accepted courses, which teach how to obtain structural information and to describe crystal structures. In the presentation we demonstrate several examples from lectures and practicals.

[1] E.V. Boldyreva, *J. Appl. Cryst.* **2010**, *43*, 1172-1180.

Keywords: crystallographic teaching

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Measures of complexity

Walter Steurer, *Laboratory of Crystallography , ETH Zurich, Wolfgang-Pauli-Strasse 10, 8093 Zurich, (Switzerland).* E-mail: steurer@mat.ethz.ch

The term *complex* is frequently attributed to crystal structures with giant unit cells containing hundreds or thousands of atoms. It is commonly used in a non-defined, fuzzy way. It would be advantageous, however, to have a quantitative measure of structural complexity, to be able to compare periodic and quasiperiodic structures, for instance. Why could this be of interest? Some physical properties, which strongly depend on medium- and long-range order, could be related to complexity and used as knowledge basis for their prediction. Another interesting question is the time evolution of a structure (crystal growth) as function of its complexity. For instance, it is obvious that a crystal with a simple cubic close packed structure such as copper will have a much simpler growth mechanism than a ternary quasicrystal.

Recently, it was suggested in different context to apply the concept of *algorithmic complexity* to crystal structures, periodic and quasiperiodic ones [1]. This way of quantifying the complexity of a system is related to the minimum size of an algorithm needed for its full description. If we apply this concept to the Fibonacci sequence (FS) in the *n*D description, for instance, then we obtain the same algorithmic complexity for the quasiperiodic FS and all its periodic approximants, from the smalls to the largest one. This is somehow counterintuitive.

If we use the concept of *symbolic complexity,* we arrive at drastically different results for periodic and quasiperiodic structures. Symbolic complexity is related to the number of different structure motifs (AET) as a function of system size, which is a function of the repeat period in case of the approximants and of the system size in case of the FS. For another example, let's start from a simple periodic structure and apply a sinusoidal incommensurate modulation. This immediately increases the period of the incommensurately modulated structure (IMS) to infinity. However, the algorithmic complexity of the IMS is only slightly higher than that of the small-unit-cell periodic structure. In case of a commensurate modulation, we can continuously increase the number of atoms per supercell without changing the algorithmic complexity of the structure, while the symbolic complexity would grow with the system size to infinity.

Another kind of complexity measure is the *combinatorial complexity,* which can best account for high symmetries of structural subunits (clusters). The less probable (symmetic) a configuration is the higher is its complexity. For instance, in case of equally sized hard spheres, close sphere packings such as the *cF*4-Cu structure are more probable from different point of views than the *cP*1-Po structure. Consequently, the latter has the higher combinatorial, but lower algorithmic complexity, and both have equal symbolic complexities.

In conclusion, no single complexity concept alone is able to reflect all facets of structural complexity, to quantify what we intuitively grasp.

[1] E. Estevez-Rams, R. Gonzaléz-Férez, *Z. Kristallogr.* **2009**, *224*, 179-184.

Keywords: complexity, quasicrystal, structure

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Frustrated Order

Rémy Mosseri *Laboratoire de Physique Théorique de la Matière Condensée, CNRS/Université Pierre et Marie Curie, Paris (France).* E-mail: remy.mosseri@upmc.fr

Frustration occurs whenever a local order (atomic configuration) cannot be extended perfectly throughout the space. A paradigmatic example is that of polytetrahedral order encountered in dense packing models. In that case, a direct connection with icosahedral order is present, which makes the frustration concept useful in different contexts, like clusters, glassy materials or quasicrystals. Similar situations can be found with covalent materials and soft matter systems; in most cases, the real structure shows intricate relations between ordered regions and topological defects[1].

We shall first recall how frustration and order interfere in the general case. Then, some new results will be presented, related to dense frustrated order in confined (cylindrical) geometry, a topic which might prove interesting in the nanophysics context. Indeed, a rich phase diagram is found, with many different types of different order occurring while increasing the cylindrical radius, showing a nice competition between chiral, icosahedral, crystalline and disclinated icosahedral order.

[1] J-F-Sadoc et R. Mosseri, " *Geometrical Frustration* ", Cambridge University Press, **1999.**

Keywords: frustration, defects, nanostructures

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Local Rules and Global Order

Nikolai Dolbilin, *Steklov Mathematical Institute of Russian Academy of Sciences, Moscow(Russia).* E-mail: dolbilin@mi.ras.ru

An appropriate concept for describing an arbitrary discrete atomic structure is the *Delone set* (or an *(r,R)-system*). Structures with long-range order such as crystals involves a concept of the space group as well.

A mathematical model of an *ideal monocrystalline matter* is defined now as a Delone set which is invariant with respect to some space group. One should emphasize that under this definition the well-known periodicity of crystal in all 3 dimensions is not an additional requirement. By the celebrated Schoenflies-Bieberbach theorem, *any space group contains a translational subgroup with a finite index.*

Thus, a mathematical model of an ideal crystal uses two concepts: a Delone set (which is *of local character*) and a space group (which is *of global character*).

Since the crystallization is a process which results from mutual interaction of just nearby atoms, it is believed (L. Pauling, R. Feynmann et al) that the long-range order of atomic structures of crystals (and quasi-crystals too) comes out local rules restricting the arrangement of nearby atoms.

However, before 1970's there were no whatever rigorous results until Delone and his students initiated developing the *local theory of crystals*. The main aim of this theory was (and is) *rigorous derivation* of space group symmetry of a crystalline structure from the pair-wise identity of local arrangements around each atoms. To some extent, it is analogous to that as, in due time, it was rigorously proved that space group symmetry implies a translational symmetry.

In the talk it is supposed to expose some results on local rules for

crystals and to outline the frontier comes through between crystalline and quasi-crystalline local rules.

Keywords: delone set, local rules, long-range order

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Aperiodic structures, order and disorder, complexity and entropy

Shelomo I. Ben-Abraham,[a] Alexander Quandt,[b] Dekel Shapira,[a] *[a]Department of Physics, Ben-Gurion University of the Negev, Beer-Sheba, (Israel). [b]School of Physics, University of the Witwatersrand, Wits, (South Africa).* E-mail: benabr@bgu.ac.il

Artificial aperiodic structures have recently been the subject of extensive and intensive research, resulting in layered quasiregular heterostructures, as well as photonic and phononic metamaterials with possible applications such as optical and acoustic bandpassfilters or photonic waveguides. The Fourier spectrum of the Prouhet-Thue-Morse sequence is known to be singular continuous; yet its dynamical spectrum has a pure point part. This confronts us with experimental challenges to produce physical realizations of the structure in one, two and three dimensions, perform diffraction experiments and devise an experiment to reveal the dynamical spectrum.

We are interested in fundamental questions about determinism, order and "disorder" and their quantification. Specifically, we study multidimensional generalizations of the standard substitution sequences. Here we present and discuss some two-dimensional instances of the Prouhet-Thue-Morse and paperfolding systems. We compute their rectangle complexities; these are at most polynomial implying zero entropy. We also report a novel substitution method to produce multidimensional paperfolding structures. We suggest to concisely characterize the complexity by the exponent of its leading term. We point out that the perfectly deterministic Champernowne and Copeland-Erdős sequences have entropy ln2 exactly like fair Bernoulli. These examples clearly show that entropy, regardless of its definition, does not distinguish between deterministic and random systems. There still remain many unanswered questions.

Keywords: aperiodic, complexity, entropy

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Inhibition of SNARE-mediated membrane fusion by VARP

Ingmar B. Schäfer,[a] Geoffrey G. Hesketh,[b] Nicholas A. Bright,[b] J. Paul Luzio,[b] David J. Owen,[b] Philip R. Evans,[a] *[a]Medical Research Council Laboratory of Molecular Biology, Hills Road, Cambridge CB2 0QH, (UK). [b]Cambridge Institute for Medical Research and Department of Clinical Biochemistry, University of Cambridge, Addenbrooke's Hospital, Hills Road, Cambridge CB2 0XY, (UK). Current address: Department of Structural Cell Biology, MPI of Biochemistry, Am Klopferspitz 18, D-82152 Martinsried.* E-mail: ischaefe@biochem.mpg.de

SNAREs are the small, mainly Type II membrane proteins that provide much of the mechanical energy and specificity to vesicle: organelle and organelle:organelle fusion events. Defined combinations of 3 Q-SNAREs from one membrane and 1 R-SNARE from another interact highly specifically and selectively to form *trans*-SNARE complexes through their SNARE motifs. Such SNARE-mediated membrane fusion processes must be tightly regulated. Members of the n-Sec1/Munc18 family regulate the incorporation of Q-SNAREs into SNARE complexes. We have identified the multidomain, endosomal rab32/38 effector VARP as the first example of an R-SNARE-binding regulator of SNARE complex formation. We demonstrate that VARP co-localises with and binds to the key R-SNARE of the late endocytic pathway, VAMP7. This crucial R-SNARE is highly conserved across species, ubiquitously expressed and is involved in many membrane traffic pathways, especially in fusion events between lysosomes and other cellular membranes including endosomes and the cell's limiting membrane. We have determined the structure of the Ankyrin repeat domain of VARP in complex with the cytoplasmic portion of VAMP7. VAMP7 is bound with its N-terminal longin domain bound back onto its SNARE motif. This closed conformation of VAMP7 is stabilized by intramolecular interactions between the SNARE motif and the longin domain as well as intermolecular interactions between the two parts of VAMP7 and the Ankyrin stack of VARP. We show that the trapping of VAMP7 in this inactive conformation by VARP inhibits the ability of VAMP7 to form SNARE complexes since the SNARE motif binding back onto the longin domain is mutually exclusive with the participation of the SNARE motif in SNARE complex formation. The mode of binding of VAMP7 to VARP contrasts with that of VAMP7 bound to the endocytic trafficking coat protein Hrb. In this latter case, it is the open conformation of VAMP7 that interacts with Hrb, which is formed when VAMP7 participates in SNARE complex formation. VARP is therefore a new and important regulatory component of the membrane fusion machinery of the endocytic pathway, which can control the fusion of VAMP7-mediated late endocytic compartments containing hydrolytic enzymes with other membranes.

Keywords: cell biology, SNARE-mediated membrane fusion, regulation

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Structure of the human histamine H1 receptor with doxepin

Tatsuro Shimamura,[a,b,c] Mitsunori Shiroishi,[a,b,d] Simone Weyand,[b,ef] Hirokazu Tsujimoto,[a,b] Graeme Winter,[f] Vsevolod Katritch,[g] Ruben Abagyan,[g] Vadim Cherezov,[c] Wei Liu,[c] Gye Won Han,[c] Takuya Kobayashi,[a,b] Raymond C. Stevens,[c] So Iwata.,[a,b,e,f] *[a]Department of Cell Biology, Graduate School of Medicine, Kyoto University, Kyoto, (Japan). [b]JST, ERATO, Kyoto, (Japan). [c]Department of Molecular Biology, The Scripps Research Institute, CA, (USA).[d]Graduate School of Pharmaceutical Sciences, Kyushu University, Fukuoka, (Japan). [e]Division of Molecular Biosciences, Imperial College, London, (UK).[f]Diamond Light Source, Oxfordshire, (UK).[g]Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California, San Diego, (USA).* E-mail: t.shimamura@mfour.med.kyoto-u.ac.jp

Histamine H1 receptor (H1R) is expressed in various tissues and involved in allergic responses. The antihistamines generally act as inverse agonists for H1R and alleviate the symptoms of allergic reactions. However, the first-generation antihistamines are known to show considerable side effects such as sedation and dry mouth, because of penetration across the blood-brain barrier (BBB) and low receptor selectivity. Second-generation antihistamines are less sedating and have fewer side effects. The improved pharmacology of the second-generation zwitterionic drugs can be attributed to a new carboxylic moiety, in combination with the protonated-amine, which reduces brain permeability and improves the H1R selectivity. However, certain second-generation drugs still show cardiotoxicity because of the interaction with cardiac potassium channels.

Using *in meso* crystallization technique, we succeeded to determine the structure of H1R overexpressed in *Pichia pastoris*. For overexpression, we replaced most of the third cytoplasmic loop with T4-