MATERIALS SCIENCE
– A CHALMERS AREA OF ADVANCE

This booklet provides brief presentations of the researchers in the Area of Advance Materials Science in Gothenburg. NO3. Oct 2019
THE EYE OF THE ROTARY STORM
Solidification of an organic monomer in a round-bottom flask during rotary evaporation. Photographed from the bottom of the flask.

Cover image: Petri Murto
This booklet contains a brief introduction to the researchers active within the Area of Advance Materials Science in Gothenburg. The Area of Advance is a strong scientific community that unites materials science activities at two universities; several departments at Chalmers University of Technology are involved as is the Department of Biomaterials at Sahlgrenska Academy, University of Gothenburg. The aim of the Area of Advance is to combine scientific excellence with societal relevance to create impact. Our activities span from undergraduate education through cutting-edge research to innovation in collaboration with industry and society.

Our vision “A sustainable society through excellence in materials science” manifests itself in our research profiles Materials for health, Materials for energy applications and Sustainable materials. All profiles address societal challenges, such as antibiotic resistance, the need for renewable energy technologies and sustainable materials from renewable feedstock. In addition, several world-leading activities in the development of materials synthesis and characterisation methods are being pursued within the Area of Advance, and we provide access to state-of-the-art research infrastructure. The combination of cutting-edge method development and excellent research lays the foundation for ground-breaking materials science advancements with strong societal relevance.

The researchers presented in this booklet are all active within one or more of the research profiles and/or in the development of new experimental and theoretical methods. Many of them are also active in centres of excellence that operate under the umbrella of the Area of Advance Materials Science and typically have long term joint industrial and governmental funding. The Wallenberg Wood Science Center 2.0, the High Temperature Corrosion Centre and Competence Centre for Catalysis are all examples of highly creative and collaborative environments that strengthen materials science in many ways and trigger interdisciplinary research collaboration.
PROFILE AREAS
The Materials Science Area of Advance has three profile areas – Materials for energy applications, Materials for health, and Sustainable materials – where multi-disciplinary research is carried out spanning from natural science to engineering, and from materials theory to processing.

The research is supported by high quality infrastructures and resources, with links to established and emerging industries. Chalmers is at the forefront of the development of advanced material synthesis and characterisation methods, crucial for successful ground-breaking materials research. Furthermore, Chalmers has a strong tradition in materials-theory research, providing modelling of materials on different length and time scales.

Materials for energy applications
Energy-related materials research at Chalmers spans across the full spectrum of energy production, transport, storage and conversion. All aspects from material synthesis and characterisation to integration of these materials into devices are covered and target global energy challenges.

Materials for health
Research at Chalmers and the University of Gothenburg on materials beneficial for people’s health is considered world leading in several areas. It is driven in a multi-disciplinary manner and covers a broad area of applications such as tissue engineering, materials for osseointegration, and materials for pharmaceuticals and personal care.

Sustainable materials
Sustainability-related materials research at Chalmers is highly interdisciplinary and aims at reducing society’s environmental impact, for example by developing new materials from renewable raw materials, improving the recycling of materials and improving the performance and life span of various materials.
FUELS AND ELECTRICITY FROM THE SUN

The research is centered around the fundamental processes needed to convert solar energy to useful forms of energy. To achieve this, we combine molecules (which provide selectivity) and functional materials to form hybrid materials which should facilitate control over multi-electron transfer reactions. We also work on materials for so-called spectrum manipulation, to better utilize the solar spectrum. For example, we work with combining two low energy photons to create one high energy photon, aiming at more efficient photocatalytic fuel forming reactions. Furthermore, we study the photophysics and photochemistry of transition metal compounds, in solution and on surfaces, both for photosensitizing purposes and spin cross-over applications. We use characterization tools such as ultrafast spectroscopy and electrochemical methods to determine rates as well as microscopy techniques to study the materials and their characteristics.

SELECT PUBLICATIONS

ENGINEERING METALS FOR DEMANDING APPLICATIONS

Johan Ahlström’s research concerns the behaviour of engineering metals both during production and for products in service. Experimental characterisation of the deformation behaviour and its relation to microstructure, temperature and strain rate combined with numerical modelling gives possibilities for physical interpretation and prediction of the behaviour in a certain environment. Johan is also interested in connected phenomena like phase transformations, fatigue, residual stresses and crack growth. Examples of industrial aims can include decreased maintenance costs and increased reliability of railways or decreased fuel consumption of road vehicles. The image attached shows how a test bar is deformed in a biaxial experiment giving high shear strains in the surface (around 200%). The following changes in microstructure and mechanical properties are characterised by microscopy (SEM, TEM) and mechanical testing under biaxial (axial-torsion) loading.

SELECT PUBLICATIONS
Microstructure and mechanical properties of the running band in a pearlitic rail steel: Comparison between biaxially deformed steel and field samples; K. A. Meyer, D. Nikas, J. Ahlström; Wear 396-397, 12-21 (2018)

6
NANOSTRUCTURED BIOMATERIALS

In my research group we utilize nanochemistry to design and form novel nanomaterials for applications in regenerative medicine, ways of preventing biomaterials associated infections, drug-delivery, water cleaning and method development. We are heavily inspired by nature’s ability to cleverly use self-assembly processes to produce materials from the bottom up. Our research is highly curiosity driven and aimed at addressing global challenges including fighting the threats from antibiotic resistance, developing medical devices for an aging society, and finding solutions for purifying water. Recently, we are also highly engaged in method development for protein structure determination using Atom Probe Tomography, where both the molecular 3D structure and chemical composition can be obtained simultaneously with near atomic resolution.

SELECT PUBLICATIONS


BIOMATERIALS • IMPLANTS • DRUG-DELIVERY • INFECTION

DETAILED MICROSTRUCTURE OF MATERIALS

We work with microscopy and microanalysis of materials using high-resolution methods such as atom probe tomography (APT) and electron microscopy.

1. Nuclear materials. With support from the Swedish Foundation for Strategic Research (SSF) and industry we study nuclear fuel more tolerant to loss-of-coolant accidents. Two types of coatings on fuel cladding tubes made from zirconium alloys are being studied: Cold sprayed pure chromium, and refractory coatings applied by laser coating. Within an international programme we also study the effect of irradiation on corrosion and hydrogen pick-up of zirconium alloys, primarily with atom probe analysis.

2. Wear resistant coatings. In an SSF-supported programme involving universities and industry we study the detailed microstructure of wear resistant coatings fabricated by CVD (chemical vapour deposition). The effect of texture of alumina coatings on cutting properties are studied, as well as the structure and morphology of epitaxially grown TiN, (Ti,Al)N and Ti(C,N) coatings.

SELECT PUBLICATIONS


A new 12% chromium steel strengthened by Z-phase precipitates; F. Liu, M. Rashidi, L. Johansson, J. Hald and H-O. Andrén; Scripta Mater. 113, 93-96 (2016)

INTERMETALLIC PHASES • THERMODYNAMIC CALCULATIONS • DISLOCATION LOOPS • SEGREGATION • HYDROGEN MICROANALYSIS • TEXTURE • EPITAXY
**MULTIFUNCTIONAL COMPOSITE MATERIALS**

Leif Asp, Professor in Lightweight composite materials and structures at Department of Industrial and Materials Science. Leif’s research is focused on several aspects of carbon fibre composite materials. The research relies on more than 25 years’ experience in damage tolerance modelling, design and certification methods for aircraft composite structures. Composite design and verification rely on combined virtual and experimental approaches in a so-called building block approach. The experimental test campaign required to complete and verify composite vehicles is costly. The research in Lightweight composites materials and structures aims to increase analysis capability to allow increased virtual testing, and hence reduce cost related to physical testing. Over the last decade Leif’s research has been focused on realization of multifunctional composites. Using carbon fibres are reinforcement and electrodes in an engineering material structural battery composites are made. The work addressed multi-physics models and characterization methods as well as materials processing and manufacture.

_A car built from multifunctional composite materials; structural materials with intrinsic energy storage, connectivity, sensing, energy harvesting and softening capabilities._

**SELECT PUBLICATIONS**


Structural power composites; L. E. Asp, E. S. Greenhalgh; Composites Science and Technology 101, 41-61 (2014)

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**MECHANICS OF LIGHTWEIGHT COMPOSITES**

My research focuses on composite process modeling and mechanics, with emphasis on multifunctionality and bio-based composites. New composite processing methods require a better understanding of the development of mechanical properties during the cure cycle. The development of accurate thermomechanical material models introduces new methods for more efficient and sustainable manufacturing. Images can be used to interpret microstructure or meso-structure in composite materials. Automated generation of virtual samples creates a virtual experimentation framework for understanding the mechanical impact of a specific micro-structure or meso-structure. This type of virtual experimentation can be used to narrow new material development options, specifically in hierarchical materials like those developed in the All-Wood Composite platform.

For a multifunctional material like a graphene polymer composite, the structural, thermal, and electrical properties may all need to be included in a virtual experimentation framework. Using computational homogenization of the microstructure, approximate properties of the overall composites can be obtained.

_A car built from multifunctional composite materials; structural materials with intrinsic energy storage, connectivity, sensing, energy harvesting and softening capabilities._

**SELECT PUBLICATIONS**


A systematic approach to transforming composite 3d images into meso-scale computational models; B. Blinzler, D. Wilhelmsson, L. Asp, K. Jespersen, L. Mikkelsen; ECCM18 proceedings (2018)

POLYMERIC MATERIALS AND COMPOSITES

The research group generally deals with useful relations between the structure and the functional properties of synthetic and renewable polymeric materials, to the benefit of making better use of polymeric materials and composites. Scientific concerns are typically on the influence of rheological properties of melts and liquids on manufacturing processes, structuring and shaping melt processing, thermal and mechanical behaviour, ageing of polymeric materials and surface appearance characteristics (gloss, surface topography and colour).

Current interests are mainly on thermoplastic composites reinforced with cellululosics (fibres, nanofibrils and nanocrystals) meant for high mechanical performance. Other current interests concern recycling of polymeric materials, processing and properties of renewable polymeric materials (hemicellulose and starch) and composites reinforced with graphene and carbon fibres. The work involves fundamental and applied materials physics, the flow behaviour of melts and dispersions, also co-operations on chemical modifications and advanced spectroscopy, towards improved manufacturing and application of current polymeric materials.

SELECT PUBLICATIONS


The influence of compatibilizer addition and gamma irradiation on mechanical and rheological properties of a recycled WEEE plastics blend; S. Tostar, E. Stenvall, A. Boldizar and M. R. S. Foreman; Recycling 1, 101-110 (2016)

POLYMERIC MATERIALS • COMPOSITES • STRUCTURE • RHEOLOGY • MELT PROCESSING • MECHANICAL PROPERTIES • THERMAL PROPERTIES • RHEOLOGY • AGEING • APPEARANCE

MATERIAL SCIENCE AND ENGINEERING

Material science and engineering focusing on characterization using modern analytical methods. Research on both applied and basic levels in the areas including coatings, corrosion and oxidation, additive manufacturing, microelectronics, nanotechnology and so on. Special emphasis on surface technology/surface characterization for traditional and new materials, focusing on analysis using X-ray photoelectron spectroscopy (XPS) and Auger electron spectroscopy (AES) having the sampling depth less than 10 nm.

Mechanical behaviours of engineering metals and the correlation with microstructure, temperature and strain rate.

SELECT PUBLICATIONS

XPS Calibration Study of Thin Film Nickel Silicides; Y. Cao, L. Nyborg and U. Jelvestam; Surface and Interface Analysis 41, 471–483 (2009)

Temperature and Strain Rate Effects on the Mechanical Behaviour of Dual Phase Steel; Y. Cao, B. Karlsson and J. Ahlström; Materials Science & Engineering A 463, 124–132 (2005)

Grain boundary microstructure and fatigue crack growth in Alvac 718 Plus superalloy; L. Viskari, Y. Cao, M. Norell, G. Sjoberg, K. Stillier; Materials Science and Engineering, A 528, 2570-2580 (2011)

SURFACE ANALYSIS • XPS • AES • THIN FILMS • METALLURGY • COATINGS • CORROSION AND OXIDATION • ADDITIVE MANUFACTURING • NANOTECHNOLOGY • MECHANICAL BEHAVIOURS
MATERIALS AND SURFACE SCIENCE
I am heading a research group that adopt a green chemistry approach to surface chemistry and catalysis. Our aim is to contribute with fundamental understanding of functional materials that have direct relevance for developing chemical technologies for environmental protection and energy conversion without putting health at risk but instead create economic growth within a sustainable societal framework. We synthesize and study materials for pollution prevention and for utilization of CO₂ and biobased routes towards chemicals, fuels and food. We want to understand the operating surface processes and link these to physicochemical properties of the materials, which typically spans from extended ideal surfaces to nanomaterials and clusters. For this we use operando spectroscopic and scattering methods in our home laboratories and at international research facilities. Thereby the paradigm of tailoring functional materials can be shifted from being traditionally intense on trial-and-error approaches to rely on a knowledge-based design.

SELECT PUBLICATIONS


SURFACE CHEMISTRY • GREEN CHEMISTRY AND CATALYSIS • OPERANDO CHARACTERISATION • CO₂ UTILISATION • BIOBASED ECONOMY

PHYSICS WITH APPLICATIONS
For an experimental physicist within the interdisciplinary area of Surface Science the scientific challenges are numerous. My research interests are towards examination of the fundamental energy and charge transfer between substrate and the adsorbed layer as result of adsorption and during electron, ion and photon irradiation. Specifically, experimental evaluation of the mechanisms of optical excitations in nanoparticle- and nanocavity arrays and the related physical and chemical processes at their interfaces. Physics and chemistry of ice and carbon materials are of special interest.

SELECT PUBLICATIONS
Photoinduced crystallization of amorphous ice films on Graphite; D. Chakarov and B. Kasemo; Physical Review Letters, 81(23), 5181-5184 (1998)


Photodesorption of NO from graphite(0001) surface mediated by silver clusters; K. Wettergren, B. Kasemo and D. Chakarov; Surface Science, 593(1-3), 235-241 (2005)

OPTICS OF NANOPARTICLES • NANO FABRICATION • SURFACE SCIENCE • WATER • ICE • CARBON
**FUNCTIONAL NANOSTRUCTURES**

I lead a research group of around 10 people working with functionalized nanostructures for various applications. We prepare our (solid state) nanostructures in the nanofabrication facilities and modify them using wet chemistry. We analyse what happens on the surface of the nanostructured materials with optical and electrical methods. Our work is currently focused on nanopores in thin films functionalized with polymers that can regulate transport of proteins through the pores. Besides addressing fundamental questions in supramolecular chemistry, these hybrid materials can be used for various bioanalytical applications such as separation and entrapment or proteins. The image is taken from a recent publication where we used antibodies as “keys” to switch nanopores with polymers between an open and a closed state with respect to protein transport.

**SELECT PUBLICATIONS**


Sensing applications based on plasmonic nanopores: The hole story; A. B. Dahlin; Analyst 140 (14), 4748-4759 (2015)

**MATERIAL MECHANICS**

Main research topic is modelling of mechanical behaviour of materials on different scales. A focus area of the research is the development of macroscopic models that should capture phenomena such as cyclic ratcheting behaviour, temperature dependence, creep deformations, damage mechanisms and, for large strains, the evolution of anisotropy in terms of texture and evolving yield surfaces. Another focus area of the research is the development of crystal plasticity models together with multi-scale modelling for polycrystals. In this area the particular focus is on modelling of dislocation pile-up, oxidation and fracture at grain boundaries.

**SELECT PUBLICATIONS**


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**NANOPORES • POLYMER BRUSHES • PROTEINS • SUPRAMOLECULAR CHEMISTRY**

**PLASTICITY • VISCOPLASTICITY • CRYSTAL PLASTICITY • ANISOTROPY • LARGE DEFORMATIONS • FINITE ELEMENT SIMULATIONS • MULTI-SCALE MODELLING • MODEL CALIBRATION**
COMPUTATIONAL MATERIALS PHYSICS

My research group applies electronic and atomic scale modeling techniques to study the fundamental properties of complex materials. Current research topics include thermal and electrical transport, thermodynamics as well as the optical properties of nanoparticles. Method and software development constitutes a substantial part of our research as we require high-performant tools to obtain efficient and accurate models of real materials.

SELECT PUBLICATIONS

- The hiphive package for the extraction of high-order force constants by machine learning; F. Eriksson, E. Fransson, P. Erhart; Advanced Simulation and Theory (2019) doi: 10.1002/adts.201800184
- Plasmon-Induced Direct Hot-Carrier Transfer at Metal-Acceptor Interfaces; P. V. Kumar, T. P. Rossi, D. Marti-Dafcik, D. Reichmuth, M. Kuisma, P. Erhart, M. J. Puska, and D. J. Norris; ACS Nano 13, 3188 (2019) doi: 10.1021/acsnano.8b08703

- Thermodynamics and optical properties of metallic nanoparticles.

COMPUTATIONAL MODELLING OF FAILURE IN LIGHTWEIGHT MATERIALS

The research in my group primarily aims to develop accurate, and at the same time, efficient computational models and methods for simulating failure in various types of materials. In current focus are lightweight materials and structures relevant for the automotive industry, the aeronautical industry and in sports. Most of the current projects concern failure in various composite materials, from high-performing carbon fibre composites to sustainable bio-composites with bio-sourced constituents. The image illustrates the numerical prediction of crack growth patterns in a fibre reinforced block of material with a central hole subjected to shear loading. As can be seen, the modelling techniques developed are able to represent a rather complex interaction of small cracks in a network which eventually coalesce into a dominating crack.

SELECT PUBLICATIONS

- A two-scale modeling framework for strain localization in solids: XFEM procedures and computational aspects; E. Svenning, F. Larsson and M. Fagerström; Computers and Structures 211, 143-54 (2018)

- The numerical prediction of crack growth patterns in a fibre reinforced block of material with a central hole subjected to shear loading.
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MICROSTRUCTURES OF INORGANIC MATERIALS

My research is concerned with relationships between microstructure and properties of hard, inorganic, structural materials. The research involves the application of different scanning and transmission electron microscopy techniques for imaging and microanalysis. The work covers three areas of materials science: (i) development and stability of nano- and microstructures, (ii) toughening and strengthening mechanisms, and (iii) deformation mechanisms. The development of nano- and microstructures under different processing and testing conditions is characterized by high resolution imaging and microanalysis, and the results are related to different parameters in the fabrication process and to the behaviour of the material under mechanical and thermal load. A significant part of the research has been concerned with the development of fine-scale microstructures during sintering and crystallisation processes in ceramics and oxynitride glass-ceramics. The mechanical and chemical behaviour of ceramic matrix composites, including nanocomposite materials, has been investigated, and the role of the internal interfaces in these materials has been addressed. My current research interest also includes the intergranular structure and properties of cemented carbide materials for cutting tool applications.

A thin (1.4 nm) intergranular film of residual glass in a silicon nitride ceramic.

SELECT PUBLICATIONS


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INDUSTRIAL MATERIALS RECYCLING AND NUCLEAR CHEMISTRY

I hold the view that my goal as a chemist in Industrial Materials recycling is to “create new chemical processes for the recycling of that which is currently impossible (or difficult) to recycle”. An important part of my work is to devise methods of recycling “difficult” materials both without causing a loss of quality of the material being recycled or the production of new wastes.

I have an interest both in recycling metals (both base and precious) and organic substances (such as polymers). I have a particular interest in solvent extraction for the recycling of metals using new and more sustainable reagents. This includes the deep eutectic solvents, I have an interest in solvent extraction from these and in their solvent properties.

I am also involved in Nuclear Chemistry where I have an interest in a range of topics including reactor accidents, automated emergency radiochemistry for analysis and advanced separations.

A neodymium complex of a new extraction reagent, two molecules of an octopus class reagent are binding to the metal.

SELECT PUBLICATIONS


Temperature effect on the distribution of lanthanides(III) in the perchlorate-malonamide-methyl isobutyl ketone systems; M. S. Tyumentsev, M. R. S. Foreman, B. M. Steenari and C. Ekberg; Journal of Chemical Thermodynamics 131, 133-148 (2019)

SILICON-BASED CERAMICS • NITRIDES • CEMENTED CARBIDES

SOLVENT EXTRACTION • DEEP EUTECTIC SOLVENTS • NEW REAGENTS • NUCLEAR REACTOR ACCIDENTS • RECYCLING • VALUE RECOVERY • NUCLEAR CHEMISTRY • NEW SEPARATIONS • AUTOMATED CHEMICAL SEPARATIONS • SOLVENT PROPERTIES
HIGH-ENTROPY ALLOYS
Sheng Guo is currently an Associate Professor at the IMS Department, Chalmers. His group mainly works on high-entropy alloys, a new type of metallic materials that comprise multi-principal elements, distinguishing them from conventional alloys where only one or two principal elements are used. The concept of high-entropy alloys opens up a massive and unexplored compositional space, and is promisingly leading to the development of novel metallic materials with unprecedented structural and functional properties. Sheng Guo’s group mainly uses the concept of high-entropy alloys to design new generation of high-temperature materials, with targets including the enabling of turbine engines to operate at higher temperatures, for an improved energy efficiency. In addition, his group also actively looks for functional applications for high-entropy alloys, for example, as constant electrical resistivity materials, low expansion materials, and corrosion-resistant and biocompatible materials.

SELECT PUBLICATIONS
More than entropy in high-entropy alloys: Forming solid solutions or amorphous phase; S. Guo, Q. Hu, C. Ng, C. Liu; Intermetallics 41, 96 (2013)

ORGANIC CHEMISTRY OF WOOD BASED MATERIAL BIOREFINERY, CELLULOSE SOLUTIONS AND MATERIALS
With organic chemistry as a platform and wood-based bio-refinery as an ultimate goal and a framework, our research is centered around chemical aspects of separation and valorization of wood polysaccharides. More specifically, the focus is on chemical approaches for recovery of wood hemicelluloses and chemistry of dissolution and modification of cellulose in aqueous alkaline systems. Our current work is focused on:
• elucidation of an overlooked CO\(_2\) chemistry active in the industrially and scientifically important cellulose/NaOH(aq) solutions, a chemistry that can be employed to affect cellulose stability and formation of coagulated structures from these solutions
• investigation of fundamental stabilizing interactions in aqueous alkaline solutions of cellulose, with the emphasis on the cation interactions
• cellulose functionalization through aqueous oxidative chemistry

SELECT PUBLICATIONS
Chemisorption of air CO\(_2\)(g) on cellulose: an overlooked feature of the cellulose/NaOH(aq) dissolution system; M. Gunnarsson, H. Theliander, M. Hasani; Cellulose, 24, 2427-2438 (2017)
The CO\(_2\) capturing ability of cellulose dissolved in NaOH(aq) at low temperature; M. Gunnarsson, D. Bomin, A. Östlund, M. Hasani, Green Chemistry, 20, 3279-3286 (2018)
PHOTO-, ELECTRO-, CHEMICAL REACTIONS AND MATERIAL DESIGN

The research of Anders Hellman focuses on pinpointing the underlying reasons (atomic and/or electronic structure) for various processes relevant to surface science, heterogeneous catalysis and materials for energy applications. This is mostly done via electronic structure calculations and multi-scale methods, e.g., kinetic Monte-Carlo or micro-kinetics, to bridge length and time scales. Research interests include charge-transfer processes, hot-electron chemistry, surface reactions, phase transformations and time evolution of catalytic reactions. He has worked on various topics related to surface science, heterogeneous catalysis and materials for energy harvesting, such as, charge transfer and non-adiabaticity in surface reaction, ammonia synthesis, CO and methane oxidation, thin oxides supported on metals, and photoelectrochemical studies of water oxidation.

As an example from my research I chose the product distribution from electrooxidation of glycerol as a function of applied potential. Such information can improve how we utilize different chemical feedstock in the future.

SELECT PUBLICATIONS

Development of Robust Powder for Additive Manufacturing.

SELECT PUBLICATIONS
Stoichiometric vanadium oxides studied by XPS; E. Hryha, E. Rutqvist, L. Nyborg; Surface and Interface Analysis, 44(8), 1022-1025 (2012)


SELECT PUBLICATIONS
Ethylene Epoxidation on Ag (100), Ag (110), and Ag (111): A Joint Ab Initio and Kinetic Monte Carlo Study and Comparison with Experiments; M. Huš, A. Hellman; ACS Catalysis 9, 1183-1196 (2018)

Electrooxidation of glycerol on gold in acidic medium; a combined experimental and DFT Study; M. Valter, M. Busch, B. Wickman, H. Grönbeck, J. Baltrusaitis, A. Hellman; The Journal of Physical Chemistry C 122, 10489-10494 (2018)
HETEROGENEOUS CATALYSIS FOR ENVIRONMENTAL APPLICATIONS

The research performed in my group focuses on catalyst design and synthesis aiming to increase the understanding of the interplay between the catalytic material and the surface reactions and mechanisms. To increase energy efficiency in various processes, catalysis plays an important role, for instance regarding emission control and for synthesis of new (green) materials and fuels. In catalyst design, atomistic insight and detailed knowledge on reaction mechanisms and catalytically active sites is vital, which is why we work with synthesis of tailored materials where e.g. composition, size, and shape can be precisely tuned.

FIRST PRINCIPLE DENSITY FUNCTIONAL THEORY

We lead development of the van der Waals density functional (vdW-DF) method as a many-body physics and materials theory. The method has broad international recognition since it permits computationally efficient, first-principle density functional theory calculations of both dense and sparse materials, for example, organics and their interfaces. The recent consistent formulations of the vdW-DF method have a high accuracy and, equally important, have proven itself useful as a general-purpose computational tool for materials theory. Since the consistent vdW-DF versions avoid all parameters, they permit usage in a sub-Ångström microscopy-type mode, using calculations to track and interpret the origin and spatial distribution of, for example, the noncovalent binding between molecules.

SELECT PUBLICATIONS

Exchange functional that tests the robustness of the plasmon description of the van der Waals density functional; K. Berland and P. Hyldgaard; Physical Review B 89, 035412 (2014)

SELECT PUBLICATIONS

Catalytically active Pd/Ag alloy nanoparticles synthesized in microemulsion template; L. Ström; H. Ström; P-A. Carlsson; M. Skoglundh; H. Härelind; Langmuir 34 (33), 9754–9761 (2018)
Silver/alumina for methanol-assisted lean NOx reduction - on the influence of silver species and hydrogen formation; M. Männikkö; X. Wang; M. Skoglundh; H. Härelind; Appl. Catal. B 180, 291-300 (2016)

DRIFT spectrum that illustrates how surface acetate species diminish upon change of gas phase forming surface formate species.
SINGLE NANOPARTICLE ANALYTICS

The lipid bilayer is probably the most fascinating example of material utilized by living organisms. Through evolutionary design, this 5 nm thick two-dimensional liquid has been selected as the boundary of all living cells, where it acts as a compartmentalizing hydrophobic barrier preventing solutes from freely diffusing in and out of cells and their organelles. In my research group, we develop surface-based bioanalytical sensors, with special emphasis on studies of cell-membrane mimics and biological nanoparticles such as viruses, exosomes and lipid nanoparticles for medical diagnostic and drug-discovery applications. Particular focus is presently put on surface-based microscopy combined with flow-cytometry like microfluidic-based analysis of the relation between nanoparticle characteristics and the nature of their multivalent interactions with cell membranes.

SELECT PUBLICATIONS


NEXT GENERATION BATTERIES

My research group creates and investigates different next generation battery concepts with real application demands in mind – hence employing both top-down and blue sky paradigms of science. Foremost we continuously combine our fundamental understanding of new materials gained at the molecular level with battery concept development and real battery performance - to make these longer-lasting, more performant, less environmentally demanding, etc. We therefore must be able to combine ab initio/DFT computational methods and IR/Raman spectroscopy with the macroscopic battery voltage and current demands via ion transport phenomena and cell performance measurements. Our special interest is electrolytes; liquids, gels, polymeric, and ionic liquids, applied to next generation batteries such as Na-ion, Li-S, Mg, Ca, Al, etc., often within large national and international projects, many involving Swedish and European industry.

SELECT PUBLICATIONS

COMPUTATIONAL SOLID MECHANICS
I am working with the computational simulation of complex materials on multiple length scales. Applications range from damage in Lithium ion batteries related to ion transport during charging-discharging cycles to the formation of crack patterns during desiccation processes of granular materials. Major aims of my work are: Speed-up multi-scale and multi-field simulations with the aid of machine learning strategies, and simulations based on 3D data, e.g. from X-Ray or FIB computed tomography.

SELECT PUBLICATIONS
Identification of viscoelastic properties from numerical model reduction of pressure diffusion in fluid-saturated porous media with fractures; R. Jänicke, F. Larsson, K. Runesson; Computational Mechanics 63, 49-67 (2019)

FINITE ELEMENT METHOD • COMPUTATIONAL HOMOGENIZATION • MULTI-PHYSICS MODELING

RHEOLOGY AND PROCESSING OF SOFT MATTER
The processing of soft matter into products typically involves rheologically complex fluids in complex flow configurations. Thus, understanding flow-field-matter/compositional interactions in relation to fundamental rheological properties is essential for obtaining products with favorable performance. In this framework, the staples of my research and current related activities and interests are:
(i) Advanced characterization methods, method development - focused on nonlinear material characterization and hypothesis rheological techniques, e.g. rheo-microscopy, rheo-SAXS, mainly applied to nanocellulose suspensions, polymer nanocomposites, adhesives and biomaterials (biofilms, tissues).
(ii) Tailoring multifunctional properties in nanostructured materials - focused on the process structuring of polymer nanocomposites based on graphene and other high aspect ratio fillers for enhanced electrical, antibacterial, thermal, mechanical, gas-barrier etc. properties.
(iii) Dynamics of simple and complex fluids for processing applications - focused on modeling, processing flow and compositional optimization of high filler content bicomposites and flow-assisted structuring of nanocrystalline cellulose dispersions.

SELECT PUBLICATIONS
First normal stress difference and in-situ spectral dynamics in a high sensitivity extrusion die for capillary rheometry via the ‘hole effect’; T. Nypelö, M. G. Naue, M. Wilhelm; Polymer 104, 193-203 (2016)
SELECT PUBLICATIONS

Unraveling the mechanisms of thermal quenching of luminescence in Ce3+-doped garnet phosphors; Y.-C. Lin, M. Bettinelli, M. Karlsson; Chemistry of Materials 31, 11, 3851-3862 (2019)


Understanding the interactions between vibrational modes and excited state relaxation in Y3-xCexAl5O12: design principles for phosphors based on 5d-4f transitions; Y.-C. Lin, P. Erhart, M. Bettinelli, N. C. George, S. F. Parker, M. Karlsson; Chemistry of Materials 30, 1865-1877 (2018)

The garnet phosphor YAG:Ce3+ exhibits a decrease in light emission and variation in color upon increasing temperature, as a result of certain vibrational motions of the CeO8 moieties.
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**SELECT PUBLICATIONS**  

**FORMULATION AND MATERIAL SCIENCE BASED ON CELLULOSIC MATERIALS**

Our group are striving to achieve molecular understanding of how molecular structures are related to and controlling the functionalities of the materials like barriers and pharmaceutics. Examples of functionalities are: molecular transport, drug release rates, thermic and mechanical properties etc. This can be exemplified by the water permeability through a film coating (barrier) based on a mixture of ethyl cellulose and hydroxypropyl cellulose. During the coating step the polymers phase separates. Upon exposure to aqueous medium the water-soluble polymer dissolves and forms water filled channels. In coated pellets formulations, the drug can then diffuse out through the coating and be released. We have shown that the structure of the polymers in the coating controls the molecular transport and release rate. Our group also relates the molecular structure to the materials’ thermic behavior and mechanical properties.

**SELECT PUBLICATIONS**

A two-scale modeling framework for strain localization in solids: XFEM procedures and computational aspects; E. Svenning, F. Larsson and M. Fagerström; Computers and Structures 211, 43-54 (2019)  
A multiscale model for reinforced concrete with macroscopic variation of reinforcement slip; A. Sciegaj, F. Larsson, K. Lundgren and K. Runesson; Computational Mechanics 63, 139-158 (2019)  

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**EFFICIENT BRIDING OF SCALES IN COMPUTATIONAL MECHANICS OF MATERIALS**

My research area is multiscale computational mechanics. In particular, we focus on developing accurate and efficient numerical models for bridging continuum length scales of materials based on the Finite Element Method. In order to increase computational efficiency, Numerical Model Reduction is applied in order to reduce the number of degrees of freedom at the microscale. In the figure, Numerical Model Reduction for an idealized microstructure is illustrated in terms of reduced basis functions used for the approximation of temperature. A key feature of the developed methodology is the accompanying error control. Current research projects range from polycrystalline metals, via various composites, to multiscale modeling of fluid-filled porous media.

**SELECT PUBLICATIONS**

Illustration of Numerical Model Reduction in microscale heat flow for an idealized microstructure (a) with reduced basis functions (b-d).

**CELLULOSE DERIVATIVES • MOLECULAR TRANSPORT • BARRIER PROPERTIES • DRUG RELEASE • PERSONALIZED MEDICINE • CELLULOSE • ADSORPTION • 3D PRINTING AND EXTRUSION OF PHARMACEUTICS AND BIOPOLYMER MATERIALS • THERMOPLASTIC CELLULOSE MATERIALS**
COMPUTATIONAL MATERIAL MECHANICS

High demands are placed on the manufacturing processes concerning machining and forming processes of high strength metal materials. The same demands apply to composites, where advanced composites are increasing due to the high interest in lightweight design. In this context my research is centered, comprising mechanics based modeling and FE-simulation of materials and structures for lightweight design and manufacturing processes. The current research is concerned with wet-out processes for composite materials, impact failure modelling of advanced composites, graphene enhanced polymers and machinability assessment of new metallic materials. My scientific challenges involve robust, accurate and cost efficient model development based on basic principles of continuum mechanics. The areas of concern relate to modeling of inelasticity mechanisms, consistent damage and fracture, porous media with free surfaces and homogenization of micro-structures.

SELECT PUBLICATIONS

Damage growth and strain localization in compressive loaded fiber reinforced composites; R. Larsson, R. Gutkin, M. Rouhi; Mechanics of Materials 127, 77-90 (2018)


X-RAY SCATTERING AND IMAGING

The focus of our research is in the development of X-ray scattering and imaging techniques and their application towards materials with hierarchical structure. The applications we are working on in different collaborations are spanning a broad range from biomimetic hierarchical nanocomposites, materials based on cellulose, industrial injection-molded plastics as well as the characterization of bone and soft tissue. A common denominator of these diverse applications is the arrangement of nanometer-sized building blocks within macroscopic samples, in particular the alignment of anisotropic constituents. To that end, SAXS tensor tomography, which allows to look at nanostructure alignment in 3D macroscopic samples is a powerful tool.

SELECT PUBLICATIONS


CONTINUUM MECHANICS • COMPUTATIONAL MATERIAL MECHANICS • STRUCTURAL MECHANICS • HOMOGENIZATION OF MICROSTRUCTURES • LOCALIZATION OF DEFORMATIONS • INTERFACES • DAMAGE AND FRACTURE MECHANICS • SHELL MODELING • POROUS MEDIA THEORY • FE-TECHNOLOGY

SAXS IMAGING • SOFT MATTER • MICROFLUIDICS • HIERARCHICAL MATERIALS • NANOSTRUCTURE ORIENTATION
MICROSTRUCTURE AND FUNCTIONALITY OF MATERIALS
We use advanced microscopy techniques to reveal structure-property relationship of materials. Our work enables design of novel materials, processing, and devices to enhance functionality and performance on a system level. Our research interests include:

- **Multifunctional composites**: We are exploring the intrinsic structural (as reinforcements) and electrochemical (as electrodes) nature of carbon fibres in a multifunctional devise – structural composite battery. We collaborate closely with Leif Asp and Patrik Johansson at Chalmers, and Dan Zenkert, Göran Lindbergh, and Mats Johansson at KTH.
- **Composites reinforced with cellulose based fibres**: We are developing a novel platform dedicated to mechanical testing of miniature cellulose fibre reinforced composites inside advanced electron microscope. We collaborate with researchers within the All Wood Composite Platform at Chalmers.
- **High temperature steels**: To overcome the trade-off between creep and corrosion resistance in conventional 9–12% Cr steels, we are exploring new concepts of designing a new generation of steels.

SELECT PUBLICATIONS


NANOMATERIALS FOR ELECTRONICS PACKAGING AND THERMAL MANAGEMENT
I am leading the research at the Electronics Materials and Packaging Group at the Electronics Materials and Systems Laboratory, Department of Microtechnology and Nanoscience. We take care of the research and education in this field at Chalmers. Our main research is to formulate, develop and characterize new materials and processes for electronics packaging, thermal management and interconnect applications. The main research question we ask is how to create and manipulate lattice structures and crystal orientation of 1D (such as carbon nanotube) and 2D (such as graphene and hexagonal boron nitride) materials to maximize thermal and electrical conductivity, significantly better than existing materials.

SELECT PUBLICATIONS
Functionalization mediates heat transport in graphene nanoflakes; H. Han et al; Nat. Commun. 7(11281), (2016) doi: 10.1038/ncomms11281
Tailoring the Thermal and Mechanical Properties of Graphene Film by Structural Engineering; N. Wang et al; Small 14, 1801346 (1 of 8) (2018)

IN-SITU MICROSCOPY • CORRELATIVE MICROSCOPY • MICROMECHANICAL TESTING • COMPOSITES • BATTERY MATERIALS • CELLULOSE BASED FIBRES • FIB/SEM (COMBINED FOCUSED ION BEAM AND SCANNING ELECTRON MICROSCOPY) • TEM (TRANSMISSION ELECTRON MICROSCOPY) • APT (ATOM PROBE TOMOGRAPHY)
**BIOPOLYMERS AND BIONANOCOMPOSITES**

A distinctive feature of studying biopolymeric materials relates to the search for relations between the structure (on different levels), the processing and the material properties. The research is often of an interdisciplinary character and covers both fundamental and applied issues. The use of such materials requires an adaptation of the processing techniques in relation to their rheological and thermal properties, with the aim of a nanostructure control for improved mechanical and/or other physical properties. Specific interests focus on understanding how the structure-modification of cellulose and lignin affects their viscoelastic properties and processability.

The research area merges polymer physics and polymer chemistry for the overarching aim of new material design. Strong attention is devoted to advances in understanding the processing-structure-properties relationships of materials, including bottom-up approaches for material engineering from the molecular design towards new routes for sustainable reactive processing, aiming at the control of the material nanostructure.

**SELECT PUBLICATIONS**


Tunable thermosetting epoxies based on fractionated and well-characterized lignins; C. Gioia, G. Lo Re, M. Lawoko, L. Berglund; Journal of the American Chemical Society 140(11), 4054-4061 (2018)

Poly(ε-caprolactone) Biocomposites Based on Acetylated Cellulose Fibers and Wet Compounding for Improved Mechanical Performance; G. Lo Re, S. Spirella, A. Boujemaa, F. Vilaseca, P. T. Larsson, F. Adås, L. Berglund; ACS Sustainable Chemistry & Engineering 6(5), 6753–6760 (2018)

**OPTICS AND ULTRAFAST DYNAMICS IN ATOMICALLY THIN 2D MATERIALS**

My research is focused on microscopic modelling of ultrafast phenomena in atomically thin 2D nanomaterials including graphene, transition metal dichalcogenides (TMDs) and Van der Waals heterostructures. These materials exhibit fascinating properties that are interesting both for fundamental science as well as for technological applications. In particular, we perform quantum mechanical calculations of time- and energy-resolved non-equilibrium dynamics of electrons, excitons, phonons, and photons in these materials. The driving force of my research is to unravel elementary processes behind ultrafast phenomena and to exploit the gained insights to propose novel concepts for technological devices. The explored scientific questions cover fundamental physics including strong many-particle phenomena (such as carrier-carrier, carrier-phonon, and carrier-photon interactions) and application-oriented research aiming at the design of future nanoelectronic devices (such as photo-emitting, amplifying, and detecting devices).

**SELECT PUBLICATIONS**


Carrier Multiplication in Graphene; T. Winzer, A. Knorr, and E. Malic; Nano Letters 10, 4839 (2010)

Proposal for dark exciton based chemical sensors; M. Feierabend, G. Berghaeuser, A. Knorr, and E. Malic; Nature Communications 8, 14776 (2017)
PROTONIC AND IONIC CONDUCTION IN IONIC LIQUIDS AND NANO-PORES

My research is focused on the study of ionic and protonic conduction in protic ionic liquids. This is investigated in pure ionic liquids, in mixtures of ionic liquids and neutral solvents (e.g. water, imidazole or ethylene glycol), and in confined environments, such as perfluorinated polymers or nano-porous silica. One relevant application for these materials is envisaged to be in proton exchange fuel cells operating at temperatures higher than 120 °C. The characterisation methods that we use on a regular basis include vibrational spectroscopy (infrared and Raman), NMR spectroscopy (1D 1H, diffusion NMR, and variable temperature solid state NMR), calorimetry (DSC & TGA), impedance spectroscopy and X-ray diffraction methods, but we also get support through collaborators from MD simulations.

SELECT PUBLICATIONS
Structural origin of proton mobility in a protic ionic liquid/imidazole mixture: Insights from computational and experimental results; N. Yaghini, V. Gómez-González, L.M. Varela, A. Martinelli; Physical Chemistry Chemical Physics 18 (33), 23195-23206 (2016)


A nano-porous carbon nano-fibre membrane that enables high capacity LiS-batteries.

SELECT PUBLICATIONS
Rational design of low cost and high energy lithium batteries through tailored fluorne-free electrolyte and nanostructured sulfur/carbon composite; M. Agostini, D-H. Lim, M. Sadd, J-Y. Hwang, S. Bruttì, J. Heo, J-H. Ahn, Y-K. Sun, and A. Matic; ChemSusChem 11, 2981-2986 (2018)


Free-standing 3-D sponged nano-fibre electrodes for ultrahigh-ate energy storage devices; M. Agostini, D-H. Lim, S. Bruttì, N. Lindahl, J. H. Ahn, B. Scrosati, and A. Matic; Applied Materials and Interfaces 10, 34140-34146 (2018)
SELECT PUBLICATIONS


NANO MATERIALS CHEMISTRY

Kasper Moth-Poulsen is leading the “Molecular Materials” research group at the Department of Chemical and Chemical Engineering at Chalmers University of Technology. He work with the design and synthesis of new self-assembled materials. Our goal is to make materials from nanoparticles, nanorods and tailor made small molecules for a broad range of applications ranging from single molecule electronics to sensors and renewable energy.

POLYMER SCIENCE

I am a materials scientist and my core expertise lies in combining classical polymer science with organic electronics. My group focuses on the physical chemistry of organic semiconductors, polymer blends and composites, and develops new plastic materials for energy technologies ranging from organic solar cells and thermoelectrics to power cables.

SELECT PUBLICATIONS


SOFT MATTER CHARACTERIZATION
Lars Nordstierna is a physical chemist devoted to surface and colloid chemistry. His research group has a focus on soft matter characterization and development of new materials. The characterization is often based on the application of NMR spectroscopy, ranging from solid-state (e.g., molecular linearity in fibers) and diffusometry (e.g., molecular association in solution) to high-resolution methods (e.g., quantification of multi-functionalized polymers). From a materials perspective, molecular and supramolecular properties of biomass-based materials is one of the main interests where cellulose is the central polymer. Another focus is formulation and physical properties of core-shell particles in order to achieve controlled release of active substances from e.g., surface coatings or wound dressings.

SELECT PUBLICATIONS
Molecular orientation distribution of regenerated cellulose fibers investigated with rotor synchronized solid state NMR spectroscopy; L. Svenningsson, T. Sparman, E. Bialik, D. Bernin, and L. Nordstierna; Cellulose 26, 4681-4692 (2019)
Controlled release of a microencapsulated arduous semi-hydrophobic active from coatings; Superhydrophilic polyelectrolyte shells as globally rate-determining barriers; J. Bergek, M. Andersson Trojer, H. Uhr, and L. Nordstierna; Journal of Controlled Release 225, 31-39 (2016)

ENGINEERING METAL SURFACES
My research focuses on the degradation of engineering metal surfaces in harsh environments. This often limits the capability of technical systems. Thorough studies of the material performance give a fundamental basis for alloy selection, and helps to identify relevant degradation mechanisms. The studies of materials degradation on scales ranging from meter to nanometer are related to the material structure and the application. This is combined with lab experiments, often mimicking complex environments, and detailed characterization of the degradation. In particular we use surface analytical tools like AES (Auger Electron Spectroscopy) and XPS on both technical surfaces from the field, and on lab material. The applications include high temperature corrosion of stainless steels in both boilers and exhaust systems, and of cast steels and iron used in engines manifolds. Regarding the running in of gear surfaces microstructural changes have been connected to the residual stresses, the surface chemistry and micropitting.

SELECT PUBLICATIONS
High temperature corrosion of cast alloys in exhaust environments I-ductile cast irons; F. Tholence, M. Norell; Oxidation of Metals 69 (1-2), 13-36 (2008)
Characterization of surface oxides on water-atomized steel powder by XPS/AES depth profiling and nano-scale lateral surface analysis; D. Chasoglou, E. Hryha, M. Norell, L. Nyborg; Applied Surface Science 268, 496-506 (2013)
POWDER METALLURGY AND ADDITIVE MANUFACTURING/SURFACE SCIENCE

Focus is placed on powder technology and surface science with particular reference to sintering of metal powder as well as metal additive manufacturing, gathered within the research group Powder Metallurgy and Additive Manufacturing. This group is also the main actor and host of the Vinnova competence centre for additive manufacturing (CAM2). How surface chemistry and powder properties affect the processing in these cases is a core research question. The research hence addresses how powder composition can be tuned and how novel powder technological approaches can be applied to arrive at improved materials and products. Core tools include the application of XPS, Auger and microscopy, theory development and processing experiments. Extensive co-operation with Swedish industry as well as other academic institutions is developed.

SELECT PUBLICATIONS

Stoichiometric vanadium oxides studied by XPS; E. Hryha, E. Rutqvist, L. Nyborg; Surface and Interface Analysis, 44 (8), 1022-1025 (2012)

Characterization of surface oxides on water-atomized steel powder by XPS/AES depth profiling and nano-scale lateral surface analysis; D. Chasoglou, E. Hryha, M. Norell, L. Nyborg; Applied Surface Science 268, 496-506 (2013)

FROM WOOD TO HIERARCHICAL MATERIALS

My research is on engineering wood-components into hierarchical materials with a function. The core is to build from liquid-rich state, gels, emulsions, dispersions, solutions, colloids toward solid organizations. I combine forest products technology, materials science and renewable resources for advancing sustainable materials engineering. The research efforts involve cellulose, hemicelluloses and lignins with emphasis on surface, interface, and intermolecular interactions.

SELECT PUBLICATIONS


THE CORRELATION BETWEEN ATOMIC STRUCTURE AND PROPERTIES OF NANOSTRUCTURE MATERIALS

My research focuses on advanced imaging and spectroscopic methods of high-resolution electron microscopy, especially transmission electron microscopy (TEM), including aberration-corrected scanning (S)TEM and in situ SEM and TEM techniques, and on the development of methods, such as holders for in situ studies in the electron microscopes and software for high spatial resolution, high spatial precision, high energy resolution and extraction of statistical significant signals and their application to topical research of functional materials and soft matter. Currently, our research is centered on (i) the direct correlation between local material structure and properties; (ii) the fundamental understanding of the mechanisms determining material transport properties; (iii) the design of new materials and structures with tailored properties; (iv) atomic resolution characterization of interfaces; and (v) method development for materials for energy technology, quantum devices, health and also soft matter. The research is carried out in close collaboration with national and international research groups in academia, industry and institutes.

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SELECT PUBLICATIONS

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MATERIALS SCIENCE, SURFACE SCIENCE, CHEMISTRY, COMPOSITES

We exploit monoatomic nanosheets of graphene featuring excellent chemical versatility, high mechanical strength and easy mass production to create materials for the automotive, aerospace and energy storage sectors. We can assemble the nanosheets together with small organic molecules, polymers, metal nanoparticles etc. using supramolecular chemistry, to obtain layered materials in the form of thin coatings, membranes or 3-dimensional foams. Our main research challenge is to use the 2-dimensional shape of the graphene nanosheets to achieve unique properties in these materials, such as high electrical conductivity, selective gas/ion transport, sensing capabilities etc. Besides their interest for fundamental research, we can use such materials also for practical applications, as example:

- Electrodes for lithium-ion batteries.
- Electrochemical sensors for drug detection.
- Metal-free, carbon-based antennas for near-field communication.
- Filters for water purification.

Computer artwork representing small molecules diffusing in between graphene sheets.

SELECT PUBLICATIONS
A robust, modular approach to produce graphene–MOx multilayer foams as electrodes for Li-ion batteries; Z. Xia, V. Palermo et al.; Nanoscale, 11, 5265 (2019)

ATOMIC STRUCTURE • INTERFACES • CORRELATION BETWEEN STRUCTURE AND PROPERTIES • ELECTRON MICROSCOPY • SPECTROSCOPY • IN SITU EXPERIMENTS • HIGH SPATIAL PRECISION • HIGH ENERGY RESOLUTION • HIGH SPATIAL RESOLUTION • FUNCTIONAL STRUCTURE

GRAPHENE • SUPRAMOLECULAR CHEMISTRY • POLYMERS • METALS • BIO-MOLECULES • BATTERIES • WATER PURIFICATION
THE HIERARCHICAL STRUCTURE AND COMPOSITION OF OSSEOINTEGRATION

My group is focused on models and methods to probe the interface between tissues and biomaterials. The use of multi-scale and multimodal analytical strategies enables detailed structural and compositional analyses at the different hierarchical levels of the tissues interfacing biomaterials and thus a greater understanding of the healing process. We work with both healthy and disease models to understand how common diseases and medication affects the tissue structure and healing capacity, and how material/surface design could improve the clinical potential. Another research focus is additive manufacturing. Here we study the role of pore geometry on bone ingrowth and how the tissue remodels in these confined spaces in order to optimize patient customized implant solutions.

The figure show the bone structure and cellular infrastructure around a titanium implant at different hierarchical levels, from macro to nano.

SELECT PUBLICATIONS

50 years of scanning electron microscopy of bone – A comprehensive overview of the important discoveries made and insights gained into bone material properties in health, disease, and taphonomy; F. A. Shah, K. Ruscsák, A. Palmquist; Bone Research (2019)


OSSEOINTEGRATION • BONE • TITANIUM • ELECTRON MICROSCOPY • RAMAN SPECTROSCOPY

FUNCTIONAL MATERIALS CHEMISTRY

We focus on development of new functional materials and synthesis methods and have expertise in studies of processes involved in the formation of nanostructured materials, structural and physicochemical characterization of materials and evaluation of their properties. We develop nanostructured materials ranging from small particles to micro- and mesoporous solids and host/guest clathrates. These materials provide high interfacial areas and a diverse range of properties of interest for a range of applications.

We use a number of methods including amphiphile-directed wet chemical sol-gel, solvothermal, solid state mixing, Czochralski crystal pulling, and spark plasma sintering for powder compaction. Examples of our research include; synthesis and evaluation of new thermoelectric materials for direct conversion of waste heat to electricity, noble metal-free fuel cell catalysts for generation of electricity, electrode materials for Li-S batteries and hybrid supercapacitors, immobilization of enzymes in porous materials for reduction of CO₂ to methanol.

SELECT PUBLICATIONS


FUEL CELL CATALYSIS • THERMOELECTRICS • BATTERY ELECTRODES • SUPERCAPACITORS • ENZYMATIC CATALYSIS • NANOSTRUCTURED MATERIALS • ZEOLITES • MESOPOROUS MATERIALS • COLLOIDAL CHEMISTRY • SURFACE CHEMISTRY
CHEMICAL BONDING AND MATERIAL PREDICTION

We are a theoretical chemistry group working on challenges in the borderlands between chemistry, physics and materials science. We believe the road to a sustainable tomorrow is intimately connected to cross-disciplinary mastery of chemical bonding. This boils down to a need for analysis and rationalization of electronic structure in a manner that is inherently understandable and useful for experimental researchers and theorists alike. Our purpose is to facilitate chemical rationales under different conditions and enable for faster search and design of functional materials. Our research includes development of chemical descriptors and methods that simplify the analysis of electronic structure in atoms, molecules, polymers and crystals. We also apply quantum mechanics to study materials and processes not readily accessible experimentally. For example, we predict materials of very high energy density, explore chemistry under high pressures conditions, and study prebiotic processes that may occur over long time scales.

SELECT PUBLICATIONS

Electronegativity Seen as the Ground-State Average Valence Electron Binding Energy; M. Rahm, T. Zeng, R. Hoffmann, J. Am; Chem. Soc 141, 342-351 (2019)

Polymorphism and electronic structure of polyimine and its potential significance for prebiotic chemistry on Titan; M. Rahm, J. I. Lunine, D. Usher, D. Shallloway; PNAS 113, 81218126 (2016)

A hypervalent and cubically coordinated molecular phase of IF8 predicted at high pressure; D. Luo, J. Lv, F. Peng, Y. Wang, G. Yang, M. Rahm, Y. Ma; Chem. Sci, 10, 2543-2550 (2019)

A new scale for electronegativity.
LIQUID CRYSTALLINE SOFT MATTER

Liquid-crystalline soft matter combines the fluidity of liquids with the macroscopic anisotropy of crystals and provides an excellent testing ground for essential concepts in condensed matter science. In my research I study the relations between molecular structures, symmetry and order parameters, and chirality effects in liquid crystals (LCs).

Chirality is fundamental for several applications of LCs but is also of fundamental scientific interest. For instance, biomolecules are homochiral and the fact that life is inevitably linked to the aqueous liquid state manifests the importance of reflection symmetry breaking in liquids and LCs. In addition, the helical organization of chiral LCs is omnipresent in living matter, and chiral LC-based systems could open up for stimuli responsive materials and devices matching the level of sophistication of biological systems. In the future I would also like to study LC formation of ultrashort DNA oligomers (nanoDNA), which might have been vital for the prebiotic development from nanoDNA to long DNA molecules.

The micrograph illustrates chiral LC structures of non-chiral lyotropic LCs under cylindrical confinement. The lines are topological defects in the form of twist disclination lines.

CONDENSED MATTER PHYSICS

Most of the materials used in today’s technologies have properties that are relatively unaffected by electron interactions. Aluminum, diamond or even graphene are materials that may be reasonably explained within the non-interacting electrons model. However, when the interactions between electrons, spins, charges, and orbitals become important, novel and fascinating physical phenomena emerge. Such materials are usually named correlated electron systems, and their understanding and possible implementation in future devices, is one of the significant challenges of condensed matter physics. Our interest is to understand why and how unusual phenomena arise, and how they can be optimized for technological applications. We are studying various types of correlated systems ranging from metal-to-insulator transition, superconductors, or magnetic materials. We are investigating their electronic and magnetic properties using a combination of techniques, and the experimental results are combined with theoretical models performed in collaboration with theoretician’s expert in the field of correlated electron systems.

SELECT PUBLICATIONS

- On the orientational distribution functions in de Vries-type smectic liquid crystals; P. Rudquist, M. A. Osipov, F. Giesselmann; Liquid Crystals, 45, 2097-2108 (2018)
- Chiral structures from chiral micellar lyotropic liquid crystals under capillary confinement; C. F. Dietrich, P. Rudquist, K. Lorenz, F. Giesselmann; Langmuir, 33, 5852-5862 (2017)
- Photon upconversion with directed emission; K. Börjesson, P. Rudquist, V. Gray, K. Moth-Poulsen; Nature Communications 7, 12689 (2016)
**ATOMIC SCALE THEORY FOR SPARSE MATTER**

Our van der Waals density functional (vdW-DF) has shown great promise in a broad range of applications, covering such varied systems as graphite, polymers, and DNA. Ground-state properties, including binding energies, equilibrium geometries, and vibrational frequencies, have been calculated with a good agreement with experimental data, as well as electronic properties, like intercalation effects and work functions.

Our work focuses on testing, developing, and applying atomic-scale computational methods. In doing so, we focus on systems with important voids or adsorption systems, such as pollution control via filtering techniques, and interactions in biomolecular systems, such as interactions between parts of DNA.

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**SELECT PUBLICATIONS**


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**CATALYSIS FOR ENERGY CONVERSION AND EMISSION CONTROL**

My main research fields are catalysis for energy conversion and emission control. By developing new catalytic materials and catalyst-based techniques to convert greenhouse gases and emissions, I want to reduce the impact of such compounds on the climate and the environment. My research is performed within the Competence Centre for Catalysis, KCK, which is an interdisciplinary research centre at Chalmers. Particularly the study of kinetics and reaction mechanisms for the catalytic reduction of nitrogen oxides, catalytic oxidation of hydrocarbons at low temperatures, and surface processes during conversion of CO₂ and methane to valuable platform chemicals is of major interest.

The research combines modern techniques, particularly in situ techniques, and methods within catalysis and nanoscience to relate catalytic properties as activity, selectivity and stability with physiochemical properties of the catalytic material studied.

An especially important issue in the research is the use of well-controlled perturbations of the reactant composition, to improve the performance of the catalyst, and to identify the surface processes that control the reaction considered. My vision is to contribute to a sustainable transport, energy and environmental system with new catalyst-based techniques.

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**SELECT PUBLICATIONS**


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**Catalysis - Heterogeneous Catalysis - Surface Science - Environmental Science - Catalyst Synthesis - Reaction Kinetics - Reaction Mechanisms - In Situ Characterisation**
MATERIALS CHEMISTRY
Materials chemistry is important for a sustainable society, e.g. for the development of new sustainable energy systems. In many cases the development of new, energy-saving and environmentally friendly techniques are limited by the degradation of materials at high temperature. My research concern mainly material chemistry for energy applications, application areas include Solid Oxide Fuel Cells (SOFC) and green electricity production from biomass. I am the director of The High Temperature Corrosion Centre (HTC). My research focuses on fundamental aspects of the oxidation and corrosion processes. The long-term scientific objective is to increase the knowledge of the oxidation and corrosion through mechanistically directed experiment. The ability of materials to withstand high-temperature corrosion is determined by the properties of the oxide scales, e.g. chromia and alumina that develop. The morphology of the protective layer and its crystal, defect and grain structure are decisive in this respect and involve a length scale from several nanometers to micrometer. Because the process that constitute corrosion occur on so different length scales, we combine methods that cover the whole range, from nanometer scale to the macroscopic object. A wide range of state-of-the-art methods for investigating and characterizing materials and surfaces, including in-situ corrosion experiments, electron microscopy and first principle model calculation is used.

SELECT PUBLICATIONS
Progress in Materials Science, Volume 89, 92-193, (2017)

SOFT MATTER PHYSICS
My group is mainly working on the role of water in biological systems. How the functions of proteins and other biomolecules often are directly dependent on the motions in the surrounding solvent. Currently, we are also elucidating how disaccharides, such as trehalose, in the solution affect the dynamical properties and stability of proteins. Such understanding is important due to the diverse applications of disaccharides for e.g. the conservation and freshness of food materials, the cryopreservation of stem cells, embryos for test-tube fertilization and body organs for transplantations, as well as medical treatments of protein aggregation related diseases, such as Alzheimer’s and Huntington’s disease.

SELECT PUBLICATIONS
BIOMATERIALS

Of fundamental interest is the way cells sense and interact with surfaces and how the cells communicate with other cells, ultimately leading to the rejection or integration of the material with the tissue. Much efforts have been devoted to get access to the material-tissue interface in order to resolve the fine structure and cell behaviour of such interface. The group has pioneered the long-term interdisciplinary collaboration between material scientists, biologists and clinicians. It has participated in numerous international and national partnerships and networks. The group has contributed to the development of oral, orthopaedic and ENT implants used globally, including membranes for guided bone regeneration (GBR), bone anchored hearing aids and orthopaedic amputation prostheses. Current fundamental research: cell-cell communication at interfaces, osseointegration in compromised conditions and mechanisms of osteoinduction of bioceramics. Current translational research: 3D printed materials for cranial bone healing, guided bone regeneration in dentistry, skin-penetrating prostheses and novel bone glues.

SELECT PUBLICATIONS


MATERIALS MODELLING AND SIMULATION

Materials modelling and simulation aims to develop fundamental relationships between the atomic structure and properties of molecules and bulk materials as well as their surfaces and interfaces, so that advanced materials with enhanced and new properties can be designed.

My research interest is in exploring the links between the electronic structure of materials, the behaviour of their atoms, the statistical thermodynamic description and materials processes. Computational techniques such as electronic structure calculations based on the density functional theory, the quantum-mechanical path integral method, classical molecular dynamics, Monte Carlo and kinetic simulation techniques are being used.

We have performed computational studies of proton motion in acceptor doped barium zirconate, a solid oxide that exhibit significant proton conductivity at elevated temperatures. Interface properties have been investigated in relation to cemented carbides, an important composite engineering material. Several of our projects are done in collaboration with experimental groups and industry.

SELECT PUBLICATIONS

Comparison of space-charge formation at grain boundaries in proton-conducting BaZrO3 and BaCeO3; A. Lindman, E. E. Helgee, G. Wahnström; Chemistry of Materials 29, 7931 (2017)

DENSITY-FUNCTIONAL THEORY • MOLECULAR DYNAMICS • PATH-INTEGRAL SIMULATIONS • MONTE CARLO • KINETIC SIMULATIONS • PROTON CONDUCTORS • HARD METALS • GRAIN BOUNDARIES • COMPLEXIONS • SPACE-CHARGE EFFECTS
**SELECT PUBLICATIONS**

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Spin injection and helicity control of surface spin photocurrent in a three dimensional topological insulator; Y. Q. Huang, Y. X. Song, S. M. Wang, I. A. Buyanova and W. M. Chen, Nature Communication 8, 15401 (2017)

SEMICONDUCTOR HETEROSTRUCTURES
Semiconductor heterostructures have feature sizes in nanometer scale and are possible to be tailor-made through band and strain engineering. Epitaxy is required to grow such structures with excellent control in thickness, alloy composition and doping. My research covers molecular beam epitaxy (MBE) growth of III-V and bismuth containing semiconductors for making optoelectronic devices and integration on Silicon. We have employed ion slicing technology to cut and transfer 2 inch III-V thin films onto SiO2/Si forming III-V on insulator (III-VOI) with good surface, structural and optical properties. Currently, we are working on improving optical and electrical properties on wafer scale III-VOIs and demonstrating optoelectronic devices. We have also synthesized various novel bismides using MBE including InPBi, GaSbBi, AlSbBi and AlAsBi thin films for the first time and also high quality Bi2Te3 thin films, and demonstrate GaAsBi lasers up to 1.41 µm at room temperature.

SEMICONDUCTOR HETEROSTRUCTURES

**SYNTHESIS OF CONJUGATED POLYMERS AND 2D MATERIALS FOR ENERGY CONVERSION AND STORAGE, ORGANIC SOLAR CELLS, ORGANIC LIGHT-EMITTING DIODES, SUPERCAPACITORS**

The focus of our research is on the development of new conjugated polymers and Graphene-like materials. The main applications of the materials are organic solar cells, photodetectors, light-emitting diodes and supercapacitors. Moreover, he has broad interests in flow battery, ferroelectric materials and thermoelectrics.

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**POLYMER CHEMISTRY • ORGANIC SEMICONDUCTORS • ORGANIC SOLAR CELLS • ORGANIC LIGHT EMITTING DIODES • SUPERCAPACITORS • 2D MATERIALS**

**A colorful solution of our conjugated polymers, which can absorb and emit at different wavelengths.**

**SELECT PUBLICATIONS**


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**SELECT PUBLICATIONS**


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BIOCOMPOSITES: CHEMICAL TUNING OF THE CELLULOSE-MATRIX INTERFACE
The group are working with controlled chemical surface modification of nanocrystalline cellulose and wood fibres for use in Composites. From systematic studies combined with multivariate analysis the relationships between the molecular surface structure, the interphase and the bulk properties are sought for.

SELECT PUBLICATIONS
Cationic surface functionalization of cellulose nanocrystals; M. Hasani, E. D. Cranston, G. Westman and D. G. Gray; Soft Matter 4, 2238–2244 (2008)

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MODELLING OF SOLAR ENERGY MATERIALS
The search for photoabsorbers has attracted much attention from researchers working in fields of materials science, chemistry, biology, and physics. This resulted in a huge amount of theoretical and experimental efforts to understand charge transport mechanisms, predict properties, synthesize new materials, and characterize them, all in search of yet more efficient, cheaper, and environmentally friendly compounds and assemblies. I complement searches for new photoabsorbers by applying advanced electronic-structure methods, and building precise models that include complex phenomena and interactions of charge carriers. I focus on emerging materials for solar cells, such as halide perovskites, and photoabsorbers for solar-to-fuel conversion, such as vanadates. Specifically, I study how charge carriers, created during illumination, interact with each other and the crystal lattice, in the bulk material and at interfaces with electrolyte or other functional layers. My long term goal is to model complete assemblies for rapid optimization of solar energy devices.

SELECT PUBLICATIONS
The Role of Polarons in Water Splitting: the Case of BiVO4; J. Wiktor, F. Ambrosio, and A. Pasquarello; ACS Energy Lett. 3, 1693 (2018)

There is increasing awareness of the imperative to accelerate materials discovery, design, development, and deployment. Our view is the material as a complex system of interacting subsystems with models and experiments at multiple scales of materials structure hierarchy to find quantitative relationships between structure-materials properties or responses to identify feasible materials.

Density of the hole polaron at the BiVO4/water interface.

NANOCRYSTALLINE CELLULOSE • SURFACE MODIFICATION • NMR • QSRR-STRUCTURE-PROPERTY RELATIONSHIPS
METAL OXIDES FOR ELECTRONICS

We are working on the electronic properties and applications of complex metal oxides and heterostructures. We are trying to understand the underlying mechanisms of the high electron mobility of two-dimensional electron gases that occurs at the interface between polar bandgap insulators, such as the LaAl\textsubscript{2}O\textsubscript{3}/SrTiO\textsubscript{3} interface. Superconductivity, giant magnetoresistance and ferroelectricity are some of the properties of these materials. We are also exploring the ultra high sensitivity of devices made from these materials in life science and in medicine.

The system in the figure has been benchmarked against a commercial low-Tc MEG-system with excellent results. Moving to high-Tc superconductors has several advantages, such as cooling (liquid nitrogen instead of the finite resource liquid helium). This makes the cooling costs negligible and brings the sensors closer to the brain with higher spatial resolution as a result.

SELECT PUBLICATIONS


Homogeneous superconductivity at the LaAl\textsubscript{2}O\textsubscript{3}/SrTiO\textsubscript{3} interface probed by nanoscale transport; A. Kalaboukhov, P. P. Aurino, L. Galletti, T. Bauch, F. Lombardi, D. Winkler, T. Claeson, D. Golubev; Physical Review B 96, 184525 (2017)

Effect of oxygen vacancies in the SrTiO\textsubscript{3} substrate on the electrical properties of the LaAl\textsubscript{2}O\textsubscript{3}/SrTiO\textsubscript{3} interface; A. Kalabukhov, R. Gunnarsson, J. Borjesson, E. Olsson, T. Claeson, and D. Winkler; Phys. Rev. B 75(12), 121404 (2007)

SENSOR APPLICATIONS OF GRAPHENE

Graphene has several unique properties that prompt for practical applications like sensitive detectors of e.g. electromagnetic radiation. The electrical resistance of graphene strongly depends on adsorbed molecules and thereby allows for building various biosensors with simple readout. We work on such devices made of CVD graphene, which offers a scalable technology for mass production of cheap graphene biosensors. The main challenge is to make the sensors specific to certain bacteria while maintaining the overall performance. In collaboration with Profs. N. Kann and I. Mijakovic.

SELECT PUBLICATIONS


CVD GRAPHENE • RADIATION DETECTORS • BIOSENSORS
CHEMISTRY OF 2D MATERIALS
Assistant Professor Xiaoyan Zhang leads the group of ‘Chemistry on 2D Materials’. His research focuses on combination of functional molecules with 2D materials through covalent and noncovalent approaches. The as-prepared molecules/2D materials hybrid systems are further explored in ad-hoc applications such as energy storage. Through the research, understanding of the structure-property-function relationship will be studied in detail, especially on how the molecules affect the properties of 2D materials.

SELECT PUBLICATIONS
Modular graphene-based 3D covalent networks: functional architectures for energy applications; Small 12, 1044-1052 (2016)
Supramolecular chemistry on graphene field-effect transistors; Small 10, 1735-1740 (2014)

METAL-ORGANIC FRAMEWORKS, TOPOLOGY, SYNTHESIS AND PROPERTIES
Our main focus is the synthesis and understanding of Metal-Organic Frameworks (MOFs), new materials with importance for “green” and sustainable chemical engineering and potential applications in catalysis and gas storage. A theoretical focus is topology questions, and applied research questions centre on PFASs removing from drinking water, machine learning in MOF synthesis, magnetism and chiral MOFs for catalysis. Recently we have also developed in interest in COFs (Covalent Organic Frameworks).

SELECT PUBLICATIONS
"PAINTING WITH CELLULOSE NANOCRYSTALS"

The image exemplifies the beautiful patterns that can be observed performing simultaneous shear rheological tests and polarized light optical visualizations in aqueous cellulose nanocrystals (CNC) suspensions. CNC organize in water suspensions in nematic or chiral nematic structures with helical arrangement of the crystals, structures observable at micro-macro levels. The photo was taken right after setting up the parallel-plate geometry to the measurement gap. A critical shear rate for beautifully oriented structures was reached during the ensuing squeeze flow. The photo also contains the randomly oriented excess fluid outside the bounds of the upper geometry.

Credit: Roland Kádár and Tiina Nypelö