

concentration of components etc., are general phenomena typical for condensed matter. Phase transitions can remarkably affect the physical properties of materials, and this behaviour is of great importance both for fundamental science and for materials applications. Establishing relationships between symmetry change at the transition, the mechanism and thermodynamics of a phase transition and the corresponding anomalous macroscopic properties of materials is an important step in understanding the microscopic nature of the effects, and in further developing the rational design of materials with desired properties. We will consider examples of structural phase transitions in materials particularly interesting due to their perspective properties: elevated hydrogen storage capacity, anomalous negative thermal expansion etc. The related structural features will be analyzed in the framework of a symmetry-based phenomenological theory. It will be shown how the formalism and methods of the theory of phase transitions can be applied to explaining anomalous effects even beyond the transformation region.

**Keywords:** phase transition; symmetry; transformation mechanism

#### KN-7

**New MOF Materials: Structure-Properties Considerations.** M. Angeles Monge. *Instituto de Ciencia de Materiales Madrid CSIC Cantoblanco Madrid, Spain.*

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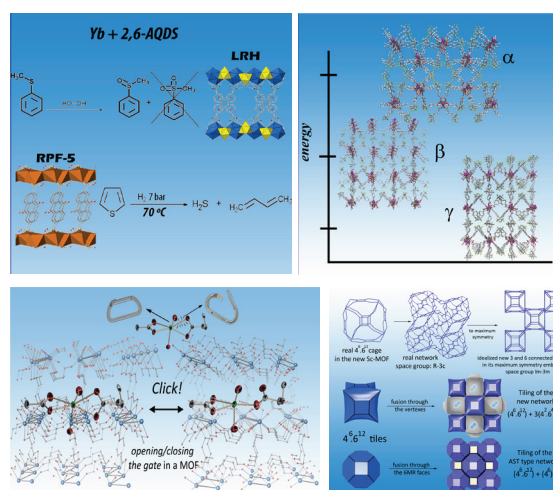
The use of rare earth elements in combination with different ligands has allowed the obtaining of several framework types, whose structural characterization, including the net topology, together with evaluation of their properties will be presented. An overview of the obtained results, on the base of structure-properties relationships allows to extract some conclusions on the properties and features of the new materials. Examples of this research will be presented:

- **Controlling the Structure of Rare Earth Arenedisulfonates towards Catalytically Active Materials.** All rare earth – anthraquinone-2,6-disulfonate materials show catalytic activity in the oxidation of methyl phenyl sulfide. Among all them, those belonging to the **LRH** family, with a 2D structure with cationic inorganic layers, are very active and selective catalysts in sulfides oxidation. Those belonging to the **RPF** families are also good catalysts for the hydrodesulphurization of thiophene. Structural features explain the differences in the activity among the materials. (Fig 1 up left).

- **Polymorphism in Rare Earth MOFs** Three Lanthanum MOF polymorphs have been obtained, their networks own unusual topologies, the three being uninodal penta-coordinated, two of them unknown up to now and the other named as **hxg-d-5-Imma**. They will be described and compared. DFT calculations of the relative energies for the three polymorphs show that the most often obtained structure is a metastable phase, which appears next to others thermodynamically more stable. Optical properties will be commented. (Fig 1 up right).

- **Reversible breaking and forming of metal-ligand coordination bonds.** A temperature triggered single-crystal-to-single-crystal phase transformation in a Metal–Organic Framework, makes this material an interesting heterogeneous catalyst. (Fig 1 down left).

- **A new Scandium Metal Organic Framework built up from Octadecasil zeolitic cages as heterogeneous catalyst.** Zeolitic cages of the AST type are found in the novel scandium-squarate MOF, and the joining of them gives rise to a new binodal network with a unique topology. This new material is an efficient heterogeneous Lewis acid catalyst (Fig 1 down right).



#### KN-8

**Complementarity of Magnetic Neutron and X-ray Scattering.** Thomas Brueckel. *Forschungszentrum Juelich GmbH / Institut fuer Festkoerperforschung / Juelich-Germany.*

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While the phenomena of magnetism is known to mankind since nearly 3 millennia, research on this macroscopic quantum phenomena is very topical as witnessed by the Nobel Prize in physics in the year 2007 awarded to Albert Fert and Peter Grünberg for their groundbreaking work in thin films magnetism. Understanding the magnetism of nanostructures paves the way to possible applications in information technology. Spintronics labels information storage, information transport and information processing using the spin of the electron and not its charge. In complex highly correlated electron systems, such as transition metal oxides, magnetism competes with other degrees of freedom leading to novel ground states and a high sensitivity to external disturbances and thus possible novel functionalities. In the quest to control functionalities in these complex materials and materials systems, it is essential to relate them with microscopic information on magnetic structures, magnetisation densities, magnetic excitations and fluctuations, which is a realm of scattering methods, namely neutron scattering complemented by magnetic synchrotron X-ray scattering.

In these fields, we witness a tremendous development: modern neutron optics allow us to apply polarisation analysis in a routine manner in neutron scattering experiments. Full vectorial polarisation analysis can be combined with spectroscopy to separate the magnetic- from the structural scattering, obtain vectorial information on magnetisation-fluctuations and chirality. High energy and resonant X-ray scattering in the hard and soft X-ray range at third generation synchrotron radiation sources provide complementary information on the electronic structure, on element and band specific spin polarisation, and on charge and orbital order directly re-lated to magnetism.

We will illustrate the potential of these novel methods on several examples ranging from magnetic nanoparticles, molecular magnets, thin film systems to highly correlated electron systems such as multiferroics, the family of the novel iron pnictide superconductors and oxide multilayers.

**Keywords:** magnetism; polarization analysis; neutron & synchrotron X-ray scattering

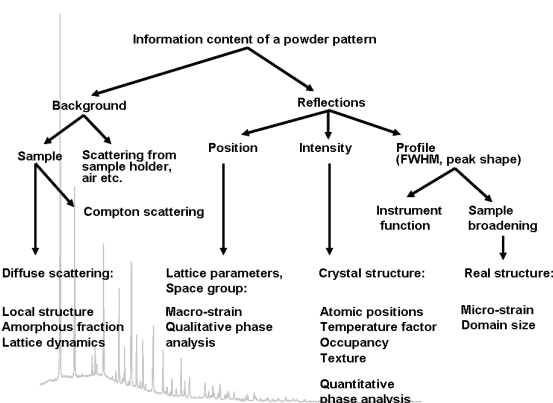
#### KN-9

**93 Years After Debye & Scherrer: Powder Diffraction in the 21st Century.** Robert Dinnebier. *Max-Planck-Institute for solid State Research, Stuttgart, Germany.*

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Although, the powder method was developed as early as 1916 by Debye and Scherrer [1], for more than 50 years its use was almost exclusively limited to qualitative and semi-quantitative phase analysis and macroscopic stress measurements. The main reason for this can be found in what is known as the principal problem of powder diffraction: accidental and systematic peak overlap caused by a projection of the three dimensional reciprocal space on to the one dimensional  $2\theta$  axis, leading to a strongly reduced information content compared to a single crystal data set. However, despite the loss of angular information, often sufficient information resides in the 1D dataset to reconstruct the 3D structure. Indeed, quantitative analysis of the pattern using modern computers and software yields the wealth of additional information about the sample structure that is illustrated in the figure below [2]. Modern instrumentation and sources are yielding data of unprecedented quality and modern analysis methods continue to increase our ability to harvest useful information from the data. The powder diffraction technique has never contributed to materials research in more diverse and important ways than now as we approach its centenary.

The information content of a powder pattern is huge, but much effort is needed to reveal the often hidden information. In the last decade, many new ideas have been successfully applied to powder diffraction, like the method of maximum entropy (MEM), fundamental parameters, global optimization in direct space, physical description of anisotropic peak broadening, parametric refinement, kinetics, distortion mode amplitudes, to name just a few. It is the intention of this talk to discuss some hot topics in powder diffraction in theory and practice.



[1] Debye, P., Scherrer, P. "Interferenzen an regellos orientierten Teilchen im Röntgenlicht," *Phys. Z.* 17 **1916** 277-282. [2] Dinnebier, R. E. (Editor), Billinge, S. J. L. (Editor) "Powder Diffraction: Theory and Practice", Publisher: Royal Society of Chemistry; 1<sup>st</sup> edition **2008** 574 pages.

**Keywords:** powder diffraction; Debye-Scherrer

#### KN-10

**When Flavins get the Blues.** Ilme Schlichting. *Max Planck Institute for Med. Research, Heidelberg, Germany.*

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Light is an important environmental variable and most organisms have evolved photoreceptors to respond to it. Photoreceptors are nano-switches that perceive the light signal by a chromophore containing sensing domain and transmit it via a structural change to an associated effector domain that subsequently gets (in)activated. Although a great deal of biochemical and spectroscopic data is known about these important relay systems, none is understood on a molecular level. This is not only frustrating from a basic science point of view but also hampers their redesign for cell biological or neurobiological applications.

Many blue-light photo-sensors rely on the light-sensitivity of the flavin cofactors, examples include the LOV- and BLUF-domains and cryptochromes/photolyases. Recent results on these different systems will be presented, sketching out the theme and variations in the paths from photon absorption to biological effects. Emphasis will be put on a blue-light activated phosphodiesterase involved in turnover of the bacterial second messenger cyclic-di-GMP. The light activation mechanism of the BLUF-photoreceptor and the catalytic mechanism of the phosphodiesterase will be presented.

**Keywords:** photoreceptor; mechanism; signaling; conformational changes

#### KN-11

**Crystallography of Complex Thermoelectrics.** Sven Lidin. *Department of Inorganic Chemistry Stockholm University, Stockholm, Sweden.*

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