Cluster of Excellence
Engineering of Advanced Materials

Dear colleagues and friends,

As the decision on the new funding round of the German Excellence Initiative draws closer, we along with our colleagues across the land wait with baited breath. We can be proud of both our highly professional proposal and well-polished presentation in Bonn in January. Hopefully, we will have a great chance to continue the fantastic developments seeded in the first funding period. Regardless of the outcome, preparations for the future of the Cluster are in full swing. At the two summer schools we will place great emphasis on EAM’s newest structural elements, the four Focal Topics. With these we aim to strengthen further the interactions between the Research Areas, ultimately catalyzing a significant impact on the university through the hiring of new academics with key competencies. Besides our internal discussions, high-caliber guest speakers at the summer schools will help breathe life into these new platforms for interdisciplinary exchange. Of course, the other structural elements of EAM will remain too, and in the first half of 2012 we continued to reap the rewards of our interdisciplinary activities, for example in the form of the 50th publication resulting from collaborations between three or more EAM members. During this period we moved into our final two new buildings and these will be inaugurated over the summer. However, the infrastructural expansion is not yet complete. In order to adequately accommodate all present activities and future growth, we will be supported by the Bavarian State Ministry of Sciences, Research and the Arts in proposing the construction of an interdisciplinary center for nanostructured films, a very welcome addition to our university’s landscape.

I look forward to further exciting scientific discussions over the summer months and thank you for your dedicated work and enthusiastic collaboration.

Wolfgang Peukert

FOCAL TOPICS – a new structural element to consolidate the EAM research strategy in the second funding period

Focal Topics are new forms of scientific collaboration, which will run orthogonal to the application-specific Research Areas of EAM. These additions to the Cluster’s structure will aim to both unify and tackle fundamental scientific challenges from different perspectives. Members of all Research Areas of EAM will work together in Focal Topics to explore these key scientific questions, which originate from a broad range of application areas and which include:

• How can thin film formation be controlled? • How can macroscopic properties be understood and tailored by interface control on the microscopic scale? • What is the impact of the dimensionality in the functionalization of building blocks? • Can we control the reaction networks that lead to nanomaterials? • Can we optimize properties and process chains based on predictive modeling?

To elucidate answers to these questions, new and improved experimental and theoretical methods will be created, optimized, and shared in a multi-disciplinary approach, thus catalyzing further coherence within EAM. Within the next few months, each Focal Topic will collect a feedstock of information (relevant scientific questions from different Research Areas, available methods etc.) that will serve as a foundation, which will be built on in the future. Furthermore, a taskforce of interested persons will be formed and the first activities will be planned, such as workshops and the upcoming EAM Summer School.

FT1 Early stages of phase transitions
Contact: Prof. Dirk Zahn, Computer Chemistry Center

FT2 Modification and characterization of interfaces
Contact: Prof. Oliver Diwald, Particle Technology

FT3 Self-organization & processing of thin films from liquids
Contact: Prof. Christoph Brabec, Materials for Electronics & Energy Technology

FT4 Numerical optimization based on predictive models
Contact: Prof. Michael Stingl, Applied Mathematics II
Success in interdisciplinary research as one of the major goals of EAM was demonstrated recently by the 50th joint publication by three or more members of the Cluster. The paper entitled “Mixed self-assembled monolayer of molecules with dipolar and acceptor character – influence on hysteresis and threshold voltage in organic thin-film transistors” was published in Applied Physics Letters by Prof. Andreas Hirsch, Prof. Marcus Halik (both Research Area B·Nanoelectronic Materials), and Prof. Tim Clark (Research Area A3·Multiscale Modeling and Simulation).

The authors investigated the impact of the molecular dipole moment and redox-active head groups (C₆₀) in pure and mixed self-assembled monolayers (SAMs), which serve as ultra-thin hybrid dielectric layers in low-voltage operating organic thin-film transistors. It was shown that the dipole of a SAM-forming molecule affects the threshold voltage, while the concentration of a redox-active molecular fragment (e.g. C₆₀) determines the hysteresis in devices. This behavior, caused by the molecular structure of the SAM forming molecules, is suggested to be general and was confirmed by the use of different organic semiconductors, which all showed the same trend. The key molecule of this study was synthesized in the Hirsch group, whereas the electronic properties of the SAM molecules were calculated by the Clark group, and the devices were fabricated and characterized in the Halik group. The work impressively represents the strong collaboration between various disciplines such as Organic Chemistry, Computer Chemistry, and Materials Science, motivated by the spirit of the Cluster of Excellence.

JEWELRY FOR PARTICLES: EAM researchers develop a new approach to produce anisotropic nanostructures

One-dimensional nanostructures comprising noble metals are promising materials for applications such as transparent conductive coatings, Raman sensing chips, and metamaterials. A major challenge is to identify scalable and sustainable routes to produce such materials. Many existing methods include multiple steps and employ functional molecules and polymers to guide one-dimensional nanostructure growth. A very simple new approach has been developed by researchers from EAM Research Areas A1 (Mathias Hanisch, Prof. Robin Klupp Taylor), A2 (Dr. Mirza Mackovic, Prof. Dr. Erdmann Spiecker) and D (Dr. Nicola Taccardi). In this method, published recently in Chemical Communications, one-dimensional silver nanoparticle necklaces are formed on silica nanospheres in the absence of explicitly added reducing and templating agents. The procedure merely involves the liquid phase treatment of colloidal silica with a common silver complex followed by washing, deposition on a substrate, and aging under ambient conditions. The fact that one-dimensional metal nanostructures result from this apparently homogeneous treatment is rather surprising and poses fundamental questions regarding the physicochemistry of metal complexes close to colloidal silica particles. Current work is focusing on this in addition to the upscaling of the technique to produce the nanostructures on the square centimeter scale, and appraisal of the optoelectronic properties of the materials.

**LIST OF PUBLICATIONS**

http://www.eam.uni-erlangen.de/fileadmin/uploads/pdfs/50_Publications_with_3_or_more_EAM_Members.pdf

**REFERENCE**

A. Jedaa · M. Salinas · C. M. Jäger · T. Clark · A. Ebel · A. Hirsch · M. Halik

M. Hanisch · M. Mackovic · N. Taccardi · E. Spiecker · R. N. Klupp Taylor
X-ray photoelectron spectroscopy (XPS) under ultra-high vacuum conditions enables the monitoring of organic reactions in solution when carried out in mixtures of reactive ionic liquids (ILs), as demonstrated by EAM scientists for a thermally activated alkylation of a nucleophilic amine by a chloroalkyl species. Ionic liquids (ILs) are a new class of materials, which have attracted vast scientific and industrial interest over the last decade. They are special salt melts exhibiting unusual physico-chemical properties (e.g. melting points even below room temperature, extremely low vapour pressure, unusual solvation and miscibility properties, and a wide electrochemical window). Possible application areas range from green chemistry, catalysis, and electrochemistry to analytics and separation technologies. The main motivation for the collaborative work of the research teams of Prof. Hans-Peter Steinrück (Chair of Physical Chemistry II) and of Prof. Peter Wasserscheid (Chair of Chemical Reaction Engineering), conducted within EAM Research Area D “Catalytic Materials”, is related to “Supported Ionic Liquid Phase” catalysis. In this context, the fundamental issue of in-situ monitoring of reactions in the near-surface IL region plays a crucial role.

Due to the high vapor pressure of conventional liquids, ultra-high vacuum-based surface science experiments are extremely difficult or even impossible. In contrast, the very low volatility of ionic liquids (ILs) allows for addressing fundamental mechanistic questions by surface science methods that were originally developed for solids, such as angle-resolved X-ray photoelectron spectroscopy (ARXPS). The EAM team has recently demonstrated that even classical organic reactions can be monitored in the near-surface region of the liquid phase under ultra-high vacuum conditions when anchoring the otherwise volatile reactive groups to ionic liquid molecules. This novel concept is successfully applied to nucleophilic substitution reactions between alkyl amine and alkyl chloride species, which are bound to cations and anions of ionic liquid molecules, respectively. For the first time, this type of reaction – belonging to the fundamental organic reaction mechanisms since the pioneering work of C. K. Ingold in the 1920s – has been thoroughly studied by ARXPS, which enables the monitoring of the fate of all elements present in the reaction in a quantitative and oxidation state-sensitive manner on the molecular level, in one experiment.1, 2

REFERENCES


New structured catalyst systems – combining high surface area carbon materials with cellular metal structures

Structured catalysts were introduced within the second half of the last century and brought with them several advantages such as a low pressure drop and high-thermal conductivity – if compared to a fixed bed of powders or pellets. Mostly they are made of ceramics such as alumina, magnesia, or silica. In addition to the well-known monolithic structures, regular and irregular open cellular structures are of increasing interest due to their improved radial heat and mass transfer. An additional improvement in the heat transfer can be achieved, if, instead of oxides, materials with high-thermal conductivity like metals are used. Metal structured catalysts and reactors are of interest for highly exothermic or endothermic reactions, where heat exchange is of utmost importance. Benefits such as higher space-time-yield and a safer process operation can be achieved.

The group of Prof. Körner and Prof. Singer (EAM Research Area E) is able to build optimized 3D open-cellular metal structures from CAD data using selective electron beam melting (SEBM). Furthermore, the group of Prof. Etzold (EAM Research Area D) has expertise in the synthesis of advanced and tuneable porous carbons. These two groups have now combined forces to study the application of cellular metal structures as catalyst supports. In this work an innovative new class of carbonaceous materials – so called carbide-derived carbons (CDC) – was applied as porous coatings on the metal structures. The carbon coating was achieved by depositing layers of silicon carbide on the metal support by chemical vapor deposition (CVD) and subsequent transformation of the carbide layer into porous carbon by exposing the structure to a chlorine containing atmosphere at 800 °C. In this second process the silicon is selectively extracted and a highly porous carbide-derived carbon remains, which provides sufficient specific surface area for catalysis. The porous carbon layer increases the specific surface area of the structure by a factor of roughly 2000. Platinum as active metal was deposited on the carbon coated metal structure by ion exchange with a platinum salt and subsequent reduction on hydrogen atmosphere. The structured CDC/metal catalyst showed improved catalytic performance in a model hydrogenation reaction when compared to a commercial Pt catalyst on activated carbon.

REFERENCES
1 T. Knorr · P. Heinl · J. Schwerdtfeger · C. Körner · R.F. Singer · B.J.M. Etzold
Process specific catalyst supports – selective electron beam melted cellular metal structures coated with microporous carbon
2 P. Heinl · A. Rottmair · C. Körner · R. F. Singer
Cellular titanium by selective electron beam melting
3 M. Schmirler · F. Glenk · B.J.M. Etzold
In-situ thermal activation of carbide-derived carbon
Carbon, 2011, 49, 3679-3686.
Merck and the Cluster of Excellence Engineering of Advanced Materials (EAM) have announced a cooperation in the field of new hybrid materials for more energy-efficient processes. This new strategic partnership centers on catalytic conversion, gas purification, and new functional surfaces. The alliance clearly underlines that the Cluster of Excellence EAM not only has a high level of expertise in materials’ development, but is also sought after as an important partner when it comes to industrial applications.

The cooperation combines the material and process expertise of the EAM scientists with a number of highly innovative classes of materials from Merck, including ionic liquids, silica-based functional materials, and fluorochemicals. The hybrid materials resulting from this cooperation promise great potential for safer, more energy-efficient and more eco-friendly processes and products. For example, the ionic liquids developed by Merck are to be integrated by EAM into novel catalyst and membrane systems intended for use in oxidation chemistry and hydrogen purification. The hybrid materials developed will be tested at EAM pilot plants and optimized in terms of material and process technology. At the same time, Merck will elaborate application scenarios and will aim to develop further the results in the form of prototypes.

Researchers from the EAM-established “Center for Nanoanalysis and Electron Microscopy” (CENEM) have scored a great success in the competition for funds in the DFG (German Research Foundation) initiative “Gerätezentren – Core Facilities”. With the proposal “CENEM – Nanocharacterization with electrons, x-rays and scanning probes”, the scientists have netted a total of € 450,000 for a period of three years. Through this funding scheme, the DFG supports the “establishment and professionalization of key analytical facilities and networks of both national and international relevance”. The new grant will drive intensification of the facility’s usage ensuring that the cutting-edge characterization of materials down to the atomic scale will be available to an even broader spectrum of internal and external clients.

Prof. Dr. Erdmann Spiecker (electron microscopy) – who filed the application, Prof. Dr. Mathias Göken (general material properties) and Prof. Dr. Tobias Unruh (nanomaterial characterization/scattering techniques) had to fight off stiff competition. However, in the end, eleven applications made it through the multi-round assessment process; according to the DFG, 57 complete applications were received after 120 preliminary enquiries. In the field of material research and structural physics, only two centers are to receive funding. In addition to Erlangen’s CENEM, the second centre to be funded is the renowned Ernst-Ruska Centre in Jülich/Aachen.

CENEM was founded in the framework of Research Area A2 of EAM in order to bring together cooperative research work and complementary high-resolution microscopic and analytical procedures within the Cluster. This project, unique in Germany, focuses on targeted methods, from which significant synergies were drawn. By combining them, new material characterization possibilities were established. This considerably enriched the profile of the university discipline in “materials and processes”.

CENEM’s flagship instrument, the Titan® 80–300 transmission electron microscope. © Jan Kneage Fotografie ’09
Research in the age of changing energy policy: Bavarian government supports two projects with strong connections to EAM

With the 2012 supplementary budget, the State of Bavaria is supporting numerous research projects related to the highly publicized change in energy policy. Two of these projects draw on results of fundamental research carried out by EAM, in the fields of catalysis and solar energy.

BAVARIAN HYDROGEN CENTER

The Bavarian Hydrogen Center will receive €3 million from the supplementary budget in addition to the €12 million already granted. This initiative is a cooperation between the FAU, the Technical University of Munich, the University of Bayreuth and Amberg University of Applied Sciences. The research project's main aim is to search for possibilities to generate, distribute and use hydrogen from exclusively renewable sources. Moreover, the researchers want to drive forward the systematic development of the chemical energy storage of hydrogen, known as Liquid Organic Hydrogen Carrier (LOHC) technology. The hydrogen released at the location where energy is required can then be transformed into electricity through fuel cells, combustion machines or turbines.

Hydrogen is one of the most sustainable energy sources and could play an essential role in changing energy policy as renewable energies, such as solar and wind power which can only be generated intermittently due to changing weather conditions. Furthermore, the amount of energy produced can vary depending on the location. For example, winds are generally stronger on the coast than inland, which means coastal locations produce more wind power. This is why technology is required that allows this excess energy to be economically and efficiently stored and transported from one location to another. In this case, using hydrogen would be the answer. Hydrogen, however, has a very low density and is extremely volatile and therefore not suitable in its natural state as an energy source. This is where the LOHC technology comes into play.

The concept was developed by Prof. Dr. Wolfgang Arlt, Chair for Thermal Process Engineering (FAU), and Prof. Dr. Peter Wasserscheid, Chair for Chemical Reaction Engineering (FAU), and is to be expanded within the framework of the Bavarian Hydrogen Center. The process under development makes it possible to store hydrogen using the hydrocarbon compound carbazole. This substance is similar in consistency to diesel fuel and reaches about 30 per cent of the heat value of fuel oil. Moreover, just like fuel oil, it can be pumped and stored or transported over large distances using tanker trucks. Furthermore, carbazole is not explosive as the hydrogen cannot escape from the compound on its own.

SOLAR TECHNOLOGIES GO HYBRID

The “Solar Technologies Go Hybrid” initiative is to receive around €6 million from the supplementary budget. In this collaborative project, research scientists from the FAU along with Bayreuth, Würzburg and both Munich universities are focusing on technologies such as photovoltaic and photoelectrolytic devices for the conversion of solar energy into electricity and chemical energy, respectively. To support these activities, the five universities have set up well equipped laboratories, known as Key Labs. The FAU Key Lab “carbon rich hybrids” will bring together highly topical and basic research on photo and light active materials from the Interdisciplinary Centre for Molecular Materials (iCMMM) and the Cluster of Excellence EAM. The lab will be coordinated by Prof. Dr. Dirk M. Guldi, Chair of Physical Chemistry I, and Prof. Dr. Timothy Clark, from the Computer Chemistry Center. The core focus will be on the concept of panchromatic absorption and light-harvesting complexes, as well as the optimization of electron transfer processes and the development of molecular photocatalysts and dye-sensitized photocathodes.

Faster and more efficient – FAU computer scientists optimize high-performance computing with graphics cards

Computer scientists at the Erlangen Regional Computing Center and the Institutes of Multiscale Simulation (founded in the framework of EAM), System Simulation and Computer Architecture at FAU have set themselves the goal of optimizing so-called GPU Computing, i.e. scientific computing using graphics cards. Under the leadership of the Central Institute for Scientific Computing (ZISC), the team has achieved success in two funding programs run by Nvidia, the global market leader in Visual and High-Performance Computing. The company will provide FAU computer scientists with financial support for their research over a one-year period. Nvidia will also provide the university with very high performance graphics cards. This will also significantly benefit students as the graphics cards are to be installed on publicly accessible computers in a CIP pool at the Faculty of Engineering.

The high-performance graphics cards will be used to speed up general computing processes. They contain a number of programs, which can be used to support a computer’s central processing unit. This makes the cards particularly appropriate for use in high-performance computing, such as simulation computing, where the computer has to conduct millions of calculations in a very short space of time. To date, the different programs on the graphics cards and on the PC are still not optimally compatible with each other. In the project at FAU the programs’ algorithms will be optimized to make high-performance computing more efficient and faster.
New EAM building: Center for Functional Particle Systems

Following the completion of the EAM chemistry building (see Winter 2011 Newsletter), the second large interdisciplinary facility for EAM researchers is almost ready. The first occupants of the Center for Functional Particle Systems could move into their new building at the beginning of May 2012. The 1420m² facility was built after being ranked no.1 for funding by the Expert Committee for Large-scale Research of the German Council of Science and Humanities (Wissenschaftsrat). The building represents a key step towards cementing EAM Research Areas A1 (Functional Particle Systems) and C (Photonic and Optical Materials) in the fabric of the university. It is located on the southern campus directly next to the existing buildings of the Department of Chemical and Biological Engineering and close to other key facilities such as the EAM funded Titan³ transmission electron microscope. The building, which includes laboratories for synthesis, characterization and optical experiments, also contains offices for researchers from project students up to the professorial level and a technical hall for large-scale studies of particle formation and handling.

The research groups of Prof. Ulf Peschel (Research Area C), EAM W2 Prof. Oliver Diwald (Research Area A1) and EAM W1 Prof. Robin Klupp Taylor (Research Areas A1, C) will now be based in the building. A key theme of research will be the synthesis and characterization of particles with well-defined shape, size, and composition. These particles are required as building blocks for a whole host of applications, which are being developed in collaboration with the other EAM Research Areas. This work will be supported by three new large acquisitions: an X-ray diffractometer with Mo-source, opening new possibilities in the analysis of defects in particles; a high resolution scanning electron microscope to be employed particularly for the optimization of novel plasmonic sub-wavelength structures (waveguides, nanoantennae, and couplers) and metamaterials; and a solvothermal reactor with a suite of analytical techniques enabling the in-situ analysis of particles of metal oxides and other compounds during synthesis and thus unraveling the mysteries of their formation mechanism.

Architects website of the project
http://www.grabow-hofmann.de/P_Bildung_FPO.htm

ZISC Annual Report 2011 published

One year after its founding, the first annual report of ZISC (Central Institute for Scientific Computing) charts an impressive development. The first year was characterized by start-up activities, including moving into a new building, the election of the executive board and chairman, the setting up and occupation of an administrative office. Of course, besides these necessary tasks, research activities were not forgotten! ZISC’s project portfolio already covers a broad spectrum of topics ranging from biomedicine to materials science as well as fundamental issues of supercomputing. The projects all share the main goals of ZISC: to promote the growth of interdisciplinary collaborations and to drive the development of modern software and algorithms for complex simulation techniques. EAM was the leading force in founding the ZISC as an essential strategic development of its core competence in Research Area A3, Multiscale Modeling and Simulation.

Special Issue in Granular Matter edited by Thorsten Pöschel

The journal Granular Matter serves as a platform for communication among researchers from various disciplines who are involved in the basic research of granular media. It helps to establish a common language and gathers articles under one single roof that up to now have been spread over many journals in a variety of fields. The Special Issue: “Isaac Goldhirsch – A Pioneer of Granular Matter Theory” edited by EAM Prof. Thorsten Pöschel and Prof. Dietrich Wolf from the University of Duisburg-Essen was published in April 2012. This issue was dedicated to the memory of Isaac Goldhirsch (1949 – 2010), former member of the EAM advisory board, and is a tribute by colleagues in this field in return for his deep insight and profound inspiration.

Graduate students donate 240 euros for charity project

Members of the Graduate School Advanced Materials and Processes (GS AMP) along with other students and researchers from EAM and neighboring programs donated € 240 during a screening of ‘The PHD Movie’ on 16 December 2011. The event was organized by GS AMP and doctoral researchers from the Cluster and other graduate schools were invited to enjoy the movie free of charge. Before the movie started, GS AMP coordinator Prof. Zaumseil and program manager Dr. Schür introduced the Erlangen Parental Initiative for Children Suffering from Cancer (Elterninitiative krebskranker Kinder Erlangen e.V., kinder-erlangen.de) and asked the audience for donations for this project, which is definitely worth supporting. The PHD Movie (http://www.phdcomics.com/movie/index.php) takes a humorous look at the life of four graduate students. It shows how they grapple with research, being a teaching assistant and finding balance in their over-worked lives. It is based on the popular PHD Comic strip series (http://www.phdcomics.com/comics.php) by Jorge Cham, which is read by more than a million readers each month (and not only graduate students!) around the world.
Joint EAM/CBI stand at ACHEMA 2012

Following the success in 2009, EAM and the Department CBI will join forces again to produce a stand at ACHEMA 2012, one of the world’s largest process engineering trade fairs, which takes place from 18 – 22 June in Frankfurt. Covering nearly 100m² in hall 9.2, the stand will showcase Erlangen’s latest developments in fundamental and applied research in the fields of catalysis, particle technology, and fluid mechanics. With energy being the main theme of ACHEMA 2012, EAM activities concerning this critical issue will be highlighted. For example, a demonstration reactor produced by selective electron beam melting (SEBM) will be shown. Such tailored reactors permit chemical reactions to be optimized for high efficiency. The SEBM process allows the fashioning of unusual reactor structures including those with variable cell sizes or additional internal cooling circuits. The internal surface of the reactor can be coated with alumina, which acts as carrier for the catalyst (see Research News p. 4). A further interest of EAM/CBI that will be shown at ACHEMA 2012 is the innovative concept for the storage of hydrogen in diesel-like organic compounds (Liquid organic hydrogen carrier LOHC). And from the area of fluid mechanics, the world’s smallest oil central heating system will be presented. This unit, which boasts a low-emission, small-scale burner and has a power modulation range between 1– 8 kW, will be suitable for highly insulated modern buildings. In the field of electricity generation, a model of a wind turbine with two rotors will be shown. The rotor blades for this system have been optimized to maximize electrical output by a combination of simulations and wind tunnel tests. The EAM/CBI stand will also give prospective students an overview of the degree programs on offer at FAU in the Department of Chemical and Biological Engineering as well as other courses related to the research field “Engineering of Advanced Materials”.

EAM Summer Schools 2012

This year, two EAM Summer Schools will take place, spotlighting the Cluster’s new structural elements “Focal Topics”.

SUMMER SCHOOL I
28 – 30 June 2012 · Kloster Banz, Bad Staffelstein
for researchers working in Research Areas A1 · A2 · A3 · B · C · E

The main subjects will be “Early Stages of Phase Transitions” (Focal Topic 1 coordinated by Dirk Zahn) and “Numerical optimization based on predictive models” (Focal Topic 4 coordinated by Michael Stingl). We are privileged to welcome three renowned guest speakers – Lorenz T. Biegler, Carnegie Mellon University, Pittsburg, USA (Multi-scale optimization for integrated design of engineering systems), Jakob Søndergaard Jensen, Denmark Technical University, Lyngby (Topology optimization of optical and elastic materials and structures), and Michael Mehring, TU Chemnitz (Formation of bismuth oxide polymorphs via metal oxido clusters) – to the first Summer School, who will surely provide interesting new perspectives.

Furthermore, we are planning additional talks from the Research Areas, tutorials and an introduction to proposal writing for EAM researchers. Poster sessions will be held in the evenings to complement the overview of the recent research activities. For EAM members, Thursday afternoon (June 28) is dedicated to a strategic meeting in direct response to the DFG decision on 15 June.

The invitation to the first Summer School and the preliminary program is available on the EAM Events webpage.

Link: www.eam.uni-erlangen.de/summerschool1

SUMMER SCHOOL II
25 – 27 July 2012 · Waldhotel Berghof, Thüringer Wald
for researchers working in Research Area D
plus selected participants of other Research Areas

The second Summer School in July will mainly be organized by Research Area D “Catalytic Materials”. However, it will also cover the Focal Topics “Modification and characterization of interfaces” (Focal Topic 2 coordinated by Oliver Diwald) and “Self-organization & processing of thin films from liquids” (Focal Topic 3 coordinated by Christoph Brabec). Similar to the first Summer School guest speakers will be invited to further stimulate future activities.

Link: www.eam.uni-erlangen.de/summerschool2
It has now become a tradition that the EAM members meet at the end of January for the annual Cluster retreat. About 40 scientists gathered together from 20 – 21 January in Muggendorf. Firstly, Prof. Peukert gave a review of the EAM evaluation which took place on 11 January in Bonn. Then, ideas and plans surrounding the new structural elements of EAM, the Focal Topics (see article p. 1) and Joint Demonstrators were discussed in detail in order to develop concepts ready for November when the new period of EAM will hopefully begin. The same applies to EAM’s activities in the area of supporting school pupils, an aspect which is being developed with Prof. Meyn from the Chair for the Didactics of Physics. In early summer, EAM will bring all interested parties from Erlangen together in order to further strengthen the network and to concretize ideas for school outreach for the new funding period of the Cluster.

International Symposium on Disperse Systems for Electronics

The second International Symposium on Disperse Systems for Electronic Applications organized by the DFG Research Training Group 1161 was held in Erlangen on 1 – 2 March 2012 and brought together scientists at the forefront of nanomaterials synthesis and characterization, modeling, particle assembly and printing, as well as the fabrication of particle based devices. During his keynote presentation, Sanjar Mathur (University of Cologne) emphasized the importance of chemistry in the development of materials science. This is due to the fact that the successful realization of building blocks like nanocrystals and nanowires often require the synthesis, modification and assembly of pre-organized molecular architectures. Tobias Kraus (INM – Leibniz Institute for New Materials, Saarbrücken) and Daniel Vanmaekelbergh (University of Utrecht) introduced the audience to the fascinating world of self-assembly of colloidal nanocrystals. In addition to presentations that focused on surface science aspects of metal oxides and related nanostructures (Thomas Mayer, TU Darmstadt, and Michael Schmid, TU Vienna), there were also contributions from theory that span the range from modeling of defects to that of drying phenomena. Brian Derby (University of Manchester) and Alberto Piqué (Naval Research Laboratory, Washington D.C.) provided insights into process fundamentals and limitations of inkjet printing of nanoparticulate systems and laser direct-write for digital microfabrication, respectively. Graduate students of the Research Training Group 1161 complemented the scientific program with reports of their research projects and demonstrated their high competency in communicating science to a broader audience. The talks, together with the lively discussions perfectly reflected the multidisciplinary nature of the Research Training Group 1161.
EVENT REVIEW

WORKSHOP: Mathematics meets Chemistry and Physics

The idea for a joint workshop to develop novel multiscale methods in molecular dynamics and continuum mechanics was born at the annual EAM Symposium 2011 in Oberhof, in which Prof. Claude Le Bris from Paris took part as EAM advisor. This idea became reality from 14 – 17 March 2012 when mathematicians, chemists and physicists from Research Area A3 along with Professor Le Bris’ group met for an interdisciplinary workshop in Schloß Weißenstein, Pommersfelden. It was clear that the interdisciplinary participants brought with them potential topics to fill a meeting for an entire week. Therefore the organizers (Le Bris, Clark, Leugering) decided to select a few specific topics, which promised to provide an ideal platform for presentations and discussions:

- Implicit solvation models
- Extending the time scale: Massively parallel molecular dynamics
- Optimization in Chemistry
- Non-periodic homogenization

Keynote lectures provided an overview and a tutorial for each topic for non-specialists from the other participating groups. Of the 30 participants, six came from France and one keynote speaker from the Technical University of Dortmund. The discussions have led to the generation of new joint projects in geometry optimization and non-periodic homogenization and to a new molecular-dynamics technique from the Paris group being used in EAM. All in all, a great success!

Symposium on Bulk Nanostructured Materials in Berlin

A symposium on bulk nanostructured materials was organized by the EAM in cooperation with the Austrian Research Network S104 (High-Performance Bulk Nanocrystalline Materials) at the German Physical Society (DPG) Spring Meeting held in Berlin from 25 – 30 March 2012. With more than 6,300 participants this conference is the largest European physics conference of the year. Chairing the symposium on bulk nanostructured materials were Prof. Mathias Göken, coordinator of EAM Research Area A2, and his colleagues Prof. Roland Würschum, TU Graz, and Prof. Gerhard Wilde, University of Münster. With more than 51 lectures the symposium was one of the largest at the conference, highlighting the very strong international research activity in this field. Nanostructured or ultrafine-grained (UFG) materials are produced nowadays by various processes such as severe plastic deformation or galvanic processes in bulk quantities with improved properties. Prof. Zenji Horita from Kyushu University in Fukuoka, Japan, opened the symposium with an impressive keynote talk on the production of UFG multifunctional materials. Also several presentations highlighting the work of EAM researchers were given. Among them, an invited talk was presented by Dr. Heinz Werner Höppel on tailoring materials properties by accumulative roll bonding. Several other contributions came from the National Research Network (Austrian Science Fund) for “High-Performance Bulk Nanocrystalline Materials” led by Prof. Michael Zehetbauer which chose the symposium at the DPG meeting for their final annual colloquium. The symposium induced intensive interdisciplinary discussions on the various opportunities of ultrafine grained materials in the fields of processing, characterization, mechanical and functional properties.
Deep-drawn outer shell of a lightweight robot arm out of high-strength aluminum with 256 single layers produced in the Accumulative Roll Bonding process.

Prototype of a tailor-made reactor with optimized geometry, e.g. for hydrogen generation from liquid organic hydrogen carriers.

EAM exhibits at Hannover Messe

EAM was represented at Hannover Messe from 23 – 27 March at the joint booth of Bayern Innovativ / Cluster Neue Werkstoffe in the hall “Research and Technology”. Two exhibits from EAM Research Areas D and E based on demonstrators from the first funding period which are close to application were on display. One was a joint demonstrator between Research Area E and D comprising a catalytic reactor based on metallic structures formed by Selective Electron Beam Melting (SEBM). The latter is an innovative process enabling the facile production of complex structures starting from metal powder. In this way, components used in process engineering (e.g. reactors and mixers) can be made in an optimized geometry and thus boast superior heat and mass transport, for example. Research Area E also showed an outer shell of a lightweight robot arm made of high strength aluminum, which is produced in a three-step-process. First, the multilayered aluminum sheet metal with 256 single layers was manufactured by Accumulative Roll Bonding by EAM cooperation partner Neue Materialien Fürth GmbH. Second, the formability was enhanced by a local short-term heat treatment according to the Tailored Heat Treated Blanks technology. Finally, the outer shells were produced by deep drawing and laser cutting.
**PEOPLE**

**Second EAM Awardee started his work in Erlangen**

Hannsjörg Freund joined the FAU as Professor for Catalytic Reactors and Process Technology at the Institute of Chemical Reaction Engineering in the Department of Chemical and Biological Engineering in January 2012. He is a recipient of the Excellence in Engineering Materials Award, which provides a €750,000 research grant over four years. The focus of his research is on the model-based design of optimal chemical reactors. For this purpose, he combines methods and tools of conceptual process design, analysis, and optimization with detailed simulations for the computer-aided catalyst support design. His strong background in chemical reaction engineering with special focus on reactor modeling and optimization along with broad competencies in process technology complements the existing expertise of EAM in a synergistic manner.

Prof. Freund studied Chemical Engineering in Erlangen and remained there for his Ph. D. under Prof. G. Emig on detailed simulations of transport processes in fixed-bed reactors. In 2005, he joined the Physical and Chemical Process Engineering Department led by Prof. K. Sundmacher at the Max Planck Institute for Dynamics of Complex Technical Systems in Magdeburg. As a senior research scientist he established his research group there in the field of process intensification with special focus on multifunctional reactors and integrated processes.

**Interview with Hannsjörg Freund**

**What led you to pursue a position in EAM?**

When I was a Ph.D. student I realized that I like research work and teaching very much, so I decided to stay in academia and pursue the goal of becoming a professor. For my further qualification phase I then joined the MPI in Magdeburg, which offered an excellent research environment. When I learned about EAM and the research areas, especially the strong link between materials sciences and catalysis, I was convinced that this would be exactly the right place for me. Therefore, the offer to join the EAM as professor came just at the right time, and I am very happy about being both a professor at the FAU as well as being a member of the interdisciplinary research environment of EAM.

**What will be your research focus in EAM’s Research Area D for the next few years?**

My research focuses on the model-based design of optimal reactors for highly efficient processes. Special emphasis is on the application of innovative materials, and here in particular novel cellular structures as catalyst support, as an option for process intensification. In order to account for the interaction of materials, reactors, and process concepts at different scales and times in the conceptual design stage, an integrated multi-scale approach is required. Only with such an approach it is possible to evaluate the potential of innovative materials and reactors and finally find an optimal solution not only on a local level but on the global process level as well. The modeling work is supported by key experiments for phenomenological investigations, data acquisition and model validation.

**Do you expect synergies and possibilities for collaboration with your colleagues at the Central Institute for Scientific Computing (ZISC)?**

Absolutely, I am delighted that we now have a dedicated Central Institute for Scientific Computing as a binding element that bridges between the disciplines and brings the expertise that is available at the different departments and institutes together. As my research work deals a lot with modeling, simulation, and optimization I am sure that we will have many opportunities for a close interaction and collaboration with ZISC. Last but not least, I would like to add that already since my time as a Ph.D. student in Erlangen I have enjoyed a close collaboration with the High Performance Computing group of the Computing Center RRZE here in Erlangen. To sum up, Erlangen offers a fantastic infrastructure with regard to scientific computing.

**You create chemical processes and the corresponding reactors on the drawing board. What kind of processes and properties do you plan to investigate?**

The general aim of my research is to develop and provide methods and tools for simulation and optimization, so I am initially not focusing on a particular system. Of course, these methods and tools are being developed and validated using example processes. One important topic of my research within EAM is to investigate structuring concepts for catalytic reactors where cellular structures will play an important role. I am excited about the experimental facilities of the materials scientists here in Erlangen, e.g. for the precise production of well-defined cellular structures. That way it is possible to both experimentally validate the optimal structures that we predict in our computations as well as to provide feedback for optimization. For example, we will investigate processes in the field of heterogeneously catalyzed gas phase reactions where heat transport is crucial and multiphase systems where a well-defined contacting of the phases is of great importance.
Sabine Maier appointed new member in the “Förderkolleg der Bayerischen Akademie der Wissenschaften”

Sabine Maier, Juniorprofessor for Scanning Probe Microscopy within the EAM’s Rising Star program and based at the Physics Department of FAU, has been announced as one of six excellent young researchers in Bavaria to be appointed to the Förderkolleg of the Bavarian Academy of Sciences. This membership is funded with € 12,000 annually for a duration of three years and requires the participation in and organization of interdisciplinary seminars and activities. Prof. Maier’s research supported by the Förderkolleg will focus on the self-assembly and molecular structure of ultrathin films on surfaces using scanning probe microscopy.

Prof. Hirsch awarded the Max Grundig Memorial Prize

Prof. Dr. Andreas Hirsch, head of the Institute for Organic Chemistry II at the FAU and coordinator of EAM Research Area B, has been awarded the 2012 Max-Grundig Memorial Prize. This € 10,000 prize, which is presented every two years in memory of the Fürth-based industrialist Max Grundig (1908 –1989), recognizes Prof. Hirsch’s pioneering and internationally acclaimed contribution to the field of molecular materials.

Five EAM Members elected to DFG Review Boards

Since 2004 the German Science Foundation (DFG) review boards have been in place to ensure quality control in the proposal reviewing process. Members of the boards are elected for three-year terms and in the most recent election, the following EAM members were elected for the period 2012 –15:

Prof. Dietmar Drummer (Plastics Engineering), Prof. Lothar Frey (Electronic Semiconductors, Components, Circuits, Systems), Prof. Mathias Göken (Microstructural Mechanical Properties of Materials), Prof. Hans-Peter Steinrück (Physical Chemistry of Solids and Surfaces, Materials Characterization), Prof. Peter Wasserscheid (Technical Chemistry). The review boards select suitable expert referees to peer review funding proposals. They then form a final recommendation to the decisions panel of the DFG, who consider this along with the proposal itself when reaching a funding decision.

New EAM Members

Prof. Rik Tykwinski
Chair of Organic Chemistry I
Dr. Milan Kivala
Chair of Organic Chemistry I
Prof. Dr.-Ing. Erik Bitzek
Juniorprofessorship Simulation and Materials Properties
Chair of General Materials Properties
Prof. Dr.-Ing. Julia Mergheim
Juniorprofessorship Computational Mechanics
Chair of Applied Mechanics

Staff News

First Evaluation for Juniorprofessors
Robin Klupp Taylor and Michael Stingl

The first interim evaluations of EAM-funded juniorprofessors have taken place. The purpose of this evaluation, which is carried out by a three-person panel appointed by the respective Faculty in addition to external referees, is to assess the teaching and research activities of the first three years of a juniorprofessorship. Based on the evaluation committee’s report, the Faculty board makes a recommendation to the university management on the outcome. Success at this stage leads to an extension of the juniorprofessorship for a maximum of three years, during which a further successful evaluation leads to a permanent W2 professorship being awarded. Prof. Robin Klupp Taylor and Michael Stingl, who were appointed to the first juniorprofessorships in the EAM Industrial Liaison and Rising Star Programs, respectively in 2009, successfully passed their interim evaluations during Winter Semester 2011/12.
German Language Course for EAM Researchers

As suggested by a group of EAM researchers from abroad, the Graduate School AMP has organized a course for German as a foreign language, specifically focusing on developing the everyday speaking and writing abilities of the participants. The course has started in Summer Semester 2012 at B1 level and takes place three times a week during lunch breaks. Topics include writing emails, discussing with colleagues, or shopping. The course is proving to be an efficient way for participants to improve their German while still being able to do full-time research. It is also not limited to doctoral students, but open to all EAM researchers. If you are interested in joining the course and your knowledge of German matches that of the other course participants (at least B1 level), please contact Dr. Carsten Schür.

Workshop Public Communication

Scientific developments are sometimes critically received by the public and it can be difficult to communicate complex issues through the mass media. As scientists, we must do justice to the trust placed in us by the public and retain the credibility that we enjoy in public opinion. To assist this, the Graduate School AMP is planning a workshop on the public communication of science and how to deal with critical public opinion. Together with Dr. R. Kötter from the Central Institute for Applied Ethics and Scientific Communication (ZIEW), GS AMP will offer a 1.5 day workshop on these questions in July. More information can be found on the GS AMP events webpage.

Pizza Seminar Postdoc Experiences

Another great suggestion by EAM researchers has led to GS AMP organizing an informal pizza dinner during which Postdocs exchanged their experiences. Being open to all EAM researchers, this was also an opportunity for doctoral researchers, to hear of and talk about ways to organize a Postdoc position, find funding and avoid pitfalls. Dr. Milan Kivala, who is currently PostDoc in Erlangen, Prof. Jana Zaumseil, Prof. Erik Bitzek, and Dr. Christian Papp, who have previously been abroad for a PostDoc and Dr. Claudia Backes, who is at present preparing for a PostDoc abroad, shared their experiences and gave advice beyond the generic funding agency leaflets. Numerous researchers took the chance to ask questions and get an idea as to why and how to become a successful Postdoc and what to do afterwards.
UPCOMING EVENTS

MPL meets ZMP
... and EAM Research Area C /
SFB 953 Synthetic Carbon Allotropes
24 MAY 2012
Max Planck Institute for the Physics of Light · Erlangen

Joint EAM/CBI stand at Achema 2012
18 – 22 JUNE 2012
Hall 9.2 · Stand E 93 · Messe Frankfurt

8th Erlangen International High-End-Computing Symposium (EIHECS)
22 JUNE 2012
Lecture Room H12 · Cauerstraße 11 · Erlangen

EAM Summer School I
28 – 30 JUNE 2012
Kloster Banz · Bad Staffelstein

EAM at VDI Technikmeile
13 – 14 JULY 2012
Pedestrian zone · Nuremberg

EAM Summer School II
25 – 27 JULY 2012
Waldhotel Berghof · Luisenthal

17th International Workshop on Microchip Plasmonics:
Enabling Optics beyond the Diffraction Limit organized by SAOT, EAM and MPL
29 – 31 AUGUST 2012
Erlangen · Germany

4th EAM Symposium
22 – 26 OCTOBER 2012
Treff Hotel · Oberhof