layers [2], selective broadening of the reflections was observed and occurrence of stacking faults was suggested.

An expression for intensity distribution in powder diffraction from a sample containing stacking faults [3] has been modified in consideration the misfit between two-dimensional lattices of the subsystems, and applied to stacking disorder in composite crystals. The analyses have been made for neutron and X-ray powder patterns of faulted $(Ca_2CoO_3)_{0.62}CoO_2$, and X-ray powder patterns of faulted $(PbS)_{1.12}VS_2$. The experimental results have been interpreted satisfactorily on the basis of stacking disorder model.

[1] Miyazaki Y., Onoda M., Oku T., Kikuchi M., Ishii Y., Ono Y., Morii Y., Kajitani T., *J. Phys. Soc. Japan*, 2002, **71**, 491. [2] Onoda M., Kato K., Gotoh Y., Oosawa Y., *Acta. Cryst.*, 1990, **B46**, 487. [3] Onoda M., Saeki M., Kawada I., *Acta. Cryst.*, 1980, **A36**, 952.
Keywords: composite crystals, stacking faults, diffuse scattering

P.22.02.2
5-D Modeling of the Co-rich decagonal Al-Co-Ni Quasicrystal
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Even twenty years after the discovery of quasicrystals, not a single structure is known with the accuracy and reliability commonly expected for regular periodic structures [1]. One way leading towards understanding the structure of quasicrystals, is given by the examination of approximants.

The main interest of this work is to investigate the complete stability field of decagonal Al-Co-Ni by 5-D modeling, starting from the W-phase [2]. The latter is of particular interest, as it is the only known approximant in this system, containing the complete atomic cluster [3]. The focus will be on order, disorder and phase transformations of the decagonal Al-Co-Ni.

First 5-D modeling results of the Co-rich decagonal phase will be discussed. Via embedding the W-phase, models of the decagonal phase are rendered and phasonic modes are being applied.

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Keywords: quasicrystal, 5-D modeling, W-phase

P.22.02.3
Modulated Structure of $[FeCl(DMPE)_2(NCC_6H_4NO_2)][PF_6]$ a Material for Use in NLO
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It is well known the recent interest in the nonlinear optical (NLO) properties of organometallic complexes [1,2]. Most efficient NLO-active complexes have a dipolar composition, with an electron-donating group linked by a π-conjugated bridge to an electron-accepting group. Our studies on complexes with this composition have been focused on metal σ-nitriles, for which the second-order NLO responses have been determined [3,4]. Since, it is also of interest to assess the importance of co-ligands in the donor metal coordination sphere, our attention has turned to an alternative coordinated Fe(II) system, namely trans-chloro(diphosphine)iron nitriles. In the solid state our main interest is to align the molecules and avoid centrosymmetric space groups. When trying to solve the structure of the title complex we had several difficulties and the structure proved to be modulated. Refinements are being done using JANA and final results will be presented in this work.

[1] Whittall I.R., et al, *Adv. Organomet. Chem.*,1999, **43**, 349. [2] Goovaerts E., et al, *Handbook of Advanced Electronic and Photonic Materials*, Ed. H.S. Nalwa, 2001, **9**, Ch. 3, 127. [3] Wenseleers W. et al, *J. Mater.Chem.*, 1998, **8**, 925. [4] Garcia M.H., Robalo M.P., Teixeira A.P.S., Piedade M.F.M., Duarte M.T., Dias A.R., *J. Organomet. Chem.*, 2001, **632**, 145.

Keywords: NLO, organometallic compound, modulated structure

P.22.02.4
Dislocation Dynamics in a Dodecagonal Quasiperiodic System
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We have developed a set of numerical tools for the quantitative analysis of defect dynamics in quasiperiodic structures, with the intention of addressing some of the open questions regarding the dynamics of dislocations in quasicrystals. We are applying these tools to study dislocation motion in the dynamical equation of Lifshitz and Petrich [1] whose steady state solutions are quasiperiodic, exhibiting dodecagonal symmetry.

Here we demonstrate - by showing real-time computer simulations - our ability to inject an arbitrary set of dislocations, parameterized by the homotopy group of the D-torus, and quantitatively follow the positions of these dislocations as the equation evolves in real time. We measure and analyze the dislocation velocity as a function of applied stress and shear, as well as the phonon and phason strains that accompany this motion as the system evolves in time. These results display intriguing differences with respect to the behavior of dislocations in periodic solutions of the dynamical equation.

[1] Lifshitz R., Petrich D.M., *Phys. Rev. Lett.*, 1997, **79**, 1261.
Keywords: dislocation dynamics, quasicrystals, computer simulation

P.22.03.1
Ab initio Simulations on the W-phase of the Al-Co-Ni System
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The W-phase [1] is the highest stable approximant of the decagonal quasicrystal known in the system Al-Co-Ni. Its structure contains the so-called "20 Å-cluster", which is a characteristic building unit of decagonal Al-Co-Ni.

The Co/Ni ratio determines which modification of decagonal $Al_{72}Co_{28-x}Ni_x$ ($8 \leq x \leq 20$) is formed. Therefore, we studied the influence of the Co/Ni ratio on the structure of the W-phase, starting from binary compositions Al-Co and Al-Ni with idealized positions. From these results a realistic ternary model was derived.

The structure models were optimized using the VASP code [2,3]. Our calculations are based on the generalized gradient approximation and utilized PAW potentials [4] supplied with VASP. The band structure, electron density districulation and electron localization function were calculated.

These calculations help to get insight into the factors governing formation and stability of this kind of complex intermetallic alloy. They also corroborate the results of the single-crystal X-ray structure analysis, from which a significantly distorted and disordered structure model was obtained.

[1] Sugiyama K., Nishimura S., Hiraga K., *Jour. Alloys Comp.*, 2002, 342. [2] Kresse G., Furthmüller J., *Comput. Mat. Sci.*, 1996, 6. [3] Kresse G., Furthmüller J., *Phys. Rev. B*, 1996, 54. [4] Kresse G., Joubert J., *Phys. Rev. B*, 1999, 59.
Keywords: quasicrystals, ab initio calculations, clusters

P.22.03.2
Interaction and Phase Transitions in a Potototype Self-assemblied Supramolecular Aperiodic Crystal
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This contribution reports on very new structural and physical

properties in self assemblied supramolecular materials, considering host-guest intergrowth crystals. A host urea molecule forms hydrogen-bonded hexagonal channels of 5.5 Å diameter in which long guest chains are densely packed in a one-dimensional arrangement [1]. This simple paradigm crystal offers a unique opportunity to address at a fundamental level the question of the nature and the roles of interactions in self-organized architectures [2]. Original physical properties in these host-guest materials are related to their aperiodic feature which, unambiguously, appears in their superspace diffraction pattern [3,4]. Here, we will present a first evidence of a superspace symmetry breaking involving only the internal variable of the superspace in these materials. These observations force a total reconsideration of the interactions in these self-organized compounds.

[1] Hollingsworth M.D., Harris K.D.M., *Comprehensive Supramolecular Chemistry*, Pergamon, New York, 1996, **6**, 177. [2] Bourgeois L., Toudic B., Ecolivet C., Ameline J.C., Bourges P., Breczewski T., Guillaume F., *Phys. Rev. Lett.*, 2004, **93(2)**, 26101. [3] Lefort R., Etrillard J., Toudic B., Guillaume F., Breczewski T., Bourges P., *Phys. Rev. Lett.*,1996, **77**, 4027. [4] Bourgeois L., Ecolivet C., Toudic B., Bourges P., Breczewski T., *Phys. Rev. Lett.*, 2003, **91(2)**, 25504.
Keywords: aperiodic materials, supramolecular assemblies, structural phase transitions

P.22.04.1
Structural Study of Single Crystalline i-Zn-Mg-Dy at high Pressure and high Temperature
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In order to understand the origin of the structural stability of quasicrystals, it is important to investigate the pressure and temperature dependence of their structures. Quasicrystalline phases in the Zn-Mg-R (R = rare-earth and Y) alloys are classified as the Frank-Kasper type. Both the icosahedral and decagonal phases have been obtained in the alloys, which are thermodynamically stable at ambient conditions and reveal a high structural perfection [1]. The icosahedral Zn-Mg-Y quasicrystal is found to be stable at high pressures up to 70GPa at room temperature [2]. The hardness seems to be primarily governed by the complexity of the structure and the bonding strength. At room temperature, Zn-Mg-R quasicrystals exhibit a strong indentation size effect with the hardness increasing with decreasing load. This effect becomes inverted at higher temperatures [3]. Therefore it is interesting to perform structural studies at HP/HT.

We will report on the results of an in-situ single crystal x-ray diffraction study on i-Zn-Mg-Dy up to ca 12GPa and 873K using a heatable diamond anvil cell. The icosahedral quasicrystal is found to be essentially stable within the experimental framework.

[1] Abe E., Sato T. J., Tsai A. P., *Mater. Sci. Eng. A*, 2000, **294**, 29. [2] Hasegawa M., Tsai A. P, Yagi T., *Phil. Mag. A*, 2000, **80**, 1769. [3] Wolf B., Bambauer K. O., Paufler P., *Mater. Sci. Eng. A*, 2001, **298**, 284.
Keywords: quasicrystal, high pressure, high temperature

P.22.04.2
Framework Structures for Quasicrystal Models based on Dense Icosahedral Sphere Packings
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Dense icosahedral sphere packings (DISP's) are known to be obtained by placing spheres on subset vertices of three-dimensional Penrose tiling (3DPT) which are called the twelve-fold packing sites [1]. The DISP's give the best known quasiperiodic cluster packings with *b*- and *c*-links along their twofold and threefold directions, respectively (b=2.75a and c=2.38a, where a is the edge length of the 3DPT). However the shapes of the possible interstices are unknown.

Instead of spheres, we consider to place rhombic triacontahedra (RT's), having an edge length of a, on the sites. As a result, the RT's share a rhombus face and an obtuse rhombohedron with *b*-link and *c*-link, respectively. These framework structures are well described by the section method in six-dimension, once occupation domains for the DISP's are specified. It is shown that the interstices can be described by acute and obtuse rhombohedra. Application of the present framework structures to p-type icosahedral quasicrystals is discussed.

[1] Henley C. L., *Phys. Rev. B*, 1986, **34**, 797.
Keywords: quasicrystals, structure modelling, higher-dimensional structure analysis

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