disk neighborhoods whose images are in general position, and no singular points of $f(S)$ lie on an axis of rotation of G. For such an immersion, there is an induced action of G on S whose Riemann-Hurwitz equation satisfies certain natural restrictions. Riemann-Hurwitz equations fulfilling these restrictions are realized by a G-general position immersion of S in most cases. Exceptions arise, in particular, for low genus and few branch points. In this talk, we review these results and consider the more general case of G containing orientation-reversing Euclidean isometries.

OLEG MUSIN, University of Texas Rio Grande Valley
Extreme Euclidean and spherical point configurations

In this talk we consider various problems of extreme sphere packings such as the densest packing problem, Tammes' problem, the maximum contact number problem, Euclidean and spherical representation of graphs as two-distance sets and contact graphs of sphere packings.

EGON SCHULTE, Northeastern University
Highly Symmetric Complexes and Graphs in Ordinary Space

The lecture is about highly symmetric skeletal polyhedra and polygonal complexes in ordinary space, and their edge graphs (nets). These polyhedra and complexes are viewed not as solids but rather as discrete geometric edge graphs in space, equipped with additional polyhedral super-structure imposed by the faces. We discuss the present state of the ongoing program to classify these structures by symmetry, where the degree of symmetry is defined via distinguished transitivity properties of the symmetry groups. A complete classification is known for the regular and chiral polyhedra, and the regular polygonal complexes. There has also been recent progress on uniform polyhedra. Remarkable new structures were discovered using a skeletal variant of Wythoff's construction in space.

MARJORIE SENECHAL, Smith College
Icosahedral Snowflakes?

Long before the discovery of H, O, and H20, Johannes Kepler proposed, incorrectly but astutely, that hexagonal snowflakes grow by the accretion of invisible spherical particles in a densely packed array. And so the science of crystallography was born. Half a milennium later, once-thought-to-be-impossible icosahedral crystals again raised the question of growth and form, but for these crystals their relation remains murky.

Two models, decorated tilings and nested clusters, have been used to describe the arrangements of atoms in icosahedral crystals. But both models have trouble with growth. In this talk I will discuss a particular case, the Yterrbium-Cadmium icosahedral crystal and its close periodic relatives, and show how a modified cluster model may show us a way out.

This is joint work with Jean E Taylor, Erin G Teich, Pablo Damasceno, Yoav Kallus ,

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ERIN TEICH, University of Michigan
Local environments in glassy hard particle systems

Soft matter systems, in which thermal fluctuations are strong enough to drive particle rearrangements, are capable of self-assembling into a staggering variety of simple and complex crystalline structures. Often, however, no such assembly occurs, and the system remains frustratingly disordered. Here, we investigate one such family of cases, in which simple systems of hard particles of a polyhedral shape, with no interactions aside from those of excluded volume, fail to assemble. Instead, these systems exhibit glassy behavior. We examine this behavior via Monte Carlo simulation, and investigate in particular the role that local particle environment plays in inducing vitrification rather than assembly.