The Danish National Research Foundation

Center for Materials Crystallography

Annual report 2012

Summary

After three exciting years the Center for Materials Crystallography (CMC) has now established itself as a world leading center for structure based materials research. Great momentum has been achieved and the CMC activities continue to expand. In 2012 CMC published more than 100 peer-reviewed papers in international journals of which 24 were in the top 10 target journals. However, it should be stressed that CMC has strong focus on fundamental science and the most important results may not appear in high impact journals and immediately be widely regarded in main stream science. Indeed the seminal works by Prof. Mark Spackman on Hirshfeld surfaces and Dr. Carlo Gatti on the Source Function were originally published in specialized journals. Yet in 2012 this work resulted in the Royal Swedish Academy of Science awarding them the Aminoff Prize of Crystallography.

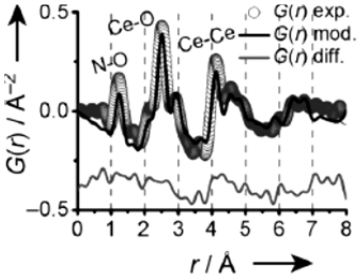
CMC has made strong progress on all the original research topics, but also opened up exciting new fields. The critical mass of CMC means that the center is acting as a scientific crossroad for novel ideas, and the evolution of CMC research topics therefore is highly dynamic. Some scientific highlights are discussed below but to mention just a few CMC published in 2012 the first direct experimental total scattering data on nanoparticle formation adding a new dimension to *in situ* studies of materials syntheses (Jensen *et al*., *J. Am. Chem. Soc*. **2012**, 134, 6785–6792). Other results include a seminal publication co-authored by three partner laboratories definitively disproving the concept of hypervalent bonding often used in chemistry text books all over the world (Schmøkel *et al., Inorg. Chem.* **2012**, 51, 8607-8616). Additionally, CMC discovered novel phases in the Zn-Sb phase diagram during synthesis of high performance thermoelectric thin films of Zn_4Sb_3 (Sun *et al*., *Adv. Mater.* **2012**, 24, 1693-1696) and gained unprecedented insight into the thermodynamics of aggregation and solvation of organilithium compound by combined X-ray crystallography and NMR (Granitzka *et al*., *J. Am. Soc. Chem.* **2012**, 134, 1344-1351).

CMC is thriving with a very large number of students and post docs, who clearly stimulate each other, and make the sum larger than mere addition of constituent parts. CMC is on course and we have strong ambitions for contributing new outstanding scientific results in the coming years.

Center for Materials Crystallography: Highlights 2012

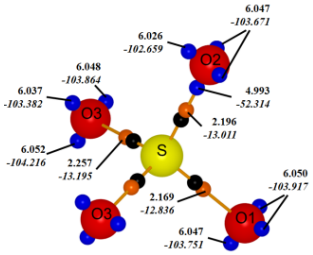
CMC continues to have an extremely large scientific output and the hard work of 11 post docs, 58 PhD students, and 16 Masters and project students led to more than 100 peer-reviewed publications. 4 PhD and 8 Master degrees were awarded, and the AU CMC group obtained 77 synchrotron and 7 neutron beam days after international peer review (with a further 34 synchrotron beam days awarded as "friendly users" to facilities). CMC activities are widely recognized, but the greatest achievement was the Aminoff Prize in crystallography, which was awarded by the Royal Swedish Academy of Science to Prof. Mark Spackman and Dr. Carlo Gatti.

Some scientific highlights:



Nanoparticle formation revealed

Using total scattering and PDF analysis experimental data for the first time directly provide a glimpse of the transformation of amorphous precursors into pristine nanocrystals (Jensen *et al.*, *J. Amer. Chem. Soc.* **2012**, 134, 6785–6792, Tyrsted *et al., Angew. Chem. Intl. Ed.* **2012,** 51, 9030–9033).

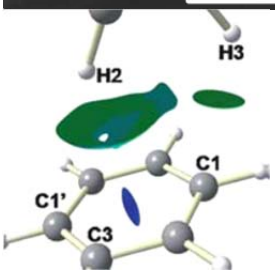


There is no such thing as hypervalent bonding

Hypervalent bonding is often used to explain bonding e.g. in sulfates. High energy synchrotron X-ray diffraction on minute crystals was used to reduce systematic errors and allow CD analysis on crystals of K_2SO_4. It was definitively shown that the hypervalent bonding model is incorrect, and this makes it necessary to revise commonly used chemistry text books (Schmøkel *et al.*, *Inorg. Chem.* **2012**, 51, 8607-8616).

Low-Cost High-Performance Zn_4Sb_3 Thin Films for Thermoelectric Applications

Zn_4Sb_3 is the cheapest thermoelectric material known, and preparation and characterization of phase pure thin films with outstanding properties was reported (Sun *et al.,* Adv. Mater. **2012**, 24, 1693-1696).

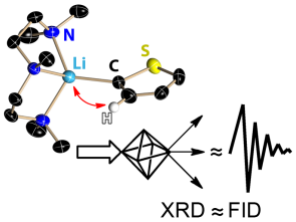


The stopping criteria in Maximum Entropy Method calculations finally defined

The MEM has been used in numerous studies of advanced materials, but since the method depends strongly on the uncertainties of the data obtaining the optimal densities has always been quite uncertain. Residual density analysis has provided the answer greatly improving the physical soundness of the method (Bindzus *et al., Acta Cryst* **2012**, A68, 750–762).

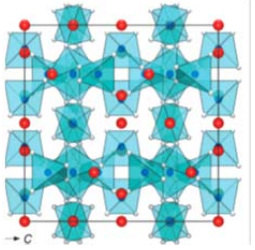
Quantifying non-covalent interaction

Non-covalent interactions form the basis of prominent research fields such as supramolecular chemistry and crystal engineering. Novel measures based on the electron density were introduced in studies of molecular crystals (Saleh *et al.*, *Chem. Eur. J.* **2012**, 18, 15523-15536).



Organolithium thermodynamics of aggregation and solvation

Organolithium compounds are indispensable reagents in materials syntheses. A highly innovative application of X-ray crystallography and solid state NMR provided unprecedented insight into the aggregation and solvation behaviour of key species (Granitzka *et al.*, *J. Am. Soc. Chem*. **2012**, 134, 1344-1351).



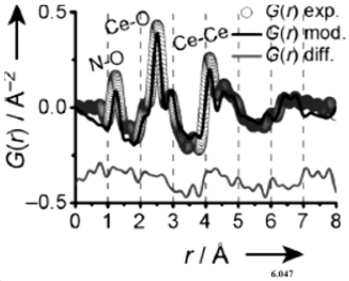
Structural diversity of borohydrides revealed by *in situ* PXRD

Borohydrides exhibit an amazing variety of crystal structures and physical properties, and mechanochemical synthesis in combination with *in situ* PXRD is shown to be an outstanding approach for exploring the diversity of these systems (Ravsnbæk *et al., Angew. Chem. Int. Ed.* **2012**, 51, 3582-3586).

Center for Materialekrystallografi: Højdepunkter i 2012

CMC har fortsat en ekstrem stor videnskabelig produktion. Hårdt arbejde fra 11 postdocs, 58 Ph.D. studerende og 16 Kandidat- og projektstuderende førte til flere end 100 peer-review publikationer. 4 Ph.D. grader og 8 Kandidatgrader blev tildelt og CMC-Aarhus opnåede 77 dages måletid ved internationale synkrotronfaciliteter, samt 7 dage ved neutronkilder, alle gennem internationalt peer-review (foruden 34 dages yderligere synkrotronmåletid tildelt som "friendly users"). CMCs aktiviteter er bredt anerkendte i det videnskabelige samfund, men den største hæder var dog Aminoff Prisen i krystallografi, som blev tildelt Prof. Mark Spackman og Dr. Carlo Gatti af det Kongelige Svenske Videnskabsakademi.

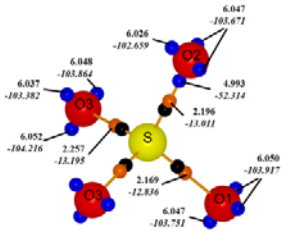
Udvalgte videnskabelige højdepunkter:



Eksperimentel måling af nanopartiklers dannelse

Ved at bruge total-spredning og PDF analyse kunne eksperimentelle data for første gang give direkte indsigt i overgangen fra atomart uordnede (amorfe) reaktanter til spæde, nydannede nanokrystaller (Jensen *et al.*, *J. Am. Chem. Soc.* **2012**, 134, 6785-6792, Tyrsted *et al., Angew. Chem. Intl. Ed.* **2012,** 51, 9030–9033).

Hypervalent binding findes ikke

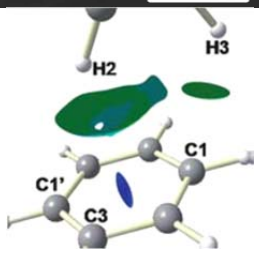


Begrebet *hypervalent binding* bruges ofte til at forklare de kemiske bindingsforhold i f.eks. sulfater. Røntgen-diffraktion med synkrotronstråling, udført på meget små krystaller, blev anvendt til at analysere elektrontætheden i K_2SO_4. Det blev definitivt vist, at den hypervalente bindingsmodel er fejlagtig. Denne opdagelse gør det nødvendigt at revidere grundlæggende lærebøger i kemi (Schmøkel *et al.*, *Inorg. Chem.* **2012**, 51, 8607-8616).

Billige, høj-effektive tyndfilm af Zn_4Sb_3 til termoelektriske anvendelser

Zn_4Sb_3 er det billigste kendte termoelektriske materiale, og CMC fremstillede og karakteriserede fase-rene tyndfilm med fremragende egenskaber (Sun *et al., Adv. Mater.* **2012**, 24, 1693-1696).

Slutkriteriet for MEM beregninger endelig defineret

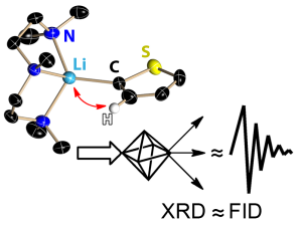


MEM har været anvendt i talrige studier af avancerede materialer, men siden metoden afhænger stærkt af usikkerheden på de anvendte data, har det altid været vanskeligt at finde de optimale elektrontætheder. Residual-tætheds analyse har skænket løsningen på dette problem, hvilket gør metoden langt mere fysisk korrekt (Bindzus *et al., Acta Cryst* **2012**, A68, 750–762).

Kvantifikation af ikke-kovalente interaktioner

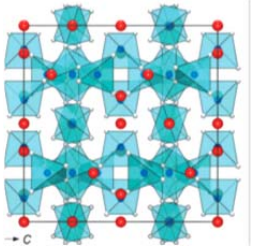
Ikke-kovalente vekselvirkninger danner basis for fremtrædende forskningsområder såsom super-molekylær kemi og *crystal engineering*. Nye metoder baseret på elektrontætheder blev introduceret i studier af molekylære krystaller (Saleh *et al.*, *Chem. Eur. J.* **2012**, 18, 15523-15536).

Termodynamikken bag aggregering og opløsning af organo-lithium afsløret



Organo-lithium forbindelser er uundværlige reagenser i materialesyntese. En yderst innovativ anvendelse af røntgenkrystallografi kombineret med NMR gav grundlag for ny indsigt i aggregering- og opløsningsfænomenet for udvalgte systemer (Granitzka *et al.*, *J. Am. Soc. Chem*. **2012**, 134, 1344-1351).

Borhydriders strukturelle diversitet afdækkes med *in situ* PXRD



Bor-hydrider udviser en fantastisk variation af krystalstrukturer og fysiske egenskaber, og mekano-kemisk syntese i kombination med *in situ* pulver-diffraktion har vist sig at være en fremragende tilgang ved udforskning af disse mangeartede systemer (Ravsnbæk *et al., Angew. Chem. Int. Ed.* **2012**, 51, 3582-3586).

CMC Science in 2012

It is impossible to review the scientific results of more than hundred papers in just 5 pages. Below we try to give an impression of the activities in each of the 12 main topics of CMC through key examples of the work.

T1: Excited state crystal structures and photoactive materials

In 2011 studies of a wide range of hetero bimetallic systems were published, but in 2012 there have not been significant new publications on photocrystallography. In relation to charge density (CD) determination of photoactive materials the main challenge has been to obtain complete crystal excitation since multipole modeling requires ordered structures. Ground state CD data has been measured on several systems, but fundamental modeling issues related to the radial functions are challenging the analysis. It may be that the new CMC-developed extended multipole model will solve the problems. Considerable synthesis efforts have focused on finding new photoactive systems, and a series of Cu-Mo complexes has some promise. As reported earlier the original plan to study a series of phosphanyl-anthracenes was delayed due to IPR issues, but these efforts are now reignited (Herbst-Irmer, *J. Phys. Chem. A* **2013**, 117, 633–641).

T2: Intermolecular interactions

Understanding the nature of intermolecular interactions is one of the main challenges in current chemistry and nanoscience, and fields such as supramolecular chemistry and crystal engineering are based on non-covalent interactions (NCI) between molecules. CMC continues to have strong and broad activities on applications of Hirshfeld surfaces to describe and quantify NCI and in particular to understand the driving forces for assembly of molecular crystals. In crystal engineering a "synthon" approach is often used, but increasing evidence suggests that the structure of molecular crystals to a large extent is governed by electrostatic complementarity and this can elegantly be visualized using the Hirshfeld surface approach. In the case of the cocrystal between hexabromoethane and $[CpRu(CO)_2Br]$ the most significant interactions arise not from the closest van der Waals contacts but rather from more distant interactions between the unsymmetrical electron distributions about the bromine atoms in the solvate and substrate molecules (Fuller *et al.,* CrystEngComm **2012**, 14, 804-811). In other studies correlations have been derived between intermolecular interactions quantified by Hirshfeld surfaces and physical properties such as melting points (Grabowsky *et al., CrystEngComm* **2012**, 14, 1083-1093). A general problem in materials chemistry is to understand which atoms are bonded to each other in intermetallic compounds. Such materials can often be extremely complex, and coupled with the heavy atoms neither theory nor experiment is yet capable of calculating accurate electron densities. Atomic Hirshfeld surface analysis using curvedness as the descriptor is a promising new tool, and it was also used to reject the hypothesis that the Mn atom in $CeMnNi_4$ can be regarded as a thermoelectric rattler atom (Jørgensen et al., *Inorg. Chem.* **2012**, 51, 1916-1924)

T3: Atomic level understanding of complex magnets

CMC studies of magnetic coordination polymers were significantly advanced with the application of Source Function analysis of both the experimental and theoretical electron density in $Zn(HCOO)_2(H_2O)_2$ (Jørgensen *et al., Inorg. Chem.* **2013**, 52, 297−305). This material is the non-magnetic reference for a series of isostructural coordination polymers exhibiting very rich magnetic behavior and they are a main target in studies of complex magnets. The source function reveals that considerable electronic communication between the metals takes place through the carboxylate group, and it will be very interesting to compare this with the bonding situation in the magnetic systems, since it is likely that this is the physical origin of the magnetic superexchange mechanism.

T4: Nanoporous materials

Following four years of vigorous experimental and theoretical investigations of the negative thermal expansion (NTE) in the archetypical metal-organic framework MOF5, CMC published a definitive study on this important issue (Lock *et al.*, *Dalton Trans.* **2013**, 42, 1996-2007 (cover page)). The extremely comprehensive study employed multi-temperature powder and single crystal X-ray and neutron diffraction, inelastic neutron scattering, EXAFS and *ab initio* calculations to provide a very elaborate explanation for the NTE. In another study electron density analysis was used to investigate bonding in zeolites, and here the analysis revealed considerable electronic interaction between oxygen atoms (Gatti *et al., J. Phys. Chem. A*. **2012**, 116, 8584-8598). Other studies have focused on improving the kinetics of hydrogen desorption by confining metal hydrides in nanoporous carbon aerogels, and a significant improvement is observed for pore sizes below 100 nm (T. K. Nielsen *et al., J. Phys. Chem. C*, **2012**, 116, 21046−21051).

T5: Nanoparticle formation, growth and structure

CMC is world-leading in the field of *in-situ* studies of hydrothermal reactions. The successes are based on the development of novel reactors for *in-situ* SAXS, WAXS, PDF and EXAFS studies. The field is rapidly developing with a range of experimental and theoretical advances coming together to bring fundamental new scientific insight. In 2012 we have for the first time reported *in-situ* total scattering (PDF) of nanoparticle formation under hydrothermal conditions. This has provided detailed insight about the formation mechanisms, which both for SnO_2, ZrO_2, and CeO_2 nanoparticles involve previously unknown dimeric metal complexes formed from the precursor before assembly of the pristine nanocluster (Jensen *et al*., *J. Am. Chem. Soc*. **2012**, 134, 6785-6792, Tyrsted *et al*., *Angew. Chem. Int. Ed.* **2012**, 51, 9030-9033, Tyrsted *et al., Chem. Eur. J.* **2012**, 18, 5759-5766). In another study the formation mechanism of rutile TiO2 under supercritical conditions was uncovered (Mi *et al., Cryst. Growth Des.* **2012**, 12, 6092-6097)

T6: Flat potential energy surface materials

After three years of technical development CMC published its first diamond anvil high pressure study of molecular crystals (Scheins *et al., Chem. Eur. J.* **2013**, 19, 195-205). The study provided highly novel insight into the electron transfer mechanism of mixed valence complexes, which previously has been shown to be strongly dependent of temperature and crystal packing effects. It was shown that isotropic compression has a different effect on the molecule than the anisotropic changes occurring during cooling. Another surprise was the fact that our new crystal batch showed a different valence trapping behavior on cooling than in previous studies even though the time and space averaged room temperature crystal structures were identical. In Aarhus CMC now has a fully equipped high pressure crystallography laboratory and a range of new studies are in progress.

T7: Energy materials

Synthesis and characterization of thermoelectric materials, Li-ion battery materials and hydrogen storage materials continues to be one of the strongest activities in CMC and also in 2012 we reported on a large number of studies in these fields. In thermoelectrics CMC had a break-through result with the synthesis and characterization of Zn_4Sb_3 thin films, showing extremely good thermoelectric properties and much better thermal stability than bulk crystals (Sun et al., *Adv. Mater.* **2012**, 24, 1693-1696). The very dedicated activities on zinc antimonides also included a comprehensive theoretical study of the defect formation, and we were finally able to explain why it has not been possible to prepare n-type materials in these systems (Bjerg *et al*., *Chem. Mater.* **2012**, 24, 2111−2116). It was furthermore shown that the main origin of thermal instability is migration of Zn ions in electric fields (Yin *et al., Appl. Phys. Lett.* **2012**, 101, 043901).

With regard to Li ion battery materials, a new supercritical flow synthesis was developed for the promising anode material $Li_4Ti_5O_{12}$, and multi-temperature X-ray diffraction was used to understand the crystal structure and especially the defects (Laumann *et al., J. Electrochem. Soc.* **2012**, 159, A166-A171).

In the field of hydrogen storage materials, many activities continue to focus on the fascinating structures and properties of borohydrides. *In situ* PXRD was shown to be an extremely powerful method for screening new systems (Ravsnbæk *et al., Angew. Chem. Int. Ed.* **2012**, 51, 3582-3586). In other work new materials were discovered that combine both Li ion conductivity properties and hydrogen storage capability (Ley *et al., Chem. Mater*. **2012**, 24, 1654-1663; Ley *et al., J. Phys. Chem. C*. **2012**, 116, 21267−21276).

T8: Development of novel crystallographic methods

One of the key problems in studies of intermolecular interactions (T2) is how to quantify and compare them. A new measure based on the reduced density gradient coined the Non-Covalent Interaction Index (NCI) has shown great promise to solve this problem, and in two publications the NCI index was for the first time applied to experimental densities (Saleh *et al., Chem. Eur. J.* **2012**, 18, 15523-15536; *Comp. and Theor. Chem.* **2012**, 998, 148-163). The NCI index has now been coded into new versatile software and is ready for general exploration. The Source Function continues to bring new insight about chemical interactions and through a large concerted effort in three partner laboratories a fundamental insight into to proposed archetypical hypervalent sulfate ion was achieved (Schmøkel *et al., Inorg. Chem.* **2012**, 51, 8607-8616). Using the SF it was shown that there are partial bonding contributions from resonant forms enabling a significant electron exchange among the oxygen atoms. However, the S-O bond is so polarized that the bond order does not exceed one, and thus there is no hypervalency.

A breakthrough in MEM CD studies was achieved when a proper general stopping criteria was finally developed based on residual density analysis (Bindzus *et al., Acta Crystallogr. Sect. A* **2012**, 68, 750-762). The same study also provided the optimal way to perform Rietveld refinement of PXRD data prior to performing MEM calculations.

T9: Structure, reactivity and chemical bonding in organolithium compounds

Organolithium compounds are indispensable reagents in materials syntheses. Insight into structure-reactivity-relationships for these compounds is very important since it is commonly accepted that the lithiated species determines the composition, yield and stereochemistry of the reaction product. In one study CMC researchers could monitor the selective and consecutive donor base addition and exchange in the same lithiumaryl carbanion complex by structural determination. Normally X-ray crystallography provides limited insight into the thermodynamics of aggregation and solvation, because the crystal structure is commonly believed to represent the least soluble derivative and not necessarily the most abundant, let alone the most reactive species. Nevertheless, different 2-thienyllithium aggregates were synthesised, crystallized and structurally characterized using a combination of X-ray diffraction and NMR (Granitzka *et al., J. Am. Soc. Chem.* **2012**, 134, 1344-1351).

T10: Materials based on silicon in low oxidation state

Tetrylenes are compounds with neutral divalent Group 14 atoms in the formal oxidation state +2. CMC researchers have now shown that tetrylenes can be stabilized and employed in a vast variety of reactions to give unprecedented products. In general they are ambiphilic in nature due to the presence of a lone pair and an empty p-orbital. In an important study a stable biradicalic $[(cAAC)_2SiCl_2]$ (cyclic-alkyl-amino-carbenes = cAAC) was synthesized and this was accessible to reduction to a silylone $[(cAAC)_2Si]$ containing a silicon

atom of the oxidation state 0 (Mondal *et al., Angew. Chem. Int. Ed.* **2013**, 52, 2963–2967). In another study stable silicon(II) fluoride were synthesized by coordination to transition metal carbonyls (Azhakar *et al., J. Am. Chem. Soc.* **2012**, 134, 2423-2428)

T11: Development of new experimental equipment

In 2011 CMC reported on a new pulsed high-pressure, high-temperature reactor for nanoparticle synthesis (Eltzholtz *et al*., *Rev. Sci. Instrum.* **2011**, 82, 084102). The same reactor can be used both in laboratory synthesis and for *in situ* studies, which solves the fundamental problem of transferring information gained from *in situ* studies to the home laboratory. CMC has now used the pulse reactor in an *in situ* study of the formation and growth of titania nanoparticles (Eltzholtz *et al., Nanoscale* **2013**, 5, 2372–2378).

Following several years of development and substantial funding from the Carlsberg Foundation the new all-in-vacuum powder diffractometer was presented (Strassø *et al., J. Synchroton Rad*. **2013**, 20, 98-104). The instrument can measure PXRD data with unprecedented accuracy and resolution, and for the first time this gives experimental access to study core electron polarization.

T12: Topological insulators

Topological insulators are bulk insulators, but surface metals, and CMC has built up a very strong collaboration with Prof. Philip Hoffman at Department of Physics, AU, and various international groups. Also in 2012 several publications were published with CMC being responsible for growing high quality crystals, structural characterization, measurements of transport properties and chemical composition analysis (Bianchi *et al., ACSNano* **2012**, 6, 7009-7015; Honolka *et al.*, *Phys. Rev. Lett*. **2012**, 108, 256811)

Milestones and challenges

In general CMC fulfilled the milestones set for the first two years, but in fact the activities have been much broader that envisioned in the original application. This emphasizes that CMC is a center for fundamental science within materials crystallography, which is driven by a strong ambition of excellence in materials crystallography not by exactly fulfilling strategic milestones.

During 2012 it became clear that the outstanding data quality previously obtained in CD measurements at ChemMatCARS at APS had been compromised. The million dollar upgrade of the beam line optics has resulted in an X-ray beam with incredible brilliance, but ironically it appears that the immense number of photons on the sample is the core of new problems. Specifically, we observe that several crystals systems (especially metalorganic crystals) now degrade in the beam during measurements and the accuracy of the recorded intensities appears inferior. During the past three beam times only few data collections have resulted in adequate data quality, and for this reason it was decided to use an entire beam time period on standardization measurements. These data are currently being analyzed, and it appears that the CCD detector hitherto used may be a major part of the problem since with the increased flux the dynamic range of the detector is no longer fully adequate. Solving these issues has high priority.

Organization

CMC in Aarhus now consists of five independent research groups: Bo Brummerstedt Iversen, Torben René Jensen, Jacob Overgaard, Mogens Christensen and Martin Bremholm. To maximize the use of experimental facilities the groups share all laboratories and equipment. Common group meetings are held every second week and furthermore CMC staff meetings are also held every second week. The latter meetings include

scientific and technical staff and they are important for the daily function of CMC. This is where overall planning and coordination is executed (purchases, renovations, teaching, strategy, information exchange etc.). The daily administration of CMC continues to be in the hands of our six technical staff members: Jacob Becker (general manager), Peter Hald (laboratory manager), Bo Richter (laboratory technician), Britta Lundtoft (laboratory technician), Karin Sutherland (accountant) and Marianne Sommer (secretary).

CMC is up to full manpower with regard to the senior participants and there is now a natural flux of new hirings and resignations in the partner laboratories. CMC is very visible in the partner Faculties, and talented students continue to be attracted to the center. One specific challenge of CMC has been the continuity of the three out-stationed post docs at large facilities. Currently Mads Ry Jørgensen is outstationed at SNS, while Lai-Chin Wu is at APS. Following the resignation of Brian Pauw, who accepted a position at National Institute of Materials Science in Japan, the SPring8 post doc position was filled twice with new people. First Hao Yin was hired, but he later resigned after being offered an attractive job in Danish industry. Subsequently, an Indian researcher was hired (Debajit Sarma), but for personal reasons he decided to withdraw just before starting the position. Following the reposting of the position an outstanding new candidate, Dipankar Saha, has accepted and started working in January 2013.

Facilities

Apart from the out-stationing of post docs, CMC staff was involved in a very large amount of beam time at international synchrotron or neutron facilities through peer-review proposals. The AU beam days were distributed as follows: PSI (Switzerland): 3 days, SNS (USA): 2 days, PETRA-III (Germany): 18 days, ESRF (France): 10 days, DORIS-III (Germany): 11 days, MAX-II (Sweden): 45 days, APS (USA): 15 days, NSLS (USA): 3 days, Diamond (United Kingdom): 4 days, FRM-II (Germany): 2 days, SPring8 (Japan): 8 days.

In Aarhus, a full renovation was launched on two CMC-laboratories in the basement of building 1514 at Dept. of Chemistry. These were not included in the renovation of all the main laboratories (buildings 1511 and 1512) back in 2010, and is now adapted e.g. for the imminent installation of the ultra-high-pressure synthesis equipment which is crucial to the research of CMC assistant professor Martin Bremholm. When completed by mid-April 2013, only the physical property laboratory remains to be renovated at CMC-AU.

Finally, CMC has been involved in the instrumentation of the new European Spallation Source (ESS) as CMC director Bo Brummerstedt Iversen agreed to chair the Scientific & Technical Advisory Panel on diffraction. The panels help guide the work of the ESS work-packages so that they deliver cutting-edge instrumentation for the European scientific community. The unique new instrumentation at ESS is expected to lead to revolutionizing new research in materials crystallography.

Signature

Ved underskriften bekræftes det, at beretning og regnskab med tilhørende noter og oversigter indeholder alle relevante oplysninger, som vedrører årets primære aktiviteter in Danmarks Grundforskningsfonds Center for Materialekrystallografi.

Bo Brummerstedt Iversen,
Aarhus, 31-03-2013