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Welcome

Dear invited guests and colleagues,

Welcome to the Institute for Molecules and Materials (IMM) at the Radboud University! It is a pleasure and honor to host you at our annual sIMMposium.

At the sIMMposium of the IMM scientists and students show their work and latest research results. We welcome our stakeholders from business, industry and societal organisations to ‘IMM meets Business & Industry’.

The sIMMposium is a great opportunity to learn more about our institute and to meet our researchers. You will hear about IMM’s research highlights and what research challenges business & industry face. We will demonstrate some fruitful collaborations between industry and IMM. For PhD candidates we have an interactive session on the challenges in careers in business and industry.

On the second day of the sIMMposium, we present an in depth scientific programme with invited speakers. Our PhD candidates and Postdocs will present their recent work in oral and poster presentations.

We hope you will have a very stimulating and inspiring meeting.

The sIMMposium organising committee
The Institute for Molecules and Materials (IMM) is an inter-disciplinary research institute in chemistry and physics at Radboud University. Our mission is to perform fundamental research and to train the next generation of leaders in science and entrepreneurship at the highest international standards.

Our research focuses on the fundamental interactions between molecules, the chemistry of complex, life-like molecular systems and the properties of matter emerging from quantum effects.

Research at IMM is focused on three closely connected themes:

**Theme 1:** Structure and Dynamics of Molecules
**Theme 2:** Chemistry of Complex Systems
**Theme 3:** Spectroscopy of Quantum Materials

Our scientists make use of unique research facilities such as the international user facilities High Field Magnet Laboratory and FELIX Laboratory, and extensive NMR, Scanning Probe and Laser Facilities.

We actively explore and promote the interaction with industry and the application of our fundamental research, ranging from electronics, photonics and data storage to medicine.
## Venue

**Monday 29 October 2018**  
Auditorium RadboudUMC  
Radboud Campus  
Geert Grooteplein 15  
6525 EZ Nijmegen

**Tuesday 30 October 2018**  
Lecture hall HG00.303, HG00.304, HG00.307  
Huygens Building  
Heyendaalseweg 135  
6525 AJ Nijmegen

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<tr>
<td>29 October</td>
<td>12:00 – 18:00</td>
<td>Plenary lectures &amp; sessions</td>
<td>Auditorium RadboudUMC, Radboud Campus</td>
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<tr>
<td>29 October</td>
<td>17:00 – 18:00</td>
<td>‘IMM &amp; Chip Integration Technology Center (CITC)’</td>
<td>Lecture room HG00.304, Huygens Building</td>
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<tr>
<td>29 October</td>
<td>18:00 – 21:00</td>
<td>sIMMposium dinner</td>
<td>South corridor Huygens Building</td>
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<tr>
<td>30 October</td>
<td>9:00 – 17:30</td>
<td>Plenary Lectures Parallel sessions</td>
<td>Lecture room HG00.307, Theme 1: HG00.303, Theme 2: HG00.307, Theme 3: HG00.304</td>
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Organising committee

Sandra Brünken  
FELIX Laboratory

Misha Titov  
Theory of Condensed Matter

Thomas Boltje  
Synthetic Organic Chemistry

Freya Senf  
Managing Director IMM

Alix McCollam  
High Field Magnet Laboratory

Brigitte Loozen  
IMM Office

Miriam Heijmerink  
IMM Office
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<tr>
<td>12:15 - 13:00</td>
<td>Welcome, registration &amp; lunch</td>
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<td>13:00 - 13:15</td>
<td>Opening by the Director IMM, Theo Rasing</td>
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<td>13:15 - 14:15</td>
<td>IMM Research highlights</td>
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<td><strong>Chair: Anouk Rijs</strong></td>
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<tr>
<td></td>
<td>Theme 1: Jonathan Martens - FELIX Laboratory</td>
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<td></td>
<td><em>Infrared Ion Spectroscopy: A New Route to -Biomarker Discovery in Metabolomics</em></td>
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<td></td>
<td>Theme 2: Oliver Maguire - Physical Organic Chemistry <em>‘How to cope with change? The effects of dynamic environments on Out-of-Equilibrium Chemical Reaction Networks’</em></td>
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<td>Theme 3: Jonathan Buhot - HFML <em>‘Exploring exotic quantum phases in high magnetic field’</em></td>
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<tr>
<td>14:15 - 14:45</td>
<td>Coffee break</td>
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<td>14:45 - 15:30</td>
<td><strong>Leiden Cryogenics &amp; Academia - A mutually inspiring relationship</strong></td>
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<td>Industry Lecture by Arlette de Waard</td>
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<td><strong>Chair: Alix McCollam</strong></td>
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<td>15:30 - 17:00</td>
<td>Parallel</td>
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<td></td>
<td>Lab tours research facilities: guided tours to High Field Magnet Laboratory (HFML), NMR Laboratory, FELIX Laboratory, SPiN labs (for invited guests only)</td>
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<td>15:30 - 17:00</td>
<td>Parallel</td>
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<td><em>‘Making Industry-University partnerships work’ - Duo presentation on fruitful collaborations industry-academia</em></td>
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<td><strong>Chair: Floris Rutjes</strong></td>
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<td>Theme 1: Christoph Gebhardt - Bruker &amp; Jos Oomens - FELIX Laboratory</td>
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<td>Theme 2: Henk Jan van Manen - AkzoNobel &amp; Jeroen Jansen - Analytical Chemistry</td>
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<td>Theme 3: Dmitry Kozodaev - Techno-nT &amp; Alexey Kimel - Ultrafast Spectroscopy of Correlated Materials</td>
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<td>17:00 - 18:00</td>
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<td>Fire side Chat on career perspectives <em>Hear and ask about differences on career perspectives between academic and industrial careers</em></td>
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<td><strong>Moderator: Alex Khajetoorians</strong></td>
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<td>Francesca Chiappini - TNO</td>
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<td>Henri van Kalker - V.O. Patents &amp; Trademarks</td>
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<td>Silvie Meeuwissen - ChemConnection B.V.</td>
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<td>Roger Rikken - Physics teacher at Fontys University of Applied Science</td>
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<td>17:00 - 18:00</td>
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<td>IMM &amp; the Chip Integration Technology Center (CITC) <em>Chair: Frans Harren</em></td>
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<td>The CITC (chip integration technology centre) is a new open innovation centre located in Nijmegen, where companies (large and small), universities and research institutes collaborate in the field of novel chip (semiconductors) integration technologies. The CITC aims to bring technology concepts from demonstrator level to manufacturability. With Radboud university optical spectroscopy based sensors will be addressed in the CITC. HGoo.304, Huygens Building, Heyendaalseweg 135, Nijmegen</td>
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<td>Barry Peet - CITC, BCSEMI NL &amp; Simona Cristescu - Life Science Trace Gas Facility, IMM</td>
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<tr>
<td>18:00 - 21:00</td>
<td>sIMMposium dinner</td>
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<td><strong>in Huygens Building, Heyendaalseweg 135, Nijmegen</strong></td>
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### Opening by Theo Rasing

#### 9:05 - 9:50

**I1 Melanie Schnell - Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany**  
Chair: Sandra Brünken

‘Mirror molecules and chemistry in the Universe - new challenges and methods’

**Coffee break**

#### 10:05 - 11:05

**Parallel session I**

**Theme 1: HG00.303**  
Chair: Musleh Munshi

- **O1 Theo Cremers - Spectroscopy of Cold Molecules**  
‘A multistage Zeeman decelerator for molecular collision experiments’

- **Theme 2: HG00.307**  
Chair: Britta Helwig

- **O2 Karina Nakashima - Physical Organic Chemistry**  
‘Chemistry inside active coacervate droplets’

- **Theme 3: HG00.304**  
Chair: Anna Gatilova

- **O3 Brian Kiraly - Scanning Probe Microscopy**  
‘An Orbitally-Derived Single Atom Magnetic Memory’

**Theme 1: HG00.303**  
Chair: Musleh Munshi

- **O4 Fleur van Zelst - Solid State NMR**  
‘Analysing complex mixtures by hyphenation of supercritical chromatography and nuclear magnetic resonance (SFC-NMR)’

**Theme 2: HG00.307**  
Chair: Britta Helwig

- **O5 Lianne Lelieveldt - Biomolecular Chemistry**  
‘Bioorthogonal click to release reactions based on vinyl boronic acids’

**Theme 3: HG00.304**  
Chair: Anna Gatilova

- **O6 Maryam Shahrokhvand - HFML**  
‘Quantum limit thermopower in the metallic semiconductor InSb’

#### 11:05 - 11:50

**I2 Jan van Maarseveen - Van ‘t Hoff Institute for Molecular Chemistry, University of Amsterdam**  
Chair: Thomas Boltje

‘Covalent approaches towards mechanically interlocked molecules’

**Lunch & Poster session**

#### 13:50 - 14:50

**Parallel session II**

**Theme 1: HG00.303**  
Chair: Wouter Franssen

- **O7 Zhongfa Sun - Molecular & Laser Physics**  
‘A simple resonance enhanced laser ionization scheme for CO via the A1Pstate’

**Theme 2: HG00.307**  
Chair: Victor Bloemendal

- **O8 Hidde Elferink - Synthetic Organic Chemistry**  
‘An integrated approach to understand stereoselective glycosylation reactions’

**Theme 3: HG00.304**  
Chair: Ivan Ado

- **O9 Marion Barbeau - Theory of Condensed Matter**  
‘Ultrafast control of exchange interactions in multi-orbital systems’
### IMM in depth - 30 October 2018
(Huygens Building, Heyendaalseweg 135, Nijmegen)

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<td><strong>O10</strong> Sjors Bakels - FELIX Laboratory</td>
<td>‘Aggregation of Isolated Neutral Dipeptides using Laser Desorption’</td>
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<td></td>
<td><strong>O11</strong> Anne Swartjes - Molecular Nanotechnology</td>
<td>‘Synthesis and Optical Resolution of Chiral Porphyrin Cage Compounds’</td>
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<td>Theme 3: HG00.304</td>
<td>Chair: Ivan Ado</td>
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<td></td>
<td><strong>O12</strong> Maarten van Delft - HFML</td>
<td>‘Quantum oscillatory phenomena in nodal line semi-metals’</td>
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<td>14:50 - 15:35</td>
<td><strong>I3</strong> Stephen Julian - Department of Physics, University of Toronto, Canada</td>
<td>Chair: Alix McCollam</td>
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<td>‘Fermi surface transitions in strongly correlated metals’</td>
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<td>15:35 - 16:00</td>
<td>Coffee break</td>
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<td>16:00 - 17:00</td>
<td>Parallel session III</td>
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<td>Chair: Sandra Wiersma</td>
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<td><strong>O13</strong> Olga Lushchikova - FELIX Laboratory</td>
<td>‘Spectroscopic characterization of copper clusters for catalytic CO2 fixation’</td>
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<td>Theme 2: HG00.307</td>
<td>Chair: Jeroen Bruekers</td>
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<td><strong>O14</strong> Sander Brugman - Solid State Chemistry</td>
<td>‘Adsorption at the muscovite mineral surface studied by surface X-ray diffraction’</td>
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<td><strong>O15</strong> Anna Gatilova - Spectroscopy of Solids and Interfaces</td>
<td>‘Laser excitation of spin dynamics in InMnAs: from THz to visible light’</td>
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<td>16:30 - 17:00</td>
<td>Theme 1: HG00.303</td>
<td>Chair: Sandra Wiersma</td>
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<td><strong>O16</strong> Arthur Christianen - Theoretical Chemistry</td>
<td>‘Unraveling the trap loss mechanism in ultracold diatomic gases’</td>
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<td>Theme 2: HG00.307</td>
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<td><strong>O17</strong> Geert van Kollenburg - Analytical Chemistry</td>
<td>‘Development of Process Path Models’</td>
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<td>Chair: Marion Barbeau</td>
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<td></td>
<td><strong>O18</strong> Ivan Ado - Theory of Condensed Matter</td>
<td>‘Anisotropy of spin-transfer torques, Gilbert damping, and Dzyaloshinskii-Moriya interaction induced by Rashba coupling’</td>
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<tr>
<td>17:00 - 17:20</td>
<td>Wrap up, prizes &amp; closing by Theo Rasing</td>
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IMM meets Business & Industry
29 October 2018

Insights into IMM, research highlights & showcases of fruitful university-industry collaborations
IMM Research highlights

Showcasing of the three IMM research themes
Metabolites, the collection of small molecules in the body, offer a fingerprint of the clinical state of an individual. Each metabolic disease presents a unique molecular signature that when unravelled, provides critical knowledge on the molecular mechanisms of the disease. Moreover, metabolites function as biomarkers - their detection and identification is critical for both the diagnosis of metabolic diseases but also to have an insight into the state of a disease and treatment.

Many metabolomics laboratories worldwide rely on liquid chromatography/high resolution mass spectrometry for metabolic profiling of individual patients. As a result of the extreme sensitivity of this technology, a completely unknown part of the human metabolome can now be examined. This, however, brings with it an entirely new challenge: approximately 80% of the molecules detected in the mass spectrometer have unknown chemical structures than cannot be assigned on the basis of this technique. This question of molecular identification is the current bottleneck in every research laboratory doing mass spectrometry-based metabolomics worldwide.

In order to overcome this challenge, we use the combination of infrared ion spectroscopy experiments at the FELIX laboratory with the untargeted metabolomics profiling used at the Translational Metabolic Laboratory at the Radboudumc, bringing together these two state-of-the-art techniques for metabolite identification for the first time. I will present how, using this new approach, we have recently uncovered a previously unidentified metabolite for Antiquitin deficiency that directly offers significant improvements for patient diagnostics and open doors to novel treatment strategies.
How to cope with change? The effects of dynamic environments on Out-of-Equilibrium Chemical Reaction Networks

Oliver R. Maguire¹, Albert S.Y. Wong², Mathieu Baltussen¹, Aleksandr A. Pogodaev¹, Wilhelm T.S. Huck¹

¹ Physical Organic Chemistry
² Department of Chemistry and Chemical Biology, Harvard University, 12 Oxford Street, Cambridge, MA 02138

One definition of Life is that it is an out-of-equilibrium chemical reaction network that consumes energy and materials in order to sustain itself. Our understanding of how to build chemical reaction networks that produce life like-behaviour is still limited but the potential of constructing these systems is enormous as it promises to transform our current chemical systems and inanimate materials into dynamic life-like systems. Life functions in a dynamic environment, yet, the governing principles guiding the behaviour of chemical reaction networks in dynamically changing environments have been overlooked and are unknown. Here, we demonstrate that the coupling of a small out-of-equilibrium chemical reaction network (Fig.1A) to its temperature environment can enrich its functional output as the network is capable of harnessing a dynamic temperature forcing to produce new emergent properties of increasing complexity (Fig.1B). Our results show new pathways to diversifying out-of-equilibrium behaviour of chemical reaction networks without the need to change the underlying network structure or composition. Through measuring the Arrhenius dependence of reactions in the network we are able to model the effect of temperature which reveals that chemical reaction networks are capable of sensing their proximity to a collapse transition and present characteristic Early Warning Signals prior to failure (Fig.1A).

Fig. 1. A) The Trypsin oscillator network is kept out-of-equilibrium in a Continuous Stirred Flow Reactor. The behaviour of the network is affected by its environment, namely temperature and flow rate, and shows oscillations only within a certain temperature range, outside of which the oscillations dampen to a steady state. The network is capable of sensing this transition in behaviour. B) In the presence of a dynamic environment the behaviour of the network increases in complexity and is able to synchronise to a sinusoidal temperature forcing and generate a new wave packet behaviour.

References:
Exploring exotic quantum phases in high magnetic field

Jonathan Buhot
High Field Magnet Laboratory

A brief overview of the recent highlights at the HFML will be given including new experimental developments. Then, this presentation will be focused on the Raman spectroscopy in high magnetic fields, technique that has been successfully updated the past two years to provide us the capability to detect low energy (down to 0.6 meV) electronic and magnetic excitations in matter and then offer new opportunities to explore quantum matter. To illustrate the scope of possibilities of this technique, recent studies on strongly correlated electrons systems including high Tc superconductors will be presented.

E-mail for corresponding author:
jonathan.buhot@ru.nl
Leiden Cryogenics & Academia - A mutually inspiring relationship

Industry lecture by Arlette de Waard
Leiden Cryogenics & Academia - A mutually inspiring relationship

Arlette de Waard
General Manager Leiden Cryogenics

Being a spin-off company from Leiden University, Leiden Cryogenics has always closely tracked the developments, demands, and trends in the academic world. Together with the customer, we have always endeavoured to find innovative solutions to challenging requirements. From gravitational wave detection to dark matter research to quantum computation, a number of such solutions is discussed.
IMM Research facilities
lab tour

Guided tours to High Field Magnet Laboratory (HFML), NMR Laboratory, FELIX Laboratory & SPiN labs (for invited guests only)
The Institute for Molecules and Materials exhibits a multitude of advanced spectroscopic tools that allow for a detailed characterisation of matter in the nano-domain. Many facilities are used both by in-house and external users. The IMM research facilities include:

**High Field Magnet Laboratory (HFML)**

The HFML is one of the few facilities with continuous high magnetic fields worldwide. Continuous field strengths of up to 37.5 tesla are possible. Also, a hybrid magnet with both superconducting and conventional electromagnets is being constructed. This will pave the way for a 45 tesla magnetic field in 2019. In these high field magnets surprising material properties come to light. Scientists use the HFML to study materials like graphene, that could one day revolutionise electronics. The facility is also coupled to the lasers of the FELIX Laboratory, and is the only place in the world where scientists can study matter under these conditions.

**NMR Laboratory**

The NMR Laboratory is a large-scale facility for high-resolution liquid Nuclear Magnetic Resonance (NMR) and solid state NMR. Located in the Goudsmit Pavilion, the laboratory houses eight NMR spectrometers, including a sensitive 850 MHz instrument. Here, new techniques are developed to optimize sensitivity and information content of NMR spectra. These methods are applied to target specific topics in materials research, like the determination of structure and functions of proteins.
**FELIX Laboratory**

The FELIX Laboratory exploits several intense pulsed (far) infrared free electron lasers that can be precisely tuned in wavelength, energy and pulsing time. The four lasers FELIX-1, FELIX-2, FELICE and FLARE each produce their own range of wavelengths and together, they provide a tuning range between 3 and 1500 µm. The facility provides the world’s most complete coverage of this spectrum and is used in a broad range of fundamental research. From exploring the limits of fibre optics networks to determining the interactions of biological molecules. The lasers can also be combined with the magnets at HFML. It is the only facility in the world that offers scientists the possibility to study matter in these conditions.

**SPiN labs**

The IMM hosts, under the supervision of the SPM department, a cluster of cutting-edge labs, which we call the SPiN labs (Scanning Probe in Nijmegen). The SPM department houses a broad range of instruments including scanning tunneling microscopes (STM) and atomic force microscopes (AFM), operating from ambient conditions down to the milliKelvin regime. The most recently constructed STILL lab facility, one of the quietest labs in the Netherlands, is situated three floors underground and is optimized for ultra-high precision measurements in large magnetic fields. It houses one of the highest resolution STMs in Europe, and is capable of vector-field magnetic characterization, including spin-polarized STM. Our microscopes are integrated in an ultra-high vacuum system allowing for in-situ sample preparation (e.g. MBE, CVD). All instruments in the SPIN labs are customized or home-built, based on strong in-house expertise in scanning probe technology, including multiple instruments capable of cryogenic operation, single-atom manipulation, and magnetic field-based measurements. These instruments are used to investigate structural, electronic and magnetic properties down to the single-atom level.
Making University-Industry partnerships work

*Duo presentations on fruitful academic-industrial collaborations*
A versatile ion trap mass spectrometer for Infrared Ion Spectroscopy at FELIX

Infrared ion spectroscopy (IRIS) is one of the major applications of the FELIX free electron laser. IRIS enables one to record an IR spectrum for a mass-selected molecular ion inside a mass spectrometer. This provides molecular structure information on the ion beyond what can be obtained from MS analysis alone and as such it has revolutionized ion chemistry. Applications include the structural characterization of gaseous coordination complexes, MS/MS reaction products and low-abundance analytes in complex mixtures. In this collaborative project, a commercial MS instrument has been modified to enable coupling with the FELIX laser for the efficient and routine recording of IRIS spectra.

Short description of the project you collaborate in:

- An ion trap mass spectrometer of Bruker Daltonics has been modified so that it can be coupled to the FELIX beamline. This combination enables us to record IR spectra of the mass-selected ions in the MS, which can be used for structural characterization. The collaboration involves the modifications made to the commercial instrument and the continuing development of hardware and software for the integration of MS and laser control.

Industry’s interest:

- Alliance with academic group experienced in coupling MS and IR laser equipment.
- Development of optical access add-on to existing MS instrument.
- Customer support and application scouting: Catch new trends early on and develop them into a market solution in close collaboration with leading research partners.

IMM’s interests:

- A sensitive and versatile MS instrument for the efficient recording of IR ion spectra.
- New MS capabilities, such as MSn, ETD, analytical applications and coupling with LC.
- Instrument is also used in many experiments of external users of the FELIX facility.
Short description of the projects you collaborate in:

- **ALBERT: Analysis of large data sets by enhanced robust techniques**
  With ALBERT we aimed to develop generic strategies and methods to facilitate better and more robust chemometric analysis to significantly reduce resources for industrial data analysis, and to boost the value of analytical measurement data.

- **OFF/On: Outfitting the Factory of the Future with On-line analysis**
  All measurements from industrial processes need to be translated into interpretable information to guide process management to guarantee end-product quality. OFF/On wants to use data analysis methods from biomedical omics technologies to improve the ‘health’ of industrial processes.

**Industries interest:**
AkzoNobel Chemicals wants to make quantifiable increases in efficiency of process management and product development based on (Process) Analytical Technologies. New chemometric algorithms should:

- automate tasks that currently require human intervention by specialist professionals
- increase prediction and classification efficiency of analytical measurements with advanced and dedicated chemometrics
- Enhance insight and understanding in comprehensive systems and processes with the insight of chemometric models.

Several RU chemometric solutions have already proven usable throughout the plant by inexperienced personnel and generically applicable for multiple applications.

**IMM interests:**
- Finding new effective and systematic ways to implement and optimize spectroscopic and other analytical technologies in a practical setting, with the associated new range of scientific challenges.
- Obtaining Big Data from well-understood chemical systems (industrial processes, developed products) to develop novel methods for quantitative analysis.
- Finding a scope for quantifiable benefit of scientific development in everyday practice.

**Mutual interest:**
Creating a place for students (BSc-PhD) to gain experience in practical problems in practical settings in internships, research projects, valorization projects etc.
Short description of the project you collaborate in:

Industries interest:
• Access to the unique expertise of the group well known in the field of experimental magneto-optics.

IMM's interests:
• Networking and new opportunities
Fire side chat on career perspectives

Hear and ask about differences in careers between academic and industrial careers
Company: V.O. Patents & Trademarks

Relation with IMM: MSc in 2009, PhD in 2013

Work-experience:
- PhD degree in synthetic organic chemistry (Rutjes group) in 2013 directed to organophosphorus catalysis to improve the sustainability of related chemical processes. More information about Henri
- Post-doctoral research position at the CPE in Lyon (France) in 2013-2014 directed to the preparation of hybrid organosilica materials and their application in NMR and MRI techniques.

Recent work:
- European and Dutch patent attorney at V.O. Patents & Trademarks (Amsterdam) in the field of chemistry and life sciences (since 2014).
Silvie Meeuwissen - principal scientist

Silvie Meeuwissen has a PhD in bio-organic chemistry, received from Radboud University in Nijmegen under the supervision of Prof.dr. Jan van Hest in 2013. Her research involved polymer chemistry, and the creation, analysis and application of nanocarriers. She worked on a postdoctoral project at FutureChemistry in cooperation with the synthetic organic chemistry group of Prof.dr. Floris Rutjes (RU), before she started as a researcher at ChemConnection in 2014.

**Company:** ChemConnection BV

**Relation with IMM:** Alumnus

**Work-experience:**
- 2014-2018: Senior scientist at ChemConnection
- 2013-2014: Post-doctoral fellow at Radboud University Nijmegen and FutureChemistry
- 2012: Visiting scholar at University of Delaware
- 2008-2013: PhD student at Radboud University Nijmegen

**Recent work:**
- 2018-now: Principal scientist at ChemConnection
- ChemConnection is part of the Ardena group, is a contractor for all chemical, pharmaceutical and (bio)analytical needs that arise in the clinical supply chain from lab to patient.
- Principal scientist and manages several projects, focusing on process development and GMP manufacture of novel nanomedicine candidates for (pre-)clinical trials.
Francesca Chiappini - research scientist

**Organisation:** TNO-Holst Centre

**Relation with IMM:** Alumnus and former employee

**Work-experience:**
- 2012-2016: PhD student at HFML (IMM, Radboud University Nijmegen)
- 2016-2018: Trainee at TNO
- September 2016-April 2017: research scientist at NanoInstrumentation (TNO, Delft)
- May 2017-January 2018: research scientist at Optomechatronics (TNO, Delft)
- February 2018-July 2018: research scientist at Holst Centre (TNO, Eindhoven)

**Recent work:**
- 2018-present: Research scientist at Holst Centre
Roger Rikken - lecturer

After finishing my PhD in 2016 I started working as a teacher in physics at the Fontys University of Applied Science (Fontys Teachers Academy Tilburg). Here, students are being trained to become a teacher in Physics. This means that beside the physics they need to know for teaching, they also get follow courses about pedagogy and didactics. Internships at secondary schools are also part of the curriculum. When I was studying at a teacher academy myself, I found out that teaching at a University of Applied Science would interest me more than teaching at a secondary school. This was one of the reasons I chose to study Natural Sciences at the RU. After completing the master, I got to stay for a PhD at the IMM and the HFML. During my PhD I had the opportunity to give some exercise classes and supervise many physics and chemistry students during their internship at the HFML. These tasks reinforced my idea that I would enjoy a job as a teacher at a University of Applied Science (HBO). My time at the RU prepared me more than enough to teach comfortably and confident at Fontys. If you have any questions about teaching at a HBO or at a secondary school I will be happy to answer them during the fire side chat.

**Organisation:** Fontys University of Applied Science / Fontys Lerarenopleiding Tilburg (FLOT)

**Relation with IMM:** Alumnus

**Work-experience:**
- Lecturer in physics at the Fontys Teacher Academy.
- PhD candidate supramolecular physics IMM and HFML, RU
- Teacher and developer of teaching materials in physics/chemistry/mathematics (elementary school De Geldershof)
- Instructor in Physics (De Delftse Examentraining)
- Physics teacher in training, Maaswaal College, Wijchen
The CITC (chip integration technology centre) is a new open innovation centre located in Nijmegen, where companies (large and small), universities and research institutes collaborate in the field of novel chip (semiconductors) integration technologies. The CITC aims to bring technology concepts from demonstrator level to manufacturability. With Radboud University optical spectroscopy based sensors will be addressed in the CITC.
The CITC (Chip Integration Technology Centre) is a new open innovation centre located in Nijmegen, where companies (large and small), universities and research institutes collaborate in the field of novel semiconductor and photonic chip integration technologies. The CITC aims to bring technology concepts from demonstrator level to manufacturability. This technology centre will focus on communication, energy transition and (bio-)medical applications.

The biosensor market is expected to reach $27 billion by 2022, and point-of-care (POC) diagnostics represents the main segment. The technological progress experienced by the nanotechnology field has significantly contributed to this expansion of the biosensor market. The increasing demand for cost-effective, portable, and easy-to-use POC platforms, which require low-sample consumption and provide sensitivity and real-time response, has considerably raised the innovation in the design of biosensors platforms.

A very promising planar platform for biosensing applications is based on two-dimensional silicon photonic crystals, where light can be confined within an optical cavity using a photonic bandgap. Photonic crystal cavities offer ultra-low modal volumes combined, also with high Q factors. Scientifically, miniaturization of the cavity brings advantages for sensing modalities, since the small optical mode volume leads to quantum-mechanical effects that are strong enough to be used to enhance detection sensitivity. In terms of sensing properties, the high Q translates into a low limit of detection, while the small volume translates into very small analyte volumes and the possibility to even measure inside cells.

At the Radboud university the concept of optical spectroscopy based sensors has been demonstrated, as well as specific biosensing medical applications. In the near future within the CITC technologies will be developed to enable a cost effective miniaturisation.

In this session an overview of the CITC and the use photonic devices for bio-medical sensing will be given, it will conclude with a discussion on integration opportunities & challenges for photonic devices.
Abstracts Invited Lectures
Mirror molecules and chemistry in the Universe – new challenges and methods

Melanie Schnell  
Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany

Polycyclic aromatic hydrocarbons (PAHs) have been of great interest to a variety of communities, especially astronomy. It is assumed that they contain up to 20% of the galactic carbon and help make up the composite of ice grains. They are also considered to be at the heart of a rich chemistry in space, for example by acting as catalysts. We investigate PAH-water complexes using chirped-pulse rotational spectroscopy and infrared spectroscopy with FELIX in the gas phase. We aim at understanding how an ice layer begins to form on a PAH surface. Recently, we extended our studies to chiral helicenes. Furthermore, we study PAH photophysics using the Hamburg FEL FLASH, by performing ultrafast XUV-UV/IR pump-probe experiments, with ionization and dissociation as competing pathways.

In another research branch, we focus on characterizing, controlling, and finally manipulating chirality. Using the new microwave three-wave mixing approach, which is non-linear and resonant, we can differentiate enantiomeric pairs of chiral molecules using tailored microwave pulses. The technique is uniquely mixture-compatible and allows for enantiomer separation, as will be discussed.

Covalent approaches towards mechanically interlocked molecules

Jan H van Maarseveen  
Van ’t Hoff Institute for Molecular Chemistry, University of Amsterdam, Science Park 904, 1098 XH Amsterdam, The Netherlands

Rotaxanes and catenanes are held together by a mechanical bond. The foundation of their synthesis was laid by Gottfried Schill in the sixties using covalent templates. It took another 20 years before the field of mechanically interlocked molecules became a popular research topic culminating in a shared Nobel prize in chemistry by Jean-Pierre Sauvage and Fraser Stoddart in 2016. Meanwhile, in 2003 the bacterial lasso peptides were discovered, showing that the unique mechanical bond is also utilized by nature. The fact that 15 years after their discovery no lasso peptide total synthesis has been published shows the hurdles that have be taken. In this talk, the latest results are discussed on our covalent template-induced backfolding methodology aimed at structurally unique rotaxanes and catenanes with the total synthesis of lasso peptides as the long-term goal.
Fermi surface transitions in strongly correlated metals

Stephen Julian
Department of Physics, University of Toronto, Canada

In the conventional theory of metals, the Fermi surface is a quasi-rigid object around which thermal and quantum fluctuations appear. While this works for most elemental metals, the Fermi surfaces of strongly correlated systems can be surprisingly unstable, appearing and disappearing as a function of doping, pressure or magnetic field. Such Fermi surface changes seem to have deep connections to superconductivity and magnetism, but the connections are not yet understood. In this talk I will discuss two examples of magnetic-field-induced Fermi surface transitions. In YbRh$_2$Si$_2$, Fermi surface transitions at high field have only a subtle effect on transport and thermodynamic properties, despite dramatic changes in the Fermi surface. In Sr$_3$Ru$_2$O$_7$, on the other hand, there are dramatic consequences when a harmless-looking Fermi surface transition occurs. The key difference seems to be that Sr$_3$Ru$_2$O$_7$ is already close to a magnetic instability, so a small change in electronic structure drives a large change in properties. I will conclude by discussing the relevance of these results to unsolved problems in high-Tc superconductivity and topological materials.
Abstracts Oral Presentations
A multistage Zeeman decelerator for molecular collision experiments

Theo Cremers, Simon Chefdeville, Vikram Plomp, Niek Janssen, Bas van de Meerakker
Spectroscopy of Cold Molecules

Molecular collision experiments are invaluable in testing theoretical models of molecular interactions. A Zeeman decelerator is a machine that uses pulsed magnetic fields to manipulate the velocities of neutral paramagnetic molecules and atoms in a supersonic beam. We have developed a multistage Zeeman decelerator consisting of 100 solenoids and 100 magnetic hexapoles, specifically designed for collision experiments. The design is modular, allowing for extension to arbitrary length, and features a cooling system that facilitates operation above 10 Hz repetition rate. We demonstrate the Zeeman decelerator using beams of atomic oxygen. We show results from deceleration and guiding of the beams that show excellent agreement with Monte-Carlo simulations that are used to predict the resulting velocity distributions. The decelerator produces high-density beams with a broad range of final mean velocities and well-defined velocity spreads. These beams are ideally suited for molecular collision experiments. Preliminary results of collisions will be shown together with prospects for future experiments.

Chemistry inside active coacervate droplets

Karina Nakashima
Physical Organic Chemistry / Soft Interfaces

Compartmentalization is one of the key features of living systems. Cells are enclosed by a membrane, but also rely on membrane-less compartments, such as nucleoli and stress granules (classified as liquid organelles). Model membraneless compartments (coacervates) can be made in vitro by liquid phase separation of oppositely charged polyelectrolytes or proteins. We developed a system in which this phase separation can be triggered by chemical reactions such as phosphorylation, like in cells. In this talk, I will discuss our ATP/polypeptide-based coacervate droplets whose assembly and disassembly can be tightly controlled by a network of enzymes supplied with phosphoenolpyruvate and glucose as substrates. Interestingly, these liquid compartments may also affect the kinetics of chemical reactions. I will discuss how coacervate droplets can act as micro-reactors, for simple reactions, such as ester hydrolysis and enzymatic phosphorylation, and for the photocatalytic generation of ATP.
Analysing complex mixtures by hyphenation of supercritical chromatography and nuclear magnetic resonance (SFC-NMR)

Fleur van Zelst, Bas van Meerten, Jan van Bentum and Arno Kentgens
Solid-state NMR

Analyzing complex mixtures, which are often only available in small amounts, is a major challenge in analytical chemistry. Nuclear magnetic resonance (NMR) is a powerful analytical technique for structural identification and quantitation of pure compounds or simple mixtures. However, for complete analysis of more complex mixtures, the molecular components should be separated by chromatography prior to spectroscopic characterisation. In our research, we have coupled supercritical fluid chromatography (SFC) to nuclear magnetic resonance spectroscopy (NMR). Due to the low sensitivity of NMR, direct analysis by NMR after SFC is impossible, since the sample is diluted in the mobile phase, CO$_2$, during chromatography. Therefore an in-line concentration step was developed. As a proof-of-principle we show the in-line SFC-NMR analysis of a mixture of four vitamin E (tocopherol) isomers.$^{1,2}$

References:

An Orbitally-Derived Single Atom Magnetic Memory

Scanning Probe Microscopy

Single atoms at the surfaces of solids have demonstrated rich electronic, chemical, and magnetic properties. In this direction, we show that we can manipulate the valency of a single cobalt atom on a crystalline black phosphorus surface (see figure). Using the local electric field generated from an STM tip, individual cobalt atoms residing at the same hollow site can be reversibly switched between two stable states, which correspond to the different valencies. Consistency between experimentally observed charge densities and density functional theory calculations reveal distinct high and low total magnetic moments for each state. We investigate the stability of each configuration, as well as compare the experimentally measured impurity states with DFT calculations. Finally, we probe the switching dynamics to determine the underlying mechanism and energy scale of the switching. This system opens up the horizon to explore complex memory based on both the orbital and spin degrees of freedom.
**Bioorthogonal click to release reactions based on vinyl boronic acids**

Lianne Lelieveldt¹, Selma Eising¹, Abel Wijen¹, Hendy Kristyanto², Hans-Ulrich Scherer², René Toes², Kimberly Bonger¹

¹ Department of Biomolecular Chemistry
² Department of Rheumatology, LUMC

Bioorthogonal reactions are used widely to achieve selective chemical modifications of biomolecules inside living cells or organisms. The bioorthogonal activation of a prodrug, so-called click-to-release reactions, have gained much interest over the years as these allow the site-selective activation of a drug. For this, the cycloaddition of a tetrazine with strained alkenes or alkynes is often used due to the high reactivity and selectivity. We recently added non-strained, highly soluble and stable vinylboronic acids (VBA) as reactants in the tetrazine ligation. We have observed exceptional high reaction rates between VBAs and dipyridyl-s-tetrazines relative to that of tetrazines lacking such dative ligand. Here, we show that we can use VBAs in a release reaction and demonstrate the potential using a VBA-protected cladribine prodrug.

**Quantum limit thermopower in the metallic semiconductor InSb**

Maryam Shahrokhvand, Teun Mass, Steffen Wiedmann, and Uli Zeitler

HFML - Semiconductors & Nanostructure

Thermopower experiments have demonstrated to be a sensitive tool to probe thermodynamic properties in various kinds of materials. Here, we present thermopower ($S_{xx}$) and Nernst effect ($S_{xy}$) in an $n$-doped InSb with $n = 2.5 \times 10^{16}/\text{cm}^3$, Fig 1. Quantum oscillations are visible in $S_{xx}$ in regime I. By entering the quantum limit (QL), regime II, where all the electron condense to the lowest Landau level, both $S_{xx}$ and $S_{xy}$ increase with increasing $B$. This trend continues to ~27 T for $S_{xx}$ and ~28 T for $S_{xy}$, where the system undergoes a magnetic-field induced Mott-Anderson transition in regime III, and consequently both $S_{xx}$ and $S_{xy}$ decreases towards zero.

Figure 1: right: $S_{xx}$ left: $S_{xy}$ at $T=1.4$ K showing quantum oscillations (regime I), and metal-insulator transition (regime III).
**A simple resonance enhanced laser ionization scheme for CO via the A1 state**

Zhongfa Sun, A. von Zastrow, and D.H. Parker  
*Molecular and Laser Physics*

We develop a new resonance enhanced multi-photon ionization (REMPI) scheme for CO, that is simple, efficient and polarization sensitive. We investigate the ionization process taking place when the CO molecule is exposed to VUV radiation resonant with the CO A(v=0) → X(v=0) transition around 154 nm, along with the ultraviolet (UV) and visible (Red) radiation used to generate VUV by difference frequency four wave mixing. By measuring the CO+ ion recoil velocity image and a room temperature gas spectrum it is possible to assign the ionization process as 1+1′+1″ REMPI where the one-photon steps refer to the VUV, UV, and Red radiation, respectively. Resonance enhancement effect of ionization of rotational states around J=12 arise due to overlap of the fixed wavelength UV (~250 nm) with the R band-head of a transition assigned to CO E(v=6) → A(v=0). The REMPI approach should have a great applicable potential in a wide range of studies involving nascent CO.

**An integrated approach to understand stereoselective glycosylation reactions.**

Hidde Elferink¹, Marion Severijnen², Jonathan Martens², Anouk Rijs² and Thomas Boltje²  
¹ *Department of Synthetic Chemistry, RU*  
² *FELIX Laboratory*

The principle challenge in oligosaccharide chemistry remains the stereoselective synthesis of glycosidic bonds (glycosylation). A central intermediate in glycosylation reactions is the oxocarbenium ion which can be attacked from the α- or β-face resulting in two diastereoisomers. To control the stereoselectivity, we recently developed a method for β-selective mannosylation using C-4 remote group participation. In order to understand the mechanism involved, we performed a study involving variation in remote participating group, sugar type and promoter system. In addition, the structure of the elusive oxocarbenium ions are difficult to study since they are unstable. Hence, we have developed new methodology to characterize the mannosylation intermediates using IR ion-spectroscopy. The structural information obtained adds unique insight into the mechanism of chemical glycosylations.
**Ultrafast control of exchange interactions in multi-orbital systems**

Marion Barbeau, Th. Rasing, M. Katsnelson and J. Mentink  
*Theory of Condensed Matter*

The exchange interaction is the strongest interaction between microscopic spins and at the origin of magnetic order. Recently, the control of exchange has attracted a lot of attention leading to opportunities to find faster and more energy efficient ways to control magnetism [1]. Here we study the ultrafast control of exchange interactions in multi-orbital systems by investigating dynamical strain and ultrashort laser pulses. We find that large modification of Dzyaloshinskii-Moriya interactions (DMI) by acoustic pulses is possible when the electronic hybridization is strong [2]. In addition, we demonstrate that the modification of DMI is sufficient to trigger toggle switching of magnetic skyrmions in thin films. Moreover, we study the effect of high-frequency laser pulses on the control of exchange interactions in a two-orbital spin system. We report that both Heisenberg and the additional biquadratic exchange interaction can be controlled as well as the competition between them.


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**Aggregation of Isolated Neutral Dipeptides using Laser Desorption**

Sjors Bakels, Sebastiaan Porskamp, Eline Meijer, Anouk Rijs  
*Molecular Structure and Dynamics, FELIX Laboratory*

The spontaneous assembly of peptides into ordered nanostructures plays a vital role in the development of a wide variety of incurable neurodegenerative diseases such as Parkinson’s disease and Alzheimer’s disease. At the same time, self-assembly can also be applied to advance the development of smart materials. The main challenge is to understand the underlying principles of peptide self-assembly; this allows one to control their growth and thus to change the course of the aggregation-related disease. This fundamental knowledge can be obtained by following peptide aggregation under controlled and selective conditions. In this project, we study the aggregation of neutral alanine-based peptides, by making use of our molecular beam set-up coupled with laser desorption and mass-selective IR-UV spectroscopy. Here, we will discuss the mechanism of the formation of these peptide aggregates and unravel their structure and structural changes upon self-assembly.
Quantum oscillatory phenomena in nodal line semi-metals

Maarten van Delft, Thomas Khouri, Claudius Müller, Steffen Wiedmann and Nigel Hussey
HFML

Nodal line semimetals (NLSMs) are a class of materials in which the conduction and valence bands cross each other along a line inside the Brillouin zone. These materials present topological aspects distinct from those of Dirac or Weyl semimetals and they are predicted to show enhanced correlation effects.

We study quantum oscillations in high magnetic fields of various materials in the class of NLSMs including ZrSiS and HfSiS, and find a rich spectrum of frequencies, low and high. Some of these frequencies arise from individual pockets of the Fermi surface, while others are due to magnetic breakdown between separate pockets.

A deeper analysis of our spectra reveals several exciting new phenomena, such as an anomalous temperature dependence of the oscillation amplitude and Klein tunneling in momentum space.

Synthesis and Optical Resolution of Chiral Porphyrin Cage Compounds

Anne Swartjes¹, Jiangkun Ouyang¹, Shaji Varghese¹,², Bram van Spierenburg¹, Johannes A. A. W. Elemans¹, Roeland J. M. Nolte¹
¹ Molecular Nanotechnology
² Department of Chemical Engineering and Chemistry, Eindhoven University of Technology, MB, Eindhoven, The Netherlands

The amount of information trafficking internet nowadays is enormous and will increase further. It can be expected that in the next decennia, the current technologies to store and process data will no longer suffice and that other strategies to handle information must be developed. We have started a program to store information on single polymer chains with chiral porphyrin catalysts that move along these chains while writing chiral epoxides (R,R-epoxide = digit 1; S,S-epoxide = digit 0). As part of this program we report here the synthesis and resolution of new porphyrin cage catalysts.
**Spectroscopic characterization of copper clusters for catalytic CO2 fixation**

Olga Lushchikova, D.M.M. Huitema, J.M. Bakker  
FELIX Laboratory

The catalytic recycling of CO₂ to liquid fuels, such as methanol, may help to control the atmospheric CO₂ content. Currently, methanol is produced industrially from syngas (CO₂·CO·H₂) under high temperature and pressure conditions over a Cu catalyst. A broad range of studies suggests that the most active parts of the industrial catalyst are Cu nanoparticles.

To increase understanding of this reaction, we study the interaction of CO₂ and H₂ with copper clusters. For this, we elucidate the structure of Cuₙ⁺ (n=1-15) clusters, both the bare clusters and their complexes with CO₂, through IR photodissociation spectroscopy in combination with Density Functional Theory.

**Adsorption at the muscovite mineral surface studied by surface X-ray diffraction**

Sander Brugman, Eleanor Townsend, Mireille Smets, Paolo Accordini, and Elias Vlieg  
Department of Solid State Chemistry

What happens when minerals come into contact with complex natural systems, such as seawater, is largely unknown. We used muscovite (KAl₂(Si₃Al)O₁₀(OH)₂), a flat layered mineral, to investigate this by looking at the adsorption of cations. Using surface X-ray diffraction, the muscovite interfacial structure was determined in contact with Cs⁺ and Ca²⁺ salt solutions. To further understand the system we have looked at competition between those cations and surprisingly we found that despite the lower valency, more Cs⁺ adsorbs to the surface than Ca²⁺. This has implications in the field of mineral growth, uptake of (radioactive) ions and enhanced oil recovery.

Illustration of the interfacial structure of muscovite after adsorption of Cs⁺.
Unraveling the trap loss mechanism in ultracold diatomic gases

Arthur Christianen, Gerrit Groenenboom
Theoretical Chemistry

In 1995 the first Bose-Einstein condensate was realized using a gas of Rubidium atoms cooled to 170 nanokelvins. Today, trapped ultracold gases of alkali atoms are used with applications ranging from optical clocks to the simulation of strongly correlated electrons in solids. Even more possibilities arise when diatoms are used instead of atoms. Ultracold gases of diatoms have already been realized, but the lifetime of the diatoms in such gases is limited due to an unknown loss mechanism. Experiments indicate that collisions between diatoms are pivotal in this loss mechanism. In our group we developed a machine learning method to construct \textit{ab initio} potential energy surfaces to study such collisions. The potential wells for alkali diatoms are very deep, meaning a huge number of quantum states are accessible. Since the collisions behave quantum chaotically, we can estimate the “sticking time” of the collisions by semiclassically calculating the density of states. For NaK-NaK collisions in electric fields, this sticking time can rise up to milliseconds, meaning they will have an important impact on the experiment.

Laser excitation of spin dynamics in InMnAs: from THz to visible light

Anna Gatilova, E. Mashkovich, A. Pogrebna, Th. Rasing, and A. Kimel
Spectroscopy of Solids and Interfaces

To reveal the role of different electronic transitions in ultrafast laser-induced magnetism, we studied laser-induced spin dynamics in ferromagnetic semiconductor InMnAs thin films excited by ultrashort far- (5 meV), mid- (500 meV) and near-infrared (1.5 eV) laser pulses. Despite qualitative similarities between spin dynamics triggered in these three cases, far-infrared (THz) pump pulses induce spin dynamics a 100 times more efficiently than mid- and near-infrared pulses. This indicates that intraband transitions may play a decisive role for both ultrafast demagnetization and change of magnetic anisotropy. In light of hole-mediated ferromagnetism in InMnAs, this result can be explained if the new magnetic anisotropy and a reduction of the magnetic moment happens through the photon excitation of holes, which influences the Mn electronic states.
Anisotropy of spin-transfer torques, Gilbert damping, and Dzyaloshinskii-Moriya interaction induced by Rashba coupling

Ivan Ado
Theory of Condensed Matter

Based on the results of microscopic analysis, we demonstrate that, in 2D ferromagnets (FMs), Rashba spin-orbit coupling leads to the rotational and, as well, to the orientational anisotropy of spin-transfer torques (STT), Gilbert damping (GD) and Dzyaloshinskii-Moriya interaction (DMI). We discuss the relevance of these results for the formation and dynamics of chiral magnetic textures. In particular, we demonstrate that, in the continuum limit, the commonly assumed form of DMI in terms of Lifshitz invariants breaks down, giving rise to previously undiscovered contributions to the micromagnetic free energy. Moreover, these contributions are of a bulk origin and can not be associated with the properties of the boundary of the sample. We show that, in certain cases, despite strong magnetic anisotropy, they favour the formation of spin spirals over domain walls. Despite significant anisotropy of torques, we reveal a general relation between STT and GD in FM Rashba model, that is responsible for a universal velocity of magnetic textures.
Abstracts Poster Presentations
Valley polarization of monolayer MoSe$_2$ and WSe$_2$ in high magnetic fields

Mariana Ballottin, Andrés Granados del Águila, Anatolie Mitioglu, Peter Christianen
HFML

Semiconducting monolayer (ML) transition-metal dichalcogenides (TMDs) have a direct band gap at degenerate, but inequivalent, valleys at the K+ and K- points of the Brillouin zone. Broken inversion symmetry and a strong spin-orbit interaction couple the spin and valley degrees of freedom. This leads to optical selection rules and these valleys can be selectively addressed by circularly polarized laser excitation, resulting in circularly polarized emission (valley polarization - VP) even at zero magnetic field.

We have measured the VP of ML MoSe$_2$ and WSe$_2$ in magnetic fields up to 30 T. In our experiments we have used four different combinations of the circular polarization of the excitation and detection channels, which allows us to distinguish between intra and inter-valley relaxation. We explain our VP data with a rate equation model. We attribute the observed differences in the VP properties of the Mo- and W-based TMDs to the reversed order of their spin levels in the conduction band.

Observation of Methane Conversion in an electrical discharge using mid Infrared dual comb spectrometer

Muhammad Ali Abbas, Amir Khodabakhsh, Qing Pan, Julien Mandon, Frans J.M. Harren
Trace Gas Facility

Dual comb spectrometer is a powerful tool for sensitive and time-resolve monitoring of fast chemical reactions. [1]

In this work, we report the conversion of methane-nitrogen sample (50% CH$_4$ in N$_2$ with pressure of 25 mbar) in an electrical discharge using the mid infrared dual comb spectrometer with ~10 GHz spectral resolution, and 20 ms acquisition time. After the electrical discharge in a 50 cm long discharge tube, C$_2$H$_6$ and HCN are identified as the main products. The absorption spectrum reveals the production of other species as well, due to electron impact excitation, ionization and dissociation reactions. At shorter time scales, e.g. in 10 µs time intervals; we can also monitor the strength of the absorption lines of CH$_4$ in the excited state, which allows measuring the relaxation rate of the populated exited states in CH$_4$ during the discharge.

**Study of Collision-Induced Absorption between atmospheric gases**

Agniva Banerjee, Tijs Karman, Julien Mandon, Wim van der Zande and David H. Parker  
*Molecular and Laser Physics*

Collisions between gas molecules lead to absorption of light due to a phenomenon called Collision-induced Absorption (CIA) which is quantum mechanically forbidden. This process also takes part in atmospheric heat balance and is important for electronic excitations of O2, which are used for remote sensing. We studied collisions between the different atmospheric gas molecules (N2, CO2 etc.) with O2 for the a’Δg (v=1) ← X3Σg− (v=0) forbidden transition of O2 at 1060 nm. As CIA is small in general, we used cavity ring-down spectroscopy to increase the path length and quantitatively determine smallest absorptions. Using analytical models and numerical quantum scattering calculations, overall transition intensities and line shape were calculated and different absorption mechanism were successful for O2-N2 & O2-N2 by theory* but seem to contradict our recent measurements for O2-CO2.

In my poster, I will explain factors affecting transition intensities for different gas molecules and the underlying mechanisms.


**Quest for a new quasiparticle: Weyl magnons in pyrochlore iridate Nd2Ir2O7**

Femke Bangma, Jonathan Buhot  
*HFML*

The family of pyrochlore iridates (R2Ir2O7) have drawn attention due to the presence of strong spin orbit coupling and magnetic frustration. At low temperatures, a metal-insulator transition sets in, concomitant with all-in-all-out magnetic ordering. In addition, theoretical and experimental studies have suggested the presence of topologically non-trivial phases [1].

In this study we focused on Nd2Ir2O7, which enters the insulating state below 15 K. A Weyl semimetallic state has been suggested to emerge when applying high magnetic fields [2]. Moreover, theoretical studies have predicted the presence of a new type of quasiparticles: Weyl magnons [3,4], the bosonic cousins of Weyl fermions. These quasiparticles, which are topologically protected from backscattering, could have a major impact in the field of magnonics. Proving the existence of Weyl magnons is, however, not trivial; their chargeless nature renders them difficult to detect. A solution is to perform Raman spectroscopy in high magnetic fields.

I will present our study of combined temperature and field dependent Raman spectroscopy and transport measurements, which have started the quest for this new quasiparticle.

**References:**

Here we report that femtosecond laser pulses are able to trigger oscillations of the magneto-optical Faraday rotation in the ferromagnetic semiconductor CdCr$_2$Se$_4$ in the presence of an applied magnetic field. The frequency of these oscillations is a linear function of the magnetic field and corresponds to the ferromagnetic resonance (FMR). Tuning the photon-energy of the pump pulses we reveal two different mechanisms, which induce FMR precession in this material. In the case of pumping from the valence band deep into the conduction band (photon energy 3.1 eV), the phase of the spins oscillations is not sensitive to the polarization of the pump, but can be reversed over 180-degrees by changing the polarity of the applied magnetic field. We assign these oscillations to the coherent spin precession triggered by ultrafast laser-induced heating. This mechanism requires a strong optical absorption in the material and becomes inactive if the pump photon energy is below the band-gap. Tuning the photon energy in a wide range from 0.88 to 2.1 eV reveals the second mechanism of optical excitation of coherent spin oscillations with a maximum around 1.2 eV, i.e. very close to the energy of the band gap in the semiconductor. Contrary to the laser-induced heating, this excitation mechanism is pump-polarization dependent being the most efficient if the pump is circularly polarized. The phase of the spin oscillations is independent on the polarity of the applied magnetic field, but changes by 180-degrees under reversing the helicity of light. We suggest that the effect can be interpreted in terms of spin transfer torque experienced by the network of the ordered Cr$^{3+}$-spins as a result of excitation of electrons from the top of the $p$-type valance band to the bottom of the $s$-type conduction band. In particular, a strong spin-orbit interaction experienced by the carriers in the valence band is responsible for the coupling of the spin of the photo generated carriers and the polarization of light. Due to strong $pd$- and $sd$-exchange interactions the spins of the photo-carriers appear to be coupled to the network of ordered spins of the Cr$^{3+}$ ions.
The role of additives during deracemization using temperature cycling

Guiseppe Belletti, H. Meekes, F. P. J. T. Rutjes and E. Vlieg
Solid State Chemistry

Temperature cycling, alongside Viedma ripening, has been proven to be a reliable approach for deracemizing racemic mixtures of chiral compounds that crystallize as a conglomerate [1-3]. Based on previous studies by Steendam et al., who showed how chiral additives can significantly increase the rate of Viedma ripening [4], here we report on how chiral additives could be used in combination with a temperature cycling process. In particular, we not only demonstrate that the speed of such a deracemization can be greatly increased when chiral additives are used, but also show that the deracemization time is considerably shorter compared to similar Viedma ripening experiments. More in detail, we reveal that, by means of continuous heating/cooling cycles, chiral phenylglycine can selectively hamper the growth of specific enantiomers of an amino acid derivative. By doing so, it allows to reach a pure solid end state with a well-defined rate, which mostly depends on the concentration of the additive used. Theoretically, higher additive concentrations lead to higher deracemization rates. However, this holds only within certain limits: indeed, a too high concentration of additives might lead to a state in which the overall process is not positively affected anymore. Furthermore, we demonstrate that, by using chiral additives, not only the speed is influenced but it also becomes possible to choose the final enantiomeric outcome of the solid phase, following Lahav’s rule of reversal [5]. Lastly, the presented method offers a concrete possibility to apply the same technique to other conglomerate-forming compounds, once a proper additive is found.


This research has received funding as part of the CORE project (October 2016 – September 2020) from the European Union’s Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie grant agreement No 722456 CORE ITN
A Revised Modular Late-Stage Approach to (−)-trans-Δ⁸-THC and Derivatives Using Suzuki-Miyaura Cross-Coupling Reactions

Victor Bloemendal
Synthetic Organic Chemistry

In the scientific field of cannabinoids, multiple preparations of (synthetic) THC are reported. Most of these syntheses rely on early stage derivatization of the resorcinol building block, and are not efficient in the late stage preparation of synthetic cannabinoids. Recently, a new modular approach of synthetic (−)-trans-Δ⁸-THC is published, and was the basis for this research into (−)-trans-Δ⁸-THC derivatives. Various derivatives were synthesized and studied in detail using NMR. This led to the discovery in which two individual scientific papers have incorrectly identified numerous THC derivatives. By conducting various cross coupling reactions with halide-THC scaffolds and investigate intrinsic regioselectivity, both natural and synthetic THC compounds were prepared. By comparing the acquired data with the previously published data, two scientific papers are hereby rectified and presented.
Proteolytic Modification of net components affects their recognition by autoantibodies

Cynthia de Bont, N. Eerden, W. Boelens, G. Pruijn
Biomolecular Chemistry

Neutrophils are able to eject their nuclear material in the extracellular space to form a Neutrophil Extracellular Trap (NET) in a process called NETosis. NETs can capture pathogens, but when not properly cleared, autoimmune responses might be elicited to NET components. Neutrophil proteases play an essential role in NET formation, but they also affect the protein content of the NETs. For example, the histones seem to be prone to degradation by proteases. We show here that the serine protease inhibitor PMSF is able to prevent histone cleavage in the NETs. Histone 3 citrullination, a molecular hallmark of NETs, was detected on PMSF-treated NET harvests but not on non-treated NETs. The conversion of NET-associated proteins by the neutrophil proteases might generate neoepitopes of autoantibodies. Alternatively, the cleavage of NET-associated autoantigenic proteins may result in the loss of autoepitopes. Preliminary data suggest that RA patient sera, which frequently contain autoantibodies to citrullinated proteins, including citrullinated histones, show more reactivity with NETs produced in the presence of PMSF than with nontreated NETs. Our data are consistent with an important role for neutrophil protease activities in the recognition of NET components by autoantibodies.
Employing paramagnetic NMR in the study of threading polymers through catalytic cage compounds

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¹ Molecular Nanotechnology
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The amount of data and data traffic grows exponentially worldwide, and new methods to store this data will be required in the near future. In our group we are developing a molecular machine that is capable of writing data in the form of epoxides on synthetic alkene-containing polymers: a manganese(III) porphyrin clip, which threads the polymer through its cavity while catalytically epoxidizing the double bonds of the chain. The (de)threading processes of these polymers through the cavity of free base and zinc porphyrin clips have been studied extensively by NMR and fluorescence spectroscopy. Yet, the kinetic and thermodynamic parameters of the threading processes of the catalytically active paramagnetic manganese(III) porphyrin clip remain unknown. In this study, the effect of the paramagnetic manganese centre on the spin-lattice relaxation during the threading process was investigated. It was found that the relaxation times of certain protons in both the paramagnetic manganese(III) porphyrin clip and the zinc(II) analogue changed upon threading a polymer chain.

References
Supervised learning of an opto-magnetic neural network with picosecond laser pulses

Ashim Chakravarty, J.H. Mentink, K.T. Yamada, A. Kimel and Th. Rasing
Spectroscopy of Solids and Interfaces

The explosive growth of data and its related energy consumption is pushing the need to develop novel, brain inspired and energy efficient schemes and materials for data processing and storage. The prospect of continuous magnetization state manipulation of a Co/Pt thin film via picosecond optical laser pulses offers the possibility of exploiting this material for brain-inspired computing. Here, we demonstrate that Co/Pt films can be used as an artificial synapse by controlling its magnetization state using circularly polarized picosecond laser pulses. We also show experimentally an efficient implementation of perceptron learning on a supervised opto-magnetic neural network, consisting out of such magnetic synapses. Importantly, we demonstrate that optimization of synaptic weights is achieved by a global feedback mechanism, such that learning does not rely on external storage or additional optimization schemes.
Discovering new cocrystals via coformer-network analysis

Jan-Joris Devogelaer, R. de Gelder, H. Meekes, E. Vlieg

Solid State Chemistry

The use of multi-component crystals, such as salts, solvates and cocrystals, is an effective way of optimizing the physicochemical and biopharmaceutical properties of active pharmaceutical ingredients (APIs) without modifying the chemical nature of the APIs [1]. Since most APIs are produced in the form of racemic mixtures, the formation of multi-component crystals may also lead to purification of the enantiomers [2]. Therefore, knowledge of the solid-state landscape of an API, in terms of polymorphism and multi-component formation, is of paramount importance during the design and optimization of the final drug product.

The experimental screening of new multi-component systems, and specifically cocrystals, is a labor and time intensive job and computational tools to understand and predict new cocrystals can significantly speed up the discovery of new solid forms. In this contribution, we present a data-mining approach that exploits the vast amount of information contained in the Cambridge Structural Database [3] in order to predict new multi-component systems. First, all information on salts, solvates and cocrystals is converted into component networks. Next, the networks are analysed to discover their organizational principles and to find the best algorithm for cocrystal prediction. These algorithms are then used to discover unknown cocrystals on the basis of the coformer network. The prediction results from this new network approach were validated for both a common coformer and an API, resulting in the discovery of several new cocrystal forms.

References

Raw Material Variability

André van den Doel¹, ², Geert van Kollenburg¹, ², Lutgarde Buydens¹ and Jeroen Jansen¹
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The ‘Outfitting the Factory of the Future with ON-line analysis’ (OFF/ON) project aims to provide innovative and generic chemometric and statistical methods for monitoring throughout the entire chemical production process. Many industrial processes have strongly variable feedstock (especially of biological origin), whose characteristics greatly affect optimal process conditions and end-product quality.

Here we show strategies to characterize the raw material feedstock and extract information that is relevant for further processing. We develop these strategies on the basis of case studies together with external partners. Together with Rijkswaterstaat and RIWA we investigate river water quality and how this affects the effort required to produce drinking water and together with RIKILT we investigate the authenticity of chicken meat.

Acknowledgement: This research received funding from the Netherlands Organisation for Scientific Research (NWO) in the framework of the Programmatic Technology Area PTA-COAST³ of the Fund New Chemical Innovations. This publication reflects only the author’s view and NWO is not liable for any use that may be made of the information contained herein.

A simple light-trapping approach for ultra-thin GaAs solar cells

Maarten van Eerden, N. Gruginskie, P. Mulder, G. Bauhuis, J. Schermer
Applied Materials Science

Solar cells based on III-V semiconductors deliver the highest efficiency of any solar cell type. However, their high fabrication cost limits their current use to space applications and concentrator photovoltaics. The use of ultra-thin active layers reduces the cost associated with the cell growth and improves the long-term stability in space environments. However, in order to maintain sufficient light absorption in ultra-thin active layers, appropriate light management schemes have to be employed. In this contribution, we present a novel light trapping concept for ultra-thin GaAs solar cells. The rear-side contact layer of the cell structure is textured by a simple wet etch and exhibits high diffuse reflectance. We integrated the textured contact layer as a diffusive mirror on the rear side of thin-film GaAs solar cells. The short-circuit current of the textured cells is 1 – 1.5 mA cm⁻² higher than the planar reference cells. External quantum efficiency measurements show that the increase in current is caused by the rear-side texture. This confirms the efficacy of this simple light trapping approach.
Investigating ultrafast quantum spin dynamics with machine learning

G. Fabiani, Th. Rasing, J.H. Mentink
Spectroscopy of Solids and Interfaces

Making magnetic data storage faster and more energy efficient is of high relevance for a sustainable information and communication technology. Recently, it was demonstrated that it is possible to achieve femtosecond control of the exchange interaction, the strongest interaction between spins in magnetic materials, and to trigger ultrafast non-dissipative quantum dynamics even at room temperature [1]. This suggests intriguing possibilities to achieve the fastest and least dissipative magnetic recording, but so far this has only been studied near equilibrium. We adopt the machine learning approach developed in [2] for the 2D Heisenberg model and show that this method is in good agreement with existing ground state calculations and reproduces the ultrafast quantum dynamics triggered by ultrashort perturbations of the exchange interaction, paving the way to explore the strongly nonequilibrium regime.


The complex magnetic structure of the Neodymium surface at 1.3 K

Umut Kamber, Andreas Eich, Alexander Khajetoorians and Daniël Wegner
Scanning Probe Materials

Chiral magnetism has gained great attention due to its potential for magnetic storage devices or computing [1,2]. Following this development lanthanide metals shift into focus as they exhibit complex magnetic structures, e.g. helical/conical spin spirals or linear spin waves [3]. However, most investigations of lanthanides so far are based on magnetic neutron scattering experiments, lacking spatial resolution. Therefore, the nano-magnetic properties of lanthanides are poorly understood.

Neodymium shows the most complicated magnetic phase diagram among the lanthanides. It exhibits several magnetic phase transitions below its Néel temperature of 19.9 K, resulting in incommensurate multi-q magnetic order [4,5].

Here, we present first results and analysis of SP-STM measurements of Neodymium (Nd) bulk-like films on W(110) taken at 1.3 K. While we can retrieve some of the q-vectors found by previous neutron scattering studies, we discover additional vectors present at the Nd surface at 1.3 K.

Increased Performance of Thin-film GaAs Solar Cells with Improved Rear Interface Reflectivity

Natasha Gruginskie¹, Federica Cappelluti², Maarten van Eerden¹, Ariel P. Cedola², Gerard J. Bauhuis¹, Peter Mulder¹, Elias Vlieg¹ and John J. Schermer¹

¹ Applied Materials Science
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The highest efficiencies in single-junction solar cells are obtained with devices based on GaAs. As this material is reaching the limit in material quality, the optimization of the design of the cell becomes more important. In this study we implement a patterning technique to the bottom contact layer of thin-film GaAs solar cells that increases the reflectance of photons to the active layers. Both shallow junction and deep junction devices were evaluated, and for deep junction cells, both the short circuit current and the open circuit voltage increase with the reflectance. The radiative saturation current density also decreases, indicating increased photon recycling. Detailed model simulations are performed to further evaluate the mechanisms leading to the improved performance of the deep junction design. Based on the same model, the possibilities for further improvements utilizing the deep junction are also identified.

Nonlinear THz Excitation of Spins in Antiferromagnetic FeBO₃

Kirill Grishunin¹, Eugen Mashkovich¹, Rostislav V. Mikhaylovskiy¹, Peter Christianen², Alexey V. Kimel¹

¹ Ultrafast Spectroscopy of Correlated Materials
² High Field Magnetic Laboratory

Terahertz electro-magnetic radiation is identified as the most direct and energy efficient interface to spins. We demonstrate that a nearly single-cycle terahertz pulse with the amplitude up to 0.5 MV/cm (0.2 Tesla) excites both modes of antiferromagnetic resonance in iron borate (FeBO₃). The quasi-antiferromagnetic mode is resonantly excited and its amplitude scales linearly with the strength of the THz magnetic field. Here we discover a nonlinear mechanism of excitation of the quasi-ferromagnetic mode, whose amplitude scales quadratically with the strength of the THz magnetic field. We propose a nonlinear mechanism of THz generation of magnons via a process similar to off-resonant stimulated Raman scattering.
Bottom-up Construction of an Adaptive Enzymatic Reaction Network

Britta Helwig, Bob van Sluijs, Aleksandr A. Pogodaev, Sjoerd G.J. Postma, Wilhelm T.S. Huck
Physical Organic Chemistry

The reproduction of emergent behaviors in nature using reaction networks is an important objective in synthetic biology and systems chemistry. Here, we report the first experimental realization of an enzymatic reaction network capable of an adaptive response. Our design is based on the dual activity of trypsin, which activates chymotrypsin while at the same time generating a fluorescent output from a fluorogenic substrate. Once activated, chymotrypsin counteracts the trypsin output by competing for the fluorogenic substrate, and producing a non-fluorescent output. We demonstrate that this network produces a transient fluorescent output under out-of-equilibrium conditions while the input signal persists. Importantly, in agreement with mathematical simulations, we show that optimization of the pulse-like response is an inherent trade-off between maximum amplitude and lowest residual fluorescence.

Sensing atomic-scale noncollinear magnetism combining magnetic exchange and spin-polarized imaging

N. Hauptmann¹, T.-C. Hung², A. K. Lemmens², D. Wegner³, A. A. Khajetoorians¹
1 SPM
2 FELIX Laboratory

The ultimate goal of magnetic-based storage is to create ultra-high density memory based on energy-efficient manipulation of the remnant magnetization state of nanomagnets such as skyrmions. Spin-polarized scanning tunneling microscopy (SP-STM) is the most routinely used method to characterize nanomagnets on surfaces, but it poses limitations that can unintentionally reverse the magnetization, and convolute the magnetic, electronic, and structural properties. We have developed a new combination of high-resolution magnetic detection utilizing SP-STM together with sensing magnetic exchange interactions (SPEX). We use SPEX to resolve the square skyrmion structure in a single iron layer on Ir(111) and demonstrate detection of different exchange regimes. We further show that the iron bilayer on Ir(111) is non-planar and use SPEX to decompose the real-space from the electronic/magnetic structure at the atomic level and the correlation with the spin-spiral ground state.
Optimisation of PTR-MS for analysis of standard compounds associated with peppermint oil

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¹ Molecular and Laser Physics
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Proton Transfer-Reaction Mass Spectrometry (PTR-MS) is a well-established technique for the analysis of trace gas volatile organic compounds (VOCs). It is a soft chemical ionisation technique that results in limited fragmentation of the measured gases. The PTR-MS consists of three regions; ionisation source (produces H₃O⁺ reagent ions), drift tube (where the VOCs are protonated) and analyser/detector region. By applying an electric field to the drift tube, it is possible to control the amount of clustering/fragmentation and hence find the optimal conditions for measuring a given VOC. We investigated the effect of changing the electric field in the drift tube on a selection of compounds that are used as ingredients in peppermint oil: menthone, menthol, limonene, α-pinene.

Design of a low-temperature scanning tunneling microscope for detection of light emission

Tzu-Chao Hung, Brian Kiraly, Alexander A. Khajetoorians, and Daniël Wegner

Scanning Probe Microscopy

Phosphorescent triplet-emitter molecules are promising candidates for highly efficient OLEDs, but it is not well understood how the optoelectronic properties are altered when they are embedded in a device environment. In order to fundamentally study such dependences with atomic-scale resolution, we upgraded a low-temperature STM (T ≈ 4K) to detect tip-induced light emission from the tunnel junction. An in-situ lens is placed close to the tunnel junction to collimate the light out of the ultrahigh vacuum system into a fiber coupler. The end of fiber is either guide to a spectrometer with an LN₂-cooled CCD detector or to a single photon counting module. This way, we are able to simultaneously study the structure, electronic properties and light-emission spectra of single molecules down to submolecular resolution and with photon yields down to a few counts per second. We will present the design and performance of the setup and show preliminary results on single-molecule light emission.
The level-spacing distribution of some fractals

Askar Iliasov, Sengjun Yuan, Mikhail Katsnelson
Theory of Condensed Matter

This work investigates spectrum statistics of some fractals. Earlier it was suggested that the spectrum of some fractals with finite ramification number is limit set of dynamical systems. It is shown that the energy-level distribution has power-law behaviour for fractals, which spectrum is the limit set of piece-wise linear functions. Therefore one can assume that such a behaviour is a general feature of fractals, and they are not described properly by random matrix theory. Several other arguments for the power-law behaviour of energy level-spacing distribution are proposed.

Multi-species trace gas detection using a mid-infrared supercontinuum source

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Trace Gas Research Group, Department of Molecular and Laser Physics

The broad spectral bandwidth of the mid-infrared (MIR) supercontinuum sources and their rather low relative intensity noise, makes them attractive for absorption spectroscopy and multi-species trace gas detection. We report the development of two different supercontinuum-based gas sensors for monitoring the quality of the fruit storage conditions by detecting ripening, fermentation and rotting-related volatiles via absorption spectroscopy.

The first system consists of a diffraction grating mounted on a galvo scanner and a single HgCdTe MIR detector. The rotation of the galvo scanner yields the spectrum which is recorded by the detector. The second system is based on nonlinear up-conversion in which the MIR beam is converted into near-infrared (NIR) in order to benefit from the efficient NIR CCD cameras. Both of the systems are capable to record the spectrum in ~3-4 µm range in a few ms, and utilize a multipass absorption cell to reach high detection sensitivities.
**Imaging of Partial Wave Resonances in Low-Energy Molecular Scattering**

Tim de Jongh, Q. Shuai, M. Besemer, S. N. Vogels, A. Van Roij, A. van der Avoird, G. C. Groenenboom, S. Y. T. van de Meerakker

*Spectroscopy of Cold Molecules*

At low energies in molecular scattering, interactions are dominated by the wavelike nature of matter. Scattering resonances are such classically forbidden processes. During a resonance, the molecules under consideration briefly form a quasi-bound complex. Its properties are extremely sensitive to the shape of the underlying interaction potential. Therefore, experimental characterization of resonances provides an excellent probe for the validity of theoretical models.

In a combined theoretical and experimental study, we investigate NO-He scattering resonances for collision energies as low as 1-10 K. We show that the currently available interaction potentials do not fully capture the experimentally observed scattering resonances. Therefore, we develop a new ab initio interaction potential at the CCSDT(Q) level. Preliminary results show better agreement between experimentally and theoretically obtained scattering resonances.

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**Atomic structure and electronic ordering in a sulfur depleted monolayer VS\(_2\) on Au(111)**

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\(^1\) Scanning Probe Microscopy

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Atomically thin transition metal dichalcogenides (TMDCs) have attracted great attention for the opportunity to study reduced dimensionality in a variety of electronic systems. Vanadium disulfide (VS\(_2\)) is of particular interest, as it is predicted to be magnetic even in its monolayer form, yet the magnetic ground state remains unclear. Here, we present an investigation with low temperature STM/STS on the structural and electronic properties of a sulfur-depleted, monolayer VS\(_2\)/Au(111). Upon annealing as grown monolayer VS\(_2\), there is a structural phase transition to a sulfur depleted phase, which exhibits a reconstructed chain-like structure. Our results shed light on the atomic structure of monolayer VS\(_2\), as well as reveal a complex Fermi surface of the striped phase. STS mapping at low temperature indicates the emergence of non-dispersive electronic ordering close to the Fermi level.
Band engineering in artificial electronic lattices

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Artificial electronic lattices, created atom by atom in a scanning tunneling microscope, have emerged as a highly tunable platform to realize and characterize the lowest-energy bands of novel lattice geometries. Here, we show that artificial electronic lattices can be tailored to exhibit higher-energy bands. We experimentally realize \( p_x \)-like bands in a four-fold and in a three-fold rotationally symmetric lattice, as well as show how an anisotropic design can be used to lift the degeneracy between \( p_x \) - and \( p_y \)-like bands. We corroborate our measurements with theoretical calculations in a muffin-tin potential. This approach to engineer higher-energy electronic bands in artificial quantum systems paves the way to exploring \( p \)-band physics in novel geometries in a controlled way.
**Developing a capacitance-based TDO technique for measuring magnetoelectric properties**

Sanne Kristensen and Alix McCollam

HFML

To examine the coupling between the magnetic and electric orders in magnetoelectric samples, it is valuable to monitor the electrical properties of these materials in high magnetic field.

One very sensitive and frequency-tunable measuring device is the Tunnel Diode Oscillator (TDO). The TDO is a device which sustains an oscillating signal with a frequency that depends on the components of a tank circuit. By inserting a sample either inside the coil or the capacitor of the tank circuit, the resonant frequency will alter and give information about the magnetic, conducting or dielectric properties of the sample. The TDO is commonly used by inserting a sample in the coil of the resonant circuit. Measuring the dielectric function of samples using the TDO has not been experimentally reported before.

I will present a new TDO set-up which has been used to measure the temperature, frequency and strain dependent dielectric function of a sample of strontium titanate. The results correspond well to data I obtained by a conventional capacitance method, as well as to earlier reported results.

**Gas Phase GrandPAHs**

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We investigate the effects of anharmonicity in the IR spectra of jet cooled large polycyclic aromatic hydrocarbons (PAHs) pentacene, coronene and dicroynylene. The photophysical properties of these molecules are of great interest for astronomy, since it is hypothesized that they are abundant in interstellar space. Comparison of our experimental cold, isolated and gas phase spectra to the widely used calculations with the harmonic approximation reveals significant shortcomings in theory. Therefore, we also present second-order vibrational perturbation theory anharmonic spectra and reveal the effects of anharmonicity in the grandPAH spectra including combination bands, Coriolis coupling and Fermi resonances.
**Chiral lead halide perovskite nanowires for second-order nonlinear optics**

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\(^1\) Spectroscopy of Solids and Interfaces
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Hybrid organic/inorganic lead halide perovskites (LHPs) have recently emerged as extremely promising photonic materials owing to the high light absorption and fluorescence efficiency and long carrier lifetimes and diffusion lengths. However, second-order nonlinear optical (NLO) responses such as second harmonic generation (SHG) have not yet been observed from the bulk of these LHP materials due to their intrinsic centrosymmetric structure.

Here we report the rational design of a new LHP material and the observation of strong bulk second-order NLO responses from nanowires based on this chiral perovskite material. We utilized the chiral \(\beta\)-methylphenethylamine as the organic component to direct the non-centrosymmetric assembly of 2D inorganic layers, resulting in perovskite crystals with a chiral P\(\overline{1}\) space group. The fabricated nanowires exhibit strong SHG with high polarization ratios and NLO circular dichroism. The novel design approach for LHP materials with intrinsic non-centrosymmetric geometries and bulk second-order optical nonlinearities is of great interest for expanding the range of applications and providing a prototype to develop new LHP functional materials and devices.

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**THz Spintronics at Interfaces of Magnetic Heterostructure Thin Films**

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Recently it was shown that circularly polarized femtosecond laser excitation in Co/Pt bilayers can effectively generate an ultrafast photocurrent pulse at the interface. The direction of this photocurrent is parallel to the in-plane magnetization of the Co layer and can be controlled by both the magnetic polarity of Co and the chirality of the circularly polarized light. Simultaneously, ultrafast spin current pulses are generated in the Co layer, which is converted to a charge current in the Pt layer via the inverse Spin-Hall effect. This charge current is in-plane and perpendicular to the magnetization of Co. Moreover, its direction can be controlled by the net spin orientation of the ultrafast spin current by switching the magnetization orientation of Co. We will present results on the role of the interfaces between the magnetic and non-magnetic layer on the generation of the ultrafast photocurrents.
**Generation of a Helium plasma using intense THz radiation and high magnetic fields**

Andrea Marchese  
HFML

We have observed the unexpected creation of a Helium (He) plasma after irradiation of He gas in a strong magnetic field by intense THz pulses generated by a free-electron-laser (FEL). The plasma is formed under resonant conditions when the frequency of the THz light and the magnetic field strength match the cyclotron energy of free electrons. We found that the plasma emits bright light, composed of the typical sharp He spectral lines split in magnetic fields due to the Zeeman effect. By measuring the plasma emission and its THz transmission, we are able to perform detailed investigations of the dynamics of the plasma formation, as a function of temperature (4-300 K), He gas pressure, laser power and field strength (up to 30 T). We find that the plasma formation is a strongly nonlinear effect and we can distinguish several different phases within the plasma dynamics.

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**Electrical resistivity across a nematic quantum critical point**

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HFML

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Of all the strongly correlated electron materials in which nematicity has been observed (Fe-pnictides and cuprates among others), FeSe$_{1-x}$S$_x$ offers a unique opportunity since nematic order exists in isolation from other forms of order. At low $x$ values, FeSe$_{1-x}$S$_x$ exhibits a nematic phase below $T = T_s$ which is gradually suppressed towards $x_c \sim 0.16$, for which $T_s = 0$ K. A superconducting phase however appears at low temperatures, preventing access to the normal state. In this work, we use static magnetic fields up to 35 T to suppress superconductivity in FeSe$_{1-x}$S$_x$ and follow the evolution of the electrical resistivity in the range $0 \leq x \leq 0.25$.

We observe signatures of quantum criticality, namely a divergence in the coefficient $A_2$ of the $T^2$ resistivity on approaching the quantum critical point (QCP) from either side and, at the QCP itself, a strictly $T$-linear resistivity. In addition to revealing the phenomenon of nematic quantum criticality, our observations suggest that nematicity could affect the transport properties of other materials too.
Magnetoplasmonic Nanoantennas for Ultrafast Magnetization Switching

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While all-optical magnetization switching is a promising alternative to magnetic-field based reading and writing of information, the bit-size attainable through this technique needs to be reduced to make it comparable to the technologies currently in use for information storage. We investigate the use of plasmonic nanoantennas to attain smaller spot-size and lower the threshold fluence over which all-optical magnetization switching can be observed. Due to the localized surface plasmon resonance in these structures, the incident electric field can be confined to a size smaller than the diffraction limit and is also enhanced in amplitude. We investigated the effect of plasmon resonances in cone-shaped Au nanoantennas on the magnetic and magneto-optical properties of Co nanoparticles, fabricated on the tips of the cones, with the goal to achieve all-optical magnetization reversal of the Co nanostructures. The Co tips show hysteresis, with an in-plane easy axis of magnetization. The hysteresis loop amplitude varies strongly with light wavelength due to resonant near-field enhancement in the nanocones. We also attempt to investigate suitable materials that could display all-optical switching to use as the magnetization-switching medium.

Statistical mechanics of crystalline membranes with dipole-dipole interactions

Achille Mauri, Mikhail Katsnelson

Theory of Condensed Matter

Thermal fluctuations play an essential role in the physical properties of two-dimensional crystalline membranes such as graphene. This is due to strong anharmonic fluctuations of the bending and stretching modes of the crystal, whose amplitudes diverge at long wavelengths. At finite temperatures, membranes are macroscopically flat but populated by thermal ripples which are akin to critical fluctuations at second order phase transitions. The correlation functions of bending and stretching modes exhibit scale invariance with anomalous critical exponents.

This work addresses the properties of fluctuating crystalline membranes subject to long-range interactions between electric dipole moments directed at each point along the local normal to the surface. This model provides a simple description of graphene derivatives and other two-dimensional materials exhibiting spontaneous out-of-plane polarization. It is shown that dipole-dipole interactions constitute an irrelevant perturbation to the large-distance correlation functions, leading to unmodified exponents. This result arises from the unexpected vanishing of a strongly relevant term of the bending mode propagator. At the same time dipole-dipole interactions corrects the behavior of correlation functions at intermediate wave vectors.
**A novel synthetic route to controlled stereoselective glycosylations**

Sam J. Moons, Rens A. Mensink, Jeroen P.J. Bruekers, Maurits L.A. Vercammen, Thomas J. Boltje

*Synthetic Organic Chemistry*

The major challenge in the chemical synthesis of oligosaccharides is the stereoselective synthesis of the glycosidic bond. 1,2-\textit{trans} glycosides can be synthesized with high selectivity by the use of neighboring group participation of a C-2 acyl group and is applicable to gluco- and manno-type sugars. The stereoselective synthesis of 1,2-\textit{cis} glycosides remains more challenging. By utilizing neighboring group participation using C-2 chiral auxiliaries, the stereoselective synthesis of 1,2-\textit{cis} gluco\textsuperscript{[1]} and manno\textsuperscript{[2]}-type sugars could be achieved. These reactions proceed \textit{via} an intermediate sulfonium ion, which is depicted in scheme 1. This intermediate can be prepared by making three disconnections, of which two have already been explored\textsuperscript{[1,3]}.

Using a thioglycoside precursor, \(\beta\)-sulfonium ion intermediates could by prepared utilizing an unexplored disconnection. Subsequently, the influence of the thioaryl moiety, as well as the benzyl protecting groups on the stereoselectivity was explored.

\[\text{Scheme 1: Retrosyntheses of the } \beta\text{-sulfonium ion}\]

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\[\text{[2]}\] Elferink, H.; Mensink, R. A.; White, P. B.; Boltje, T. J. \textit{Angew. Chem., Int. Ed.} 2016, 55, 11217−11220

**Magnetic Breakdown in the Nodal Line Semimetal HfSiS**

Claudius Müller, M.R. van Delft, T. Khouri, N.E. Hussey, S. Wiedmann  
*Correlated Electrons – High Field Magnet Laboratory*

By performing magneto-transport experiments up to 31 T, we investigate the Fermi surface of the nodal line semimetal HfSiS. We observe pronounced quantum oscillations superimposed on a positive magneto-resistance (fig. 1a). By taking the Fast Fourier Transform (FFT), we find two frequencies, labelled as $\beta$ and $\alpha$ which correspond to individual closed orbits around an electron and a hole pocket (fig. 1b), respectively. In addition, a frequency corresponding to the difference in frequencies, $\beta - \alpha$ is found in the FFT, which can be explained by magnetic breakdown between adjacent pockets, giving rise to a ‘figure of eight’ orbit enclosing both individual orbits $\beta$ and $\alpha$ (fig. 1c).

**FIG. 1.**

(a) Magnetic field dependency of the longitudinal resistance $R_{xx}$ at 1.3 K.

(b) Fast Fourier Transform of (a).

(c) Sketch of the individual orbits and the ‘figure of eight’ orbit in the Z-R-A plane.

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**A magnetic response in ensemble’s crossover of Random Matrix Theory**

Bektur Murzaliev, M. Titov and M. I. Katsnelson  
*Theory of Condensed Matter*

Magnetic susceptibility of quantum mesoscopic systems is calculated within a framework of the Random Matrix Theory. Magnetic field applied drives the system from the Gaussian Symplectic (GSE) or Gaussian Orthogonal Ensemble (GOE) to the Gaussian Unitary Ensemble (GUE). While GOE-GUE crossover is realized in the absence of spin-orbit interaction, the GSE-GUE crossover is characteristic for the systems with sufficiently strong spin-orbit coupling. We demonstrate that magnetic susceptibility is generally of opposite sign in these two cases. Our analytical results are compared to numerical simulations.
Compact optical absorption cells for trace gas sensing

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Trace Gas Research Group

Recently, we modeled and compared intensity enhancement and effective enhanced path-length of a compact 5 cm-long cavity with a 50cm-long absorption cavity [1]. The calculated results showed that a short cavity can yield equivalent sensitivity compared to a long cavity (proportional to the product of enhanced intensity transmission and effective path-length). Here, we will demonstrate the optical properties of such a short three-mirror system (cavity finesse ~ 15700) at near-IR wavelengths. For this we used a single absorption line of 100 ppmv CO₂ in N₂ at 6240.1 cm⁻¹ to verify the intensity enhancement effect with the reinjection mirror. Amongst others, we will compare the modelled (1400 and 101) with the experimentally determined intensity enhancement, and detection sensitivities, for short and long cavities, respectively.

References:

Improving Industrial Process Control with Multivariate Predictive Modelling

Tim Offermans, Jeroen Jansen
Analytical Chemistry/Chemometrics

This study shows the potential of using Partial Least Squares regression for predicting end-product quality in process control solutions for the industrial-scaled production of lactose (milk sugar) and casein (milk protein) powder. To optimize the yield and energy consumption of industry-scaled (bio)chemical production facilities, dedicated process control and monitoring solutions are required. Controllers used in such solutions typically act on real-time measurements of parameters such as temperatures, pressures or flow rates. Although those variables accurately reflect the status of the production installation, they do not directly reflect the quality of the actual end-product. Optimizing end-product quality is however a primary goal of the process. Multivariate statistical models therefore have a large potential for improving process control, as they can be used for predicting the quality of the end-product while it is still being produced, based on real-time process parameter measurements. This allows for better detection of production faults, identification of process faults and formulation of control actions, and contributes to more accurate and goal-oriented process control.
**Infrared spectroscopy of protonated fullerenes**

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FELIX Laboratory, Molecular Structure and Dynamics group

We investigate protonated fullerenes in an ion trap mass spectrometer with IR multiple photon dissociation (IRMPD) spectroscopy using the wide wavelength tunability and high pulse energies of the FELIX free electron laser. For ionization, we use an atmospheric pressure chemical ionization (APCI) source which is efficient for less polar molecules.

With this measurement, we present the first gaseous IR spectra of \( C_{60}H^+ \) and \( C_{70}H^+ \). When one proton attaches to the highly symmetrical neutral fullerene, their symmetry is significantly reduced causing many bands that were inactive in the unprotonated system to become IR-active, resulting in a rich vibrational spectrum. The spectra of the protonated species are therefore entirely different in appearance from those of the neutral \( C_{60} \) and \( C_{70} \). Experimental data are supported by results from quantum-chemical calculations at the DFT level.

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**Combination of UV-Vis and resonance light scattering as a probe to measure kinetics of TPPS J-aggregates in situ**

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HFML-EMFL

We have previously demonstrated that the handedness of helical supramolecular aggregates formed from achiral porphyrin molecules (tris-(4-sulfonatophenyl)phenylporphyrin, TPPS3) can be directed by applying rotational and magnetic forces during the self-assembly process. Interestingly, the growth of the aggregates and their chirality proceed at entirely different timescales, which can be caused by either a slow structural reorganization or by a hierarchical (stepwise) aggregation process. To identify the actual mechanism we have developed a method to simultaneously measure resonance light scattering (RLS, sensitive to aggregate size) and electronic absorption (UV/Vis, sensitive to local chromophore order) as a function of time. Our method allows to completely disentangle the absorbance and scattering contributions during porphyrin aggregation.
Controlling magnetic domain wall velocity by photo-induced localization of Bloch lines

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Understanding domain-wall dynamics is important for realizing faster and energy-efficient information processing systems. Several experiments have demonstrated that the domain-wall position can be optically controlled [1]. Here we report about an experimental investigation of the effects of femtosecond laser pulses on a moving domain wall in (Bi,Y)₃Fe₅O₁₂. The domain-wall motion is captured with the method of double photography [2]. Our results reveal that an ultrashort optical pulse applied during the domain-wall motion is able to slow down that motion. We found that the effect strongly depends on the domain-wall velocity and the optical fluence. To explain our observations, we suggest that the mechanism involves laser-induced localization of Bloch lines in slowly-moving domain walls, which are known to reduce domain-wall velocities [2].


Potent metabolic sialyltransferase inhibitors

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1 Synthetic Organic Chemistry
2 RUMC, Radiation Oncology

Sialic acid sugars are abundantly expressed on mammalian glycans outside the cell, regulating numerous biological processes. However, sialic acids are also the targets of several pathogens and aberrant sialylation of cancer cells mediates immune evasion, migration and metastasis. Sialyltransferase (ST) enzymes catalyze the addition of sialic acids and are therefore prime targets for inhibition. We developed highly potent ST inhibitors based on C-5 modified 3-fluoro sialic acid. We found that the addition of carbamates to the C-5 position allows for the inhibition of sialylation at lower concentration, for a longer period of time and in more resistant cell lines. This qualifies them as good candidates for therapeutic development and as a tool for elucidating the role of sialic acid in both health and disease.
IR characterization of reaction products created in an electrical discharge for astrochemical research

Daniël Rap, Jan Thunnissen, Alexander Lemmens, Anouk Rijs
FELIX Laboratory

In the chemically rich interstellar medium (ISM), a large variety of molecules have already been detected. However, none of the proposed ubiquitous polycyclic aromatic hydrocarbons (PAHs) has been confirmed. In this research we have tried to mimic the physical and chemical conditions of the ISM using an electrical discharge. Naphthalene, a PAH from which there is an indication of existence in the ISM, is used as precursor in our discharge. The formed fragments and reaction products are studied by IR/UV ion dip spectroscopy using infrared free electron laser FELIX. By scanning the IR fingerprint region, we have been able to identify multiple products among which are aromatic molecules with additional ethynyl and diacetylene side chains. The ethynyl addition is often seen in pyrolysis experiments and follows the HACA mechanism. However, the measured compounds with diacetylene side chain suggest that also larger acetylenic groups may have a role in the fragmentation and formation mechanisms of PAHs in the ISM.

Probing electric polarization induced by very high magnetic fields in a frustrated spinel

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Materials that exhibit magnetic frustration often have complex non-collinear spin ground states that can give rise to multiferroicity. In magnetic compounds with the spinel structure, the pyrochlore sub-lattice can host geometrical frustration: one such compound is the antiferromagnetic spinel CdCr₂O₄. This material exhibits a magnetostructural transition at the Neél temperature of 7.8 K to a spin spiral state. When a magnetic field of 28 T is applied, the material undergoes another magnetostructural transition to a ferrimagnetic phase. We used dilatometry to map the low-temperature phase diagram up to 30 T, and observed Negative Thermal Expansion in the ferrimagnetic phase. We also performed polarization and Electrostatic Force Microscopy measurements up to 30 T. We find a magnetic field-induced electric polarization, which increases with field up to the ferrimagnetic transition, where it collapses to zero. The field-induced polarization may arise due to the spin spiral state.
**Metabolic engineering of sialic acids to visualize host-pathogen interactions and inhibit bacterial and viral infections.**

**Emiel Rossing**  
*Synthetic Organic Chemistry*

Sialic acids play a major role in host-pathogen interactions. The influenza virus infection cycle depends on the binding and eventual hydrolysis of host sialic acids. Pathogens, like non-typeable *Haemophilus influenzae* (NTHi) evade the immune system by presenting host-derived sialic acids. Recently, we reported sialic acid-based probes to visualize sialic acid stealing by NTHi in an in vitro model of the human respiratory tract. We modified the bronchial epithelial cell sialic acids with either azidoacetyl (Az)-, or propargyloxycarbonyl (Poc)- modified sialic acids. We visualized decoration of NTHi with Az-sialic acid and demonstrated efficient sialic acid inhibition, abrogating NTHi serum resistance. Poc-sialic acid, was not transferred. We showed that Poc-modified sialic acids are largely resistant to neuraminidase cleavage and influenza cell-to-cell transmission is strongly reduced in Poc sialic acid glycoengineered host cells.

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**Neel Spin Transfer Torques in Dirac Anti-Ferromagnet**

**Robert Sokolewicz, Mikhail Titov**  
*Theory of Condensed Matter*

Two-dimensional anti-ferromagnet (AFM) s-d model on a honeycomb lattice is proposed as a generic microscopic model to investigate dynamics of Neel vector in the presence of electric field or current. Using microscopic analysis we derive coupled dynamic equations on Neel and magnetization vectors in the presence of non-trivial AFM magnetic textures. We single out leading contributions to the Neel spin-transfer torques and discuss their dependence on disorder strength, Fermi energy, and s-d exchange interaction strength.
Product-pair correlations in complete state-resolved bimolecular inelastic collisions

Guoqiang Tang, Zhi Gao, Matthieu Besemer, Gerrit C. Groenenboom, Ad van der Avoird, Sebastiaan Y.T. van de Meerakker
Spectroscopy of Cold Molecules

A detailed understanding of molecular interactions is crucial for the interpretation of microscopic dynamics. The crossed molecular beam technique proved to be a sophisticated approach to obtain detailed information of potential energy surface. Despite the success studying collisions between molecules and rare-gas atoms [1], quantum-state resolved bimolecular collisions are experimentally more challenging because of the low particle density in the colliding beams. We used a Stark decelerator and a hexapole in a crossed molecular beam configuration to produce two molecular beams of NO and ND$_3$ with an almost perfect quantum-state purity. State-resolved inelastic collisions between NO(X$^2$Π$_{1/2}$, $j$=1/2, $f$) and ND$_3$(J$_k$=1, $p$=1) molecular beams are studied. From the measurement, we successfully observed the correlated energy transfer in rotationally NO-ND$_3$ inelastic collisions.


High Field Quasiparticle Mass study in PrOs$_4$Sb$_{12}$

N. Hesp, Lucas Tang, B.Vlaar and A. McCollam
HFML-EMFL

PrOs$_4$Sb$_{12}$ is a heavy fermion system that initially attracted interest due to being the first Pr-based unconventional superconductor. The renormalisation of the quasiparticle mass, in the absence of the Kondo effect, suggests that PrOs$_4$Sb$_{12}$ is not a typical heavy fermion system, and may have a novel mechanism of both mass renormalisation and superconductivity. A field induced antiferroquadrupolar (AFQ) phase, arising near the crossing of Zeeman-split crystal electric field states, could provide fluctuations or means to mediate the superconductivity and the renormalised quasiparticle mass. However, clear experimental evidence for these effects is still missing.

I will present de-Haas van Alphen (dHvA) measurements on PrOs$_4$Sb$_{12}$, in high magnetic fields up to 33T. Our results show that the quasiparticle mass saturates at high magnetic field, above 20 T. In combination with the tracking of the dHvA phase, we propose that the mass enhancement at high fields is not solely mediated by AFQ fluctuations, and that other interactions in the crystal electric fields begin to influence the system.
**Ultrathin crystalline alloys of Gd and Fe on W(100)**

Werner van Weerdenburg, Brian Kiraly, Daniël Wegner, Alexander Khajetoorians

*Scanning Probe Microscopy*

The challenge to find small, topologically protected chiral magnetic structures, e.g. skyrmions, concurrently stable at room temperature, motivates the search for new magnetic materials. An ultrathin ordered alloy, consisting of 3d transition metal and 4f rare-earth metal elements, contains the ingredients necessary to support chiral magnetic order with high thermal stability. Alloys of GdFe are especially promising as the bulk material is ferrimagnetic, displays ultrafast switching and can be tuned to antiferromagnetic ordering.

Here we show the emergence of two atomically thin crystalline phases of GdFe, accessible by varying the stoichiometry, probed at the atomic scale with a scanning tunneling microscope. Both structural phases are matched with isomorphic growth on the W(100) substrate, stabilized by a wetting layer. Finally, both phases are spectroscopically characterized as the first step toward spin-polarized measurements.

**Supramolecular transformers: towards microscale shape changes in artificial systems**

Mitch Winkens

*Physical Organic Chemistry*

Microscale shape changes play a great role in biological systems. Changes in the shape of cells can be a driving force for shrinking, growing, folding and movement of tissues,¹ and they even play a role in cell division² and intercellular signal transduction.³ While small-scale shape changes are already being applied in artificial systems, we are only scratching the surface of what is possible if biology provides any indication.

In the current study, the focus will be on the developing and understanding of smart supramolecular systems on the microscale level. The project should lead towards the construction of new tunable shape-changing systems. Outlined here are the first results of experiments on the self-assembly of alcohol ethoxylate surfactant molecules under osmotic pressure.

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Visible light-induced active site switch in flavinium catalysis

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Mass spectrometry with capillary tip irradiation is a powerful technique for the study of photocatalytic reactions.¹ We have used this technique in combination with infrared photo-dissociation spectroscopy and quantum-mechanic calculations to determine possible reaction intermediates and the mechanism of recently developed flavinium salt 1 photocatalytic system. We have observed formation of an atypical hydroperoxyhydroflavinium 1+H₂O₂ intermediate during this reaction which is unprecedented in literature so far. This intermediate differs from the usual one in the position of the hydroperoxy group. This active site switch is driven by the change from ionic to radical mechanism during the photocatalytic cycle.

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