In these fields, we witness a tremendous development: modern neutron optics allow us to ap-ply 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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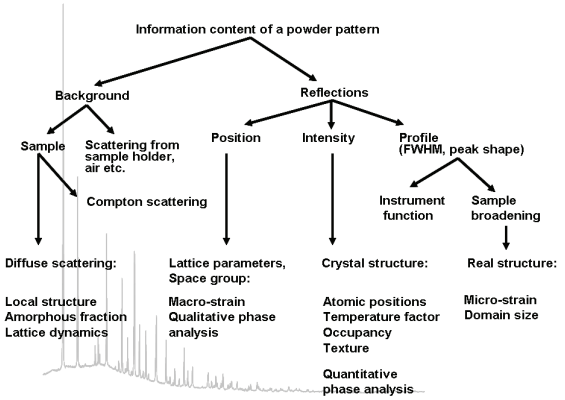
Although, the powder method was developed as early as 1916 by Debye and Scherrer [1], for more than 50 years its use was almost exclusively limited to qualitative and semi-quantitative phase analysis and macroscopic stress measurements. The main reason for this can be found in what is known as the principal problem of powder diffraction: accidental and systematic peak overlap caused by a projection of the three dimensional reciprocal space on to the one dimensional 2θ 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; 1st 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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An efficient thermoelectric material should be a good electronic conductor and a bad thermal conductor. Slack[1] introduced the concept of "electron crystal – phonon glass" to illustrate how such a material could be conceived. Among the classes of materials that fulfill these somewhat contradictory prerequisites and that have been studied extensively are Zintl-phase clathrates, layered main group metal structures and complex antimonides. What these all have in common is a complex crystallography, often caused by a super structure ordering within a simple basic structure. While the average structure forms the basis for the electronic properties of the compounds, and the carrier concentration can be optimized by doping, the super structure order (or disorder) is responsible for lowering the thermal conductivity. The crystallographic challenge lies in elucidating the super structure ordering (commensurate of incommensurate) caused by a relatively small number of scatterers. Since the super structure often adopts a lower symmetry than the basic structure, a frequent further complication is pseudo merohedral twinning, and in more severe cases epitactic intergrowth between different phases.

[1] Slack, G. A. in Solid State Physics, Vol 34, Ehrenreich H., Steitz F., Turnbull D. Eds.: Academic Press, New York, **1979**; pp1-71

**Keywords: thermoelectric; complex structure; intermetallic phases**

## KN-12

**Macromolecular Electron Crystallography.** Jan Pieter Abrahams[a], Linhua Jiang[a], Irakli Sikhuralidze[a], Igor Nederloff[a], Henny Zandbergen[a], Dilyana Georgieva[a]. [a]*Leiden Institite of Chemistry, Leiden University, The Netherlands.* [b]*Kavli Institute, Delft University, The Netherlands.*
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If protein crystals have multiple layers, but are smaller than 1 mm, they are currently beyond the reach of crystallographic structure determination, whether by X-rays or electrons. For structure determination of 3D protein crystals that are smaller than about 0.5 μm, it can be shown that electrons are more suited for structure determination than X-rays, as they are less damaging by several orders of magnitude when normalised to the amount of elastically scattered quanta. Indeed, if only two-dimensional, single-layer crystals of proteins are available, electron diffraction already is the method of choice for structure determination. However, if such crystals have multiple layers, practical problems include the data acquisition, the lack of software to process such data and the absence of successful pilot studies. These drawbacks currently prompt most protein crystallographers into putting their efforts into growing larger crystals that diffract X-rays, and make them abandon projects if such crystals cannot be obtained.
In this seminar, the implications of the fundamental differences between electron refraction and X-ray diffraction of 3D crystals will be discussed and potential solutions to many of the practical problems in electron 3D nanocrystallography will be evaluated. These include sample preparation and handling routines, data collection strategies, the use of quantum area detectors, data processing software and the potential of novel approaches towards phasing the diffraction data.

**Keywords: protein crystallography; electron diffraction**

## KN-13

**The Structural Bases of Chromosome Segregation**
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Equational division of the genetic material during mitosis is based on the establishment of secure interactions of chromosomes with the mitotic spindle, a microtubule- and motor-based structure [1]. The point of attachment of chromosomes to spindle microtubules is a complex protein scaffold (80-100 proteins) named the kinetochore. Kinetochores can be conceptually dissected into four modules: 1) a DNA-binding module that is built around a specialized nucleosome containing the Histone H3 variant CENP-A; 2) a microtubule-binding module, that is physically tethered to the DNA-binding module, and that is based on a proteinaceous microtubule receptor that goes by the name of the KMN network; 3) an attachment correction module, that removes improper attachments by activating microtubules "saws" such as MCAK and Aurora B; and 4) a safety device known as the spindle assembly checkpoint, that coordinates the chromosome attachment process with a cell cycle oscillator consisting of cyclin-dependent kinases and associated cyclins. Our current challenge is to reduce the functional and structural complexity of kinetochores to a set of basic organizational principles. This requires the construction of an accurate topological map of the kinetochore's modules, an understanding of their points of contact, and the availability of high-resolution structures of kinetochore components. Our work concentrates on three of the modules (modules 2-4) described above. Specifically, we are applying a combination of structural and functional investigations to unravel the architecture of the microtubule-kinetochore interface (module 2) [2], and its interactions with the error correction mechanism (module 3) [3] and with the spindle assembly checkpoint (module 4) [4]. I will present our main results, and discuss them in the framework of an integrated model of checkpoint function that explains many apparently contradictory aspects of kinetochore biology.

[1] Musacchio A and Salmon ED, *Nat Rev Mol Cell Biol* **2007**, 8, 379 [2] Ciferri C, Pasqualato S, Screpanti E, Varetti G, Santaguida S, Dos Reis G, Maiolica A, Polka J, De Luca JG, De Wulf P, Salek M, Rappsilber J, Moores CA, Salmon ED, Musacchio A, *Cell* **2008**, 133, 427 [3] Sessa F, Mapelli M, Ciferri C, Tarricone C, Areces L, Schneider T, Stukenberg P, Musacchio A, *Mol Cell* **2005**, 18, 379 [4] Mapelli M, Massimiliano L, Santaguida S, Musacchio A, *Cell* **2007**, 131, 730

**Keywords: cell cycle proteins; chromosome dynamics; biological macromolecules**