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The Institute for Molecules and Materials (IMM) is an interdisciplinary research institute in chemistry and physics at the Radboud University Nijmegen. Its mission is to fundamentally understand, design and control the functioning of molecules and materials. The institute is a centre of excellence that trains the next generation of leaders in science and entrepreneurship.
Preface

The American physicist John Bardeen is the only person to have won the Nobel Prize in Physics twice. In 1956 he won it for the invention of the transistor and in 1972 for the fundamental theory of conventional superconductivity, known as the BCS theory. Bardeen once noted that ‘Science is a field which grows continuously with ever expanding frontiers. Further, it is truly international in scope. Any particular advance has been preceded by the contributions of those from many lands who have set firm foundations for further developments.’

In 2014 the Institute for Molecules and Materials (IMM) has continued to build on its strong national and international reputation and to push the expanding frontiers of science. Nigel Hussey and his team from the High Field Magnet Laboratory acquired a €14.9 million grant from the National Roadmap for Large-scale Research Facilities. Furthermore they set a new world record by the generation of a continuous magnetic field of 37.5 tesla in a resistive, non-superconducting magnet. Last but not least, the headquarters and legal entity of the European Magnet Field Laboratory were established in Brussels.

More international borders were crossed in 2014. Alexey Kimel obtained a MegaGrant (90 million roubles) from the Russian Federation for establishing a state-of-the-art laboratory in Moscow. Alan Rowan and Dave Parker were among the first scientists to acquire a Horizon 2020 grant for an Innovative Training Network from the European Union. On top of this, the IMM scientists and research facilities became part of a new pan-European partnership focusing on the innovation in ‘raw materials’. This consortium, named ‘KIC Raw MatTERS’, includes more than 100 partners from 22 European countries representing leading partners from industry, research and academia.

Long ago John Bardeen already said that ‘Science is a collaborative effort. The combined results of several people working together is often much more effective than could be that of an individual scientist working alone.’ With the scientific excellence and the team spirit that we have cultured within the IMM, the institute is optimally positioned for the future!

Elias Vlieg and Iwan Holleman

Director and Managing Director of the Institute for Molecules and Materials
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SUPERGEL - biomimetic extra cellular matrix

It has long been known that cell behaviour – motility, embryogenesis, stem cell differentiation, wound healing, tumorgenesis, etc – are extremely sensitive to the biophysical cues from the extracellular matrix (ECM) in which the cells reside. Yet in spite of considerable research, it remains unclear exactly how the chemical composition and the properties of the materials on the outside, control cell behaviour on the inside. Once the exact nature of this ‘outside-in’ communication is unraveled, the full potential of regenerative medicine can be realized [1]. Numerous studies have indicated that biophysical properties essential for controlling cell behaviour include ECM stiffness, the number and type of cell attachments and the pore size. Another biophysical property, unique to all biological ECM materials, that may be essential in controlling cell behaviour, is that of material ‘strain stiffening’; biological ECMs become several orders of magnitude stiffer when strained by the cells. However, to date strain stiffening has hardly been studied since there are virtually no synthetic materials, which exhibit strain stiffening and none that stiffen at the very low forces a cell can apply.

In 2001 the group of Professor Roeland Nolte (IMM-Nano science) published in Science the discovery that a helical polymer could be stabilized by supramolecular interactions to form one of the stiffest polymers in the world. (Figure 1). After years of applications of these stiff nano-rods as scaffolds for nanoelectronics and nanodevices, in the group of Prof Alan Rowan (IMM- Molecular Materials), a request appeared for the use of the unique spectroscopic signatures of these materials as a security measure in paper used for bank notes. To stabilize these polymers in paper they needed to become more water-soluble. An Australian Postdoc Heather Kito and a French Postdoc Mathiu Koepf, set about decorating the polymers with ethylene glycol tails.

Figure 1. left AFM image of the extremely long and stiff polymers formed by peptidopolyisocyanides invented in 2001. Right The addition of water solubilizing PEG side-arms resulted in a polymer which gelates in water upon warming.
In 2012 together with Dr Paul Kouwer we discovered a new class of biomimetic materials, based upon helical stiff peptidopolyisocyanides (PICs). [2,3] Hydrogels based on oligo(ethylene glycol) grafted polyisocyanopeptides mimic almost precisely the strain stiffening properties of biological ECMs.[4] These extremely stiff helical polymers [3] form gels upon warming at concentrations as low as 0.005 % wt polymer, with materials properties almost identical to these of intermediate filaments and extracellular matrices. The macroscopic behaviour of these gels can be described in terms of the molecular properties of the basic stiff helical polymer and a multi-step hierarchical self-assembly, which results in strain stiffening [5]. For the first time, we now have a tool that allows us to examine cell behaviour in a synthetic ECM. Preliminary results of experiments with the PIC-gels are ideal as wound dressing materials and indicate that stem cell fate can indeed be directed by varying the ‘strain stiffening’ properties of this new supergel.


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**Figure 2.** AFM 2 µm x 2 µm image of the hydrogel (1.5 mg/ml). Revealing the fibrellar bundles and nanoporous nature of the gel. (right) Change in PIC-gel stiffness as a function of the applied stress.
IMM News 2014

Tenth Ewald Prize for Aloysio Janner and Ted Janssen
January 2014

Emeritus professors Aloysio Janner and Ted Janssen were awarded the tenth Ewald Prize for the development of super-space crystallography and its application to the analysis of aperiodic crystals.

HFML sets world record with a new 37.5 tesla magnet
March 2014

In March HFML set a new world record: the generation of a continuous magnetic field of 37.5 tesla in a resistive (i.e. non-superconducting) magnet. Strong magnetic fields of this type are crucial for materials research.

Royal decoration for emeritus prof. Ad van der Avoird
April 2014

On Friday April 25, Emeritus Prof. Van der Avoird received a Royal decoration (Knight in the Order of the Dutch Lion) for his lifelong contribution to theoretical chemistry and training students.

Prof. Mikhail Katsnelson (Theory of Condensed Matter) member of KNAW
May 2014

Prof. Katsnelson became an elected member of the Royal Netherlands Academy of Arts and Sciences (KNAW). Other members from IMM are professors Huck, Nolte, Rasing, and Van der Avoird.
**HFML acquires 14.9 million from National Roadmap**  
*July 2014*

Professor Nigel Hussey and his team from the HFML acquired an extremely prestigious – and substantial – grant (€14.9 million) from the National Roadmap for Large-scale Research Facilities. They will use it to build new magnets and to further expand the operating capacity of the laboratory.

**European Magnet Field Laboratory gets headquarter in Brussels**  
*November 2014*

The European Magnet Field Laboratory (EMFL), which the HFML is part of, has been formally established in Brussels. On 27 November the involved institutes, RU, FOM, CNRS, and HZDR, signed a collaboration agreement and on 27 January 2015 they also signed for the founding of the legal entity, an ‘Association Internationale sans but lucratif’ (AISBL).

**Kick-off meeting IMM PhD’s 2014**  
*December 2014*

On Monday 8 December, IMM Director Elias Vlieg, Jan van Hest, and Iwan Holleman had a successful kick-off meeting with a group of about 20 IMM PhD students who started in 2014. It is the intention that these PhD students form a year group of the Graduate School for Molecules and Materials (GSMM) and that they undertake several joint activities each year.

**European consortium on ‘raw materials’ kicks off**  
*December 2014*

Scientists and research facilities at the IMM will be part of a large pan-European partnership focusing on innovation in ‘raw materials’. The consortium ‘RawMatTERS’ includes more than 100 partners from 22 countries in the EU, representing leading partners from industry, research and academia. This ‘Knowledge and Innovation Community’ will stimulate the competitiveness and growth of the European raw materials sector through intensive innovation and entrepreneurship.

**Teaching Award 2014 for Floris Rutjes**  
*December 2014*

On 18 December, professor Floris Rutjes has received the Faculty’s Teaching Award 2014. The nomination for this award and the selection of the winners were fully arranged by the students’ representatives in the faculty.
Newly appointed professors

- On 1 September Ad Bax was appointed professor by special appointment in Biophysical NMR Spectroscopy. Bax has a magnificent track record in the research field of NMR development and application. He is employed by the National Institute Health in Bethesda, USA., and will spend a few weeks per year at IMM.

- On 1 September Alex Khajetoorians was appointed as full professor of the Scanning Probe Microscopy group. Before Khajetoorians was a research leader of an Emmy Noether Group embedded in the Wiesendanger group at the University of Hamburg.

Leaving professors

- On 23 May a Farewell Symposium was organized for Jan Kees Maan, former director of the High Field Magnet Laboratory and professor on Condensed Matter Physics. Lectures were amongst others given by Kostya Novoselov (Nobel Prize in Physics 2010) Greg Boebinger (Director National High Magnetic Field Laboratory in Tallahassee) and Jochen Wosnitza (Director Hochfeld Labor Dresden).

- On 27 June a symposium was organized on the occasion of the 65th birthday of Rob de Groot, professor on Electronic Structure of Materials. Lectures were given by Thom Palstra (University of Groningen), Reinder Coehoorn (Philips), Ekkes Bruck (Technical University Delft), and Peter de Boer.

- On 1 Augustus Professor Wim van der Zande of the Molecular and Biophysics group and chair of the FELIX board left our institute to become a group leader in the research department of ASML in Veldhoven.
IMM Awards and Prestigious Grants 2014

- **Misha Katsnelson** became an elected member of the Royal Netherlands Academy of Arts and Sciences (KNAW).
- **Ad van der Avoird** received a Royal decoration (Knight in the Order of the Dutch Lion) for his lifelong contribution to theoretical chemistry and training students.
- **Aloysio Janner** and **Ted Janssen** were awarded the **Tenth Ewald Prize**, for the development of superspace crystallography and the analysis of aperiodic crystals.
- **Nigel Hussey** and the HFML acquired an extremely prestigious – and substantial – grant (€14.9 million) from the National Roadmap for Large-scale Research Facilities.
- **HFML** participates in an approved FOM Program (€2.9 million) on conducting interfaces in insulating oxides, together with four other Dutch universities.
- **Theo Rasing** and colleagues from other universities obtained one of the six grants for a FOM Free Program (€2.2 million) on ‘Exciting Interactions’.
- **Alexey Kimel** and **Bas van de Meerakker** were each granted a subsidy in the FOM Project Ruimte.
- **Nadine Hauptmann** was awarded a prestigious fellowship from the “Alexander von Humboldt Foundation” for postdoctoral researchers.
- **Alexey Kimel** obtained a MegaGrant from the Ministry of Education and Science of the Russian Federation. This grant is worth €1.2 million for three years.
- **Britta Redlich** obtained a subsidy from the COMPASS (Coherent Optical Microwave Physics for Atomic-Scale Spintronics in Silicon) project for measurements at the FELIX Laboratory.
- **Wilhelm Huck** acquired a prestigious NWO TOP-PUNT grant (€2 million) – together with colleagues at Delft and Groningen Universities – for the bottom-up construction of a synthetic cell using complex enzymatic networks.
- **Lutgarde Buydens**, **Jeroen Jansen**, and **Herma Cuppen** each received an NWO ECHO subsidy.
- **Jeroen Jansen** obtained a project on in-flow multidimensional particle analysis that is funded through TA-COAST.
- **Kim Bonger** (Biomolecular Chemistry) and Rene Toes (from Leiden UMC) received a grant from the Institute of Chemical Immunology (ICI).
- **Dave Parker** and **Alan Rowan** each acquired a Horizon 2020 grant for an Innovative Training Network.
- **Michael Taylor** (Solid State NMR) received a Marie Curie International Outgoing Fellowship (IOF).
- **Alan Rowan** has received the 2014 Soft Matter and Biophysical Chemistry Award of the Royal Society of Chemistry.
- **Alex Khajetoorians** received the Nicholas Kurti Prize, sponsored by Oxford Instruments.
- **Anouk Rijs** was awarded the Mildred Dresselhaus Award which includes a guest professorship in Hamburg.
- **Mark van Eldijk**, former PhD student in Bio-Organic Chemistry, has won the DPI Golden Thesis Award 2014.
- **Floris Rutjes** has received the Faculty’s Teaching Award 2014.
Magnetifiek

Door monnikenwerk en ingenieursgeduld heeft Nijmegen sinds deze week de sterkste elektromagneet van Europa. Hoe de minimale brainwave van een technicus een revolutie werd.

Door Martijn van Calmthout
Foto’s Jiri Büller

Magnetifiek in the media

Het bezwete kopen staan ze in een kleine werkploeg: technici Jos van Velsen en Frits Janssen van het Nijmeegse High Field Magnetic Laboratory. Met witte stofhandschoentjes aan legt Frits dunne plaatjes koperen ringen ter grootte van een oud singelrijtje met een speciaal patroon van gaten en inkepingen in de zachtjes brommende borstelmachine, aan het andere eind telt Jos ze er schoongemaakt weer uit. Frits heeft nog stapels te gaan, Jos stapelt de blinkend schone schijven aan zijn kant netjes op, een enkel begeschadigd exemplaar gaat eruit.

Monnikenwerk. Maar iemand moet het doen, glimlachen Jos en Frits. De geoorlogde Bitterplaatjes worden verzet bij een gespecialiseerd bedrijf buiten de deur. Waarna ze, uiteindelijk, één voor één volgens een voorafgekozen schema op elkaar zullen worden gestapeld. Zodanig dat ze samen de soep vormen van een bal beet van een elektromagneet, met een veld van 37,5 tesla. De sterkste van Europa. En met een beetje behendig redeneren zelfs de sterkste van de wereld.

Om precies te zijn, vertelt projectleider Frans Wijnen van het HFML, werken de heren technici aan een kopie van de magneteer die net klaar is en waarmee de afgelopen weken het beoogde megamagnetenveld is bereikt.

Aan de vooravond van de festiviteiten staat Radboud Universiteit-physicus Uli Zeitler aan de voet van het nieuwe
Nieuwe chemische reactie verklaart ontstaan van leven

Mijnmeeste chemie hebben voor het eerst een reactie laten plaatsvinden die mogelijk het ontstaan van leven nabootst.

Het van de RU Nijmegen hebben belangrijke stap in het verklaren van het ontstaan van levensvormen gepland en deze opties geopend door ze op aminezuur liggende moleculen, die niet als aminezuur in de natuur aanwezig zijn. De eerste linkshandige aromatische moleculen kennen zo zijn ontstaan, op aarde of in de kosmos. Zij publiceren volgende week in het vakblad Natuur Communicaties.

Jan Kees Maan gaat nu voor Europa

Strategisch denken leerde Jan Kees Maan (63) al begin jaren zevenentwintig, toen hij betrokken was bij de bezetting van de TU in Delft. Hij had politicus kunnen worden, maar ging voor natuurkunde. Vandaag neemt hij officieel afscheid als hoogleraar en baas van het HI.MFL (High Field Magnet Laboratory).

Jan Kees Maan kon er niet goed tegen dat de TU Delft, waar hij natuurkunde studeerde, autonoom werd bestuurd. Hij was een van de voortrekkers van de studentenbeweging in 1972. Tijdens de bezetting van de faculteit was hij het die de onderhandelingen met het college voerde. Hij leerde strategisch denken, een talent dat hem verder bracht in de natuurkunde. In 2003 opende het geavanceerde laboratorium voor hoge magneten (HI.MFL) aan het Torremoosveld in Nijmegen. Er staan vijf — binnenkort zes — magnetomeren tot 38 tesla (ter vergelijking: een koelkomkastmagnet is 0.1 tesla).


Andre Geim en Konstantin Novoselov, Maers promovendus, kregen in 2010 de Nobelprijs voor hun ondertekening van graafite. Ze deden hun meeting in het HI.MFL. Meer bevestiging had Maan raak kunnen interpreteren.

"Ik voorzie ongelofelijke mogelijkheden"

De Nijmeegse emeritus hoogleraar organische chemie en Nolde bedrijft reeds wetenschappelijke toppost. "Ik heb het gevoel dat je moet vroeg worden geboren."

CORRY VAN DRIEL

"Ik voorzie ongelofelijke mogelijkheden"

"Ik voorzie ongelofelijke mogelijkheden"

Interview

Jan Kees Maan gaat nu voor Europa

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Mikhail Katsnelson peilt die diepte onder de werkelijkheid
‘Wij fysici praten langs elkaar heen’

Vorig jaar ontving hij de Spinozapremie. Toch vindt de uit Rusland afkomstige vaste-stoffenfysicus Mikhail Katsnelson dat zijn vak degeneereert. ‘We zijn de eenheid van de natuurkunde aan het kwijtraken. Dus werkt hij aan een alternatief.

door Robert Dulmers

‘MAGNETEENTEN’ stond als je echte hier gewoon op zat - je kon er echt spijtige zoer aan toevoegen; dat was opvredend. Magneteenten, stad in de Oeral. Honden rolende schietbessen aan de horizon, nog steeds, met zwarte, rode en zwartwolfsige plekken, maar de magnetische berg waar Stalin staatzaal naar is verzonden is al lang geleden afgegraven. Nog Mikhail Katsnelson, (Magneteenten, Sojoez, 1957). ‘Ze importeren nu jerrycans van ledere en verkeer.’

Maar we zijn niet in Magneteenten, maar in Nijmegens, waar Katsnelson – ‘neg dat liever Masa’ – al weer bijna tien jaar hoogstaande theoretische natuurkunde is aan de Radboud University.

Iedereen is nu zo vol van kwantuminformatica, maar waar is de grote discussie die de denkers van de eerste uur meesteed? Universiteit.

Vorig jaar ontving hij de hoogste Nederlandse wetenschapssluitkampioen, de Spinozapremie, voor zijn haardendravende werk in de vaste-stoffenfysica. Hij is mede-auteur de theoretici van het grafen, het nieuwe wondermateriaal van één laag, dat bijzondere eigenschappen, waarnaar elektronen kunnen reageren met de snelheid van het licht. Grafen is toegewijd aan de mogelijkheid, supersterke en lichtgewicht, niet zonder de komende jaren de wereld te veranderen. Hij heeft een vijfjarig plan om het structurele en elektrische domein van grafen te versterken en bij te dragen aan de toekomstige rekenmachines.

Ik ben dus de meest oostelijke Cao-European die er bestaat. De gigantische hoogte werden in de grond gestampt in 1928, in Shanghai eerste Vierjarenplan, en de nucleaire Miganetekniek kreeg spoedig de status van gesloten stad. Het was juist: op een gegeven moment oosteinde woedende, schijf en spindel, tot onze grote vertaling dat bijna iedereen in onze kleine ouderdom had gehoord die waren. Veel waren kinderen van koekjes, rijke boeren, en slaven in de slavenhuis, of kinderen van de intelligentie. Onze grootmoeder was naar deze uithoek verbannen. Wat Stalin deed, was natuurlijk verschrikkelijk, maar een overwicht in die tijd, en ik vroeg me af waarom. Nu denk ik dat het was omdat we eeuwig geen keuze hadden. Als je gipsbroodschuur in de mensenscholen, in geschiedenis, in literatuur, in filosofie, was onmiddellijk op een beeld meestreekt. Je moest niet weten wat als artikelen werd beschouwd, en je zou moeten kunnen inschatten en een disident worden omwreven, iets wat maar weinig mensen wegrekken is. Bijvoorbeeld, kinderen van de nazipartij, waren natuurlijk verschrikkelijk, maar mensen die in de omgeving van militairen werden afgezet.

Aan de andere kant als je in we- en natuurkunde gezelschapsvoelen was, je meer dan welkom. Literatuur was natuurlijk te krijgen, maar mislukken. We waren kinderen van koekjes, rijke boeren, en slaven in de slavenhuis, of kinderen van de intelligentie. Onze grootmoeder was naar deze uithoek verbannen. Wat Stalin deed, was natuurlijk verschrikkelijk, maar een overwicht in die tijd, en ik vroeg me af waarom. Nu denk ik dat het was omdat we eeuwig geen keuze hadden. Als je gipsbroodschuur in de mensenscholen, in geschiedenis, in literatuur, in filosofie, was onmiddellijk op een beeld meestreekt. Je moest niet weten wat als artikelen werd beschouwd, en je zou moeten kunnen inschatten en een disident worden omwreven, iets wat maar weinig mensen wegrekken is. Bijvoorbeeld, kinderen van de nazipartij, waren natuurlijk verschrikkelijk, maar mensen die in de omgeving van militairen werden afgezet.

Citeert om een uitleg genoeg, vraag ik: hoeveel filosofie of theologische geloofsdiensten dan natuurkunde. Of politiek.

‘Ik houd van een beetje noogtekort. Ik probeer wat te je hoofd. En het is tegenwoordig van: dit was een vreselijke gewoon goed.’

Katsnelson leest, waar Britse Sterren, niet, niet... We hebben een boodschap, een boodschap een bediener, Tot de bediening, dat je eraan denkt. Is het er in een enge, niet: heteloven.

Vier jaar oude, in heel met keukencorrelatie, het eerste inzicht. In een plaschen beer.

31 maart 2014, 2014/11

HFM vestigt wereldrecord met nieuwe 38 tesla magnete

Het High Field Magnet Laboratory aan de Radboud Universiteit vestigde vandaag een wereldrecord: een continu magnetisch veld van 38 tesla in een resistieve (niet-supergerelieerde) magnet. Dit soort hoge magneten zijn cruciaal voor materiaalonderzoek. Het ontwerp van het HFM toont aan dat er geen dure supergerelieerde spoelen nodig zijn om 38 tesla te halen, wat de afscherming met een factor tien verlaagt. Op 10 april 2014 wordt de nieuwe magnete in gebruik genomen.

Materiaalonderzoekers hebben behoefte aan sterkere magneten: in een magnetisch veld van 38 tesla zijn sommige effecten wel honderd keer beter dan in een veld van 33 tesla, het huidige maximum in het Nijmeeuw lab voor hoge magnetenveld HM. Daarom begon het HFM in 2011 met een ambitieus project: het ontwerpen en bouwen van een magnet die de huidige wereldrecord van 36 tesla terdeed.

Sprong voor de wetenschap

Volgens HFM-onderzoeker dr. Uli Zeitler is het veld van 38 tesla een grote sprong voor de wetenschap. “In een veld van 33 tesla naar 38 tesla is een sommige effecten wel honderd keer beter te zien dan in een veld van 33 tesla, het huidige maximum in het Nijmeeuw lab voor hoge magnetenveld HM. Daarom begon het HFM in 2011 met een ambitieus project: het ontwerpen en bouwen van een magnet die het huidige wereldrecord van 36 tesla terdeed.”

Figuur 1. Magnetspoelen

Materiaalonderzoekers hebben behoefte aan sterkere magneten: in een magnetisch veld van 38 tesla zijn sommige effecten wel honderd keer beter dan in een veld van 33 tesla, het huidige maximum in het Nijmeeuw lab voor hoge magnetenveld HM. Daarom begon het HFM in 2011 met een ambitieus project: het ontwerpen en bouwen van een magnet die de huidige wereldrecord van 36 tesla terdeed.
Research Report 2014

The Institute for Molecules and Materials (IMM) is an interdisciplinary research institute in chemistry and physics at Radboud University. Its mission is to fundamentally understand, design and control the functioning of molecules and materials. The institute is a centre of excellence that trains the next generation of leaders in science and entrepreneurship.

The IMM is composed of twenty research groups, each headed by a full professor. The four research themes are:

1. Structure and Dynamics of Molecules
2. Molecular Life-like Systems
3. Quantum Matter

The institute employs around 140 PhD students and every year some 30 of them graduate. There is a strong focus on interdisciplinary research between theorists and experimentalists as well as between physicists and chemists.

Structure and Dynamics of Molecules
The focus within this research theme is on the constellation and motion of the atoms within molecules, molecular complexes, molecular and atomic collisions, and even chemical reactions. Examples include small organic molecules, non-covalently bounded complexes, and collisions between diatoms and noble gases. Experiments are often based on advanced spectroscopic techniques such as Nuclear Magnetic Resonance (NMR), various laser techniques, and velocity-map imaging. Theoretical approaches include \textit{ab initio} calculations, simulations and DFT methods.

Molecular Life-like Systems
This research theme involves the design, synthesis and characterization of molecules and molecular assemblies in order to elucidate the structure and function of natural systems. Examples include artificial cells and organelles, enzyme-mimetic structures, orthogonal chemistry in living cells and analysis of biomolecular interactions. This research is based on expertise in bio/organic chemistry, supramolecular chemistry, microfluidics, microscopy, NMR spectroscopy techniques, and data analysis/chemometrics.

Quantum Matter
Researchers working on this theme focus on studying the properties of matter that is dominated by interactions between quantum particles, quantum coherence, and quantum correlations and topology. The goal is to understand and develop new materials and concepts based on collective, emergent quantum effects. Examples include the study and control of magnetic materials at energy and time scales of the exchange interaction, sub-nanometre metal clusters (including metal-oxide clusters), and graphene and quantum dots. Properties are often studied under extreme conditions such as high magnetic fields, ultra-short laser pulses, and low temperatures.

Nanostructured Materials
This research theme involves the design, growth, synthesis and characterization of materials in which the properties partly stem from their nanoscale dimensions, with the aim of exploring novel property-function relationships. This includes supramolecular assemblies, nanoreactors, self-assembled monolayers, chiral clusters and solar cells. These materials are typically studied using microscopy (including SPM) and X-ray diffraction.
Research facilities

The national and international position of the IMM is enhanced by the availability on the university campus of a number of large-scale experimental research facilities, including:

- A High Field Magnet Laboratory (HFML) for continuous fields up to 37.5 Tesla. A hybrid magnet for achieving 45 Tesla in 2017 is being constructed.
- Free Electron Lasers for Infrared and Terahertz Experiments (FELIX) Laboratory. The infrared lasers (FELIX/FELICE) and the terahertz laser (FLARE) are fully tunable between 3 and 1,500 microns.
- A Large-Scale Facility for high-resolution liquid NMR and a Solid-State NMR Facility for advanced material science, including an 850 MHz proton NMR instrument.
- A Scanning Probe laboratory (NanoLab) with a wide range of Scanning Tunnelling Microscopy (STM) and Atomic Force Microscopy (AFM) techniques.
- A Trace Gas Facility for the application of laser diagnostics in biology and medicine.

In March 2014 the HFML set a new world record by generating a continuous magnetic field of 37.5 Tesla in a purely resistive (i.e. non-superconducting) magnet.

Collaboration

The organic chemistry groups at the IMM have a longstanding collaboration with the Institute for Complex Molecular Systems (ICMS) at the Eindhoven University of Technology and the Stratingh Institute for Chemistry at the University of Groningen. The IMM also collaborates intensively with the Catholic University of Leuven in Belgium and several organic chemistry groups collaborate with the University of Barcelona. Within graphene research, the groups at the IMM led by Profs. Katsnelson and Maan collaborate closely with their ex-colleagues Profs. Geim and Novoselov, who now work at the University of Manchester. Prof. Katsnelson also works closely together with scientists at the Universities of Uppsala, Hamburg, and Moscow. There are numerous bilateral collaborations with other research groups, including those at a range of European and non-European universities e.g. Tsinghua, Jilin, and Peking University in China, are numerous.

The IMM is a partner in two formal collaborations with the Foundation for Fundamental Research on Matter (FOM). One partnership relates to the relocation and the decade-long exploitation of the free electron lasers ‘FELIX and FELICE’ in Nijmegen, and the other involves the joint running of the HFML and the promotion of materials research with high magnetic fields. The Engineering and Physical Sciences Research Council (EPSRC, UK) transferred a research contract on solid-state physics with free electron lasers to Nijmegen.

The EU-FP7 project on the European Magnet Field Laboratory (EMFL), which is coordinated by HFML, involves investigating all legal, financial, organizational, and employment issues required for a Founding Agreement for the EMFL. On 27 November the three founding partners (Radboud University, Helmholz Zentrum Dresden-Rossendorf (HZDR) and le Centre National de la Recherche Scientifique (CNRS) in Grenoble/Toulouse) signed an agreement to formally start working together as a single entity that develops and operates world-class high magnetic field facilities.

Scientists and research facilities at the IMM will be part of a large pan-European partnership focusing on innovation in ‘raw materials’. The consortium ‘RawMatTERS’ includes more than 100 partners from 22 countries in the EU, representing leading partners from industry, research and academia. This ‘Knowledge and Innovation Community’ will stimulate the competitiveness and growth of the European raw materials sector through intensive innovation and entrepreneurship.
Research results

Highlights are listed below under the Institute’s four main research themes.

**Structure and Dynamics of Molecules**

Dr Rijs and her colleagues at Molecular and Biophysics have imaged peptides in unprecedented detail using far-infrared spectroscopy. Conformation selective far-infrared action spectroscopy – in combination with the novel Born-Oppenheimer Molecular Dynamics theoretical method – has proved to be a promising new tool for the detailed structural characterization of peptides.

Dr Harren and his colleagues at Molecular and Laser Physics have carried out broadband mid-infrared dual-comb spectroscopy with a two-crystal optical parametric oscillator, measuring absorption and dispersion spectra in gas phase simultaneously. The broad spectral coverage and the fast acquisition time associated with extreme sensitivity will enable extensive spectral studies of rarefied samples and real time monitoring of processes. (Optics Letters)

The Molecular Structure and Dynamics group (led by Prof. Oomens) has carried out infrared spectroscopy of negatively charged gaseous polyaromatics, which are probably present in the interstellar medium. The experimental IR spectra provide an important benchmark for quantum-chemical calculations of IR spectra. Comparison of experimental and theoretical spectra suggests that good agreement can be obtained.

Dr Cuppen, Dr de Wijs, and their colleagues at Theoretical Chemistry have studied the interactions of adsorbed CO$_2$ on water ice at low temperatures. Interstellar water ice is thought to be the precursor of cometary ice and even water on Earth. Whether, how, and in what form interstellar ice survives during the evolution of a dense molecular cloud into a planetary system is far from understood. (Phys. Chem. Chem. Phys.)

**Molecular Life-like Systems**

Prof. Pruijn and his colleagues at Biomolecular Chemistry have studied the specificity of protein citrullination, which is involved in several physiological processes. These include regulation of gene expression and are associated with various diseases, such as cancer, multiple sclerosis, rheumatoid arthritis and Alzheimer’s disease. (Biochim. Biophys. Acta)

Prof. Buydens and her colleagues at Analytical Chemistry have linked odours to compounds identified in data from gas chromatograph and mass spectrometers using a chemometrical data science approach. They have developed two approaches that revolutionize the interpretation and speed of this analysis. These approaches were demonstrated via analyses of flavoured beverages from Heineken.

Researchers in the Bio-Organic Chemistry group (led by Prof. Van Hest) studied enzymatic cascade reactions in multicompartment polymersomes. A simple cell mimic with subcompartments was created based on polymer building blocks. The final product of the cascade reaction was produced locally and confined in an organelle subcompartment if the last enzyme of the reaction sequence was enclosed in the same compartment. These concepts may lead to a better understanding of the structure and functioning of the living cell. (Angew. Chemie Int. Ed.)

Prof. Huck and his Physical Organic Chemistry group are exploiting reaction-diffusion systems in smart materials. Chemistry in a traditional round-bottom flask is completely different from chemistry within a living cell, where the typical diffusion times of components are of a magnitude that is similar to their reaction times. These so-called reaction-diffusion systems can reveal extremely complex behaviour and the aim is to understand and harness this complexity. (Angew. Chem. Int. Ed.)
A fascinating question in science is how molecular single handedness arose from an achiral abiotic world. The Solid State Chemistry and Synthetic Organic Chemistry groups (led by Profs. Vlieg and Rutjes) have jointly developed a reaction in which an enantiopure product can be obtained from achiral reactants in a single reaction. They envision that a wider range of chiral molecules is likely to be accessible in enantiopure form and are currently extending this method to other pharmaceutically relevant molecules. (Nature Communications)

Dr Tessari (Biophysical Chemistry) and his colleagues have developed a technique in which the NMR signals of small molecules in solution are enhanced without any chemical modification. Signal Amplification By Reversible Exchange (SABRE) is based on the reversible association of both para-Hydrogen and a substrate molecule to a mediating Iridium complex. The proposed approach results in a dramatic reduction (ca. 100-fold) of measuring time. (J. Am. Chem. Soc.)

Quantum Matter
The group led by Prof. Hussey (Correlated Electron Systems, HFML) obtained experimental support for proposed supersolid phase in a magnetically frustrated metal. Magnetically frustrated materials are those in which the preferred alignment of electronic spins cannot be achieved due to the geometrical arrangement of atoms on the crystal lattice. Evidence has been found for intriguing additional magnetic transitions within the proposed supersolid phase. (Phys. Rev. B)

Dr Zeitler and his colleagues at Semiconductors and Nanostructures, HFML have found a temperature-driven transition from a classical semiconductor to a two-dimensional topological insulator. Topological insulators are a new state of quantum matter, which is characterized by an insulating gap in the bulk and gapless edge states.

The Spectroscopy of Surfaces and Interfaces group (led by Prof. Rasing) studied laser induced spin precession in a granular film of FePt. This will be the recording medium used in next generation hard disk drives as it has an exceptionally high magneto crystalline anisotropy that allows for higher data storage densities than can be achieved with current recording media. (Appl. Phys. Lett.)

Profs. Katsnelson and Fasolino (Theory of Condensed Matter) have studied the use of moiré patterns as a probe of interplanar interactions. The superposition of crystalline layers – with either slightly different lattice constants or different orientations – creates moiré patterns. The strain distribution and out-of-plane displacement in moiré patterns can provide direct information on the interplanar interactions in van der Waals heterostructures. (Phys. Rev. Lett.)

Nanostructured Materials
The Applied Materials Science (led by Dr Schermer) group worked on Ultra-thin, high performance tunnel junctions for III-V multi-junction solar cells. Due to lower absorption compared to a standard tunnel junction, the wavelength dependent response of the underlying Gallium Arsenide cell improved, which led to higher efficiency of the double junction cell.

The group led by Prof. Christianen (Soft Condensed Matter, HFML) demonstrated –together with the Bio-Organic Chemistry group – that high magnetic fields can be used to reversibly open and close nano-sized polymer capsules. This finding makes it possible to capture and release cargo particles, which is a crucial first step towards applications in magnet-assisted drug delivery. It is the first time that such a magneto-valve nanosystem has been realized. (Nature Communications)

Prof. Rowan and his colleagues at Molecular Materials reported on strain stiffening of biomimetic materials. They described the effect of easily controllable variables (concentration, polymer length and temperature) on the mechanical properties of semi-flexible polymer hydrogels. The outlook is a class of materials for which the mechanical properties can be readily adjusted by changing the external conditions. (Nature Communications)
Prof. Nolte and his colleagues at Molecular Nanomaterials are developing a molecular Turing machine. A great challenge for the future is how to develop computers that can perform calculations at the molecular level. This molecular Turing machine should be able to read and write data on a polymer chain using information from a ring attached to a molecular device that moves along this chain. (*J. Am. Chem. Soc.*)

Dr Elemans (Scanning Probe Microscopy) used an STM tip to induce chemical reactions with manganese porphyrins at a solid/liquid interface. Besides using an STM for observations, an exciting possibility is to use it to trigger local chemical reactions. This opens up the possibility of manipulating chemical reactions locally at the nanoscale, in particular at solid/liquid interfaces. (*J. Am. Chem. Soc.*)

The Solid State NMR group (led by Prof. Kentgens) demonstrated high-resolution solid-state NMR of nanolitre sample volumes. The resolution achieved makes it possible to exploit the proton chemical shifts for structural assignments in the solid-state. The group will use this setup to study specific regions of polymers and aligned polymer fibers to arrive at new insights into their local physical properties.

**Awards and grants**

Prof. Hussey and his team from the HFML acquired an extremely prestigious – and substantial – grant (€14.9 million) from the National Roadmap for Large-scale Research Facilities. They will use it to build new magnets and to further expand the operating capacity of the laboratory. In addition, the HFML participates in an approved FOM Program (€2.9 million) on conducting interfaces in insulating oxides, together with four other Dutch universities.

Prof. Rasing and colleagues at the Technical University Eindhoven and the University of Twente obtained one of the six grants for a FOM Free Program (€2.2 million) on ‘Exciting Interactions’. This programme focuses on the non-equilibrium states of magnetic systems and the time dependence of the magnetic exchange interaction. Moreover, Dr Kimel and Dr Van de Meerakker were each granted an award in the FOM Project Ruimte.

Dr Kimel also obtained a MegaGrant from the Ministry of Education and Science of the Russian Federation. This grant is worth 90 million roubles (€1.2 million) for three years. During this period Kimel will establish a state-of-the-art lab specialized in developing novel methods for ultrafast control of magnetization and electric polarization at Moscow State Technical University for Radio Engineering, Electronics and Automation.

Prof. Huck acquired a prestigious NWO TOP-PUNT grant (€2 million) – together with colleagues at Delft and Groningen Universities – for the bottom-up construction of a synthetic cell using complex enzymatic networks. Prof. Buydens, Dr Jansen, and Dr Cuppen each received an NWO ECHO subsidy. Dr Jansen also obtained a project on in-flow multidimensional particle analysis that is funded through TA-COAST.

Profs. Parker and Rowan each acquired a Horizon 2020 grant for an Innovative Training Network. Dr Redlich obtained a subsidy from the COMPASS (Coherent Optical Microwave Physics for Atomic-Scale Spintronics in Silicon) project for measurements at the FELIX Laboratory. COMPASS is subsidized by the Engineering and Physical Sciences Research Council (EPSRC) in the UK.

Dr Hauptmann was awarded a prestigious fellowship from the “Alexander von Humboldt Foundation” for postdoctoral researchers.
Prof. Rowan received the 2014 Soft Matter and Biophysical Chemistry Award from the Royal Society of Chemistry for his pioneering work on processive catalysis, functional self-assembly and the development of biomimetic extracellular matrices. Dr Rijs was awarded the Mildred Dresselhaus Award, which includes a guest professorship at the Hamburg Centre for Ultrafast Imaging. Prof. Katsnelson became an elected member of the Royal Netherlands Academy of Arts and Sciences (KNAW).

Emeritus Prof. Van der Avoird received a Royal decoration (Knight in the Order of the Dutch Lion) for his lifelong contribution to theoretical chemistry and training students. Emeritus professors Janner and Janssen were awarded the tenth Ewald Prize for the development of super-space crystallography and its application to the analysis of aperiodic crystals.

**Societal impact**

IMM has cooperative arrangements with leading companies in the Netherlands, including ASML, DSM, Philips, NXP, Solvay, Unilever and AkzoNobel. And, in recent years, the IMM has given birth to many spin-off companies, including Chiralix, Encapson, FutureChemistry, Mercachem, ModiQuest, Noviotech, Pansynt, ReRa Systems, SensorSense, Sphere Fluidics, Spinovation, SynAffix, Syntarga, Synthon, TeraOptronics, and tf2 devices.

Grants for new chemical innovations (the so-called KIEM subsidy) were awarded to Prof. Pruijn, Prof. Rutjes, and Dr Feiters. Prof. Pruijn and NovioSmart plan to develop a new blood test for detecting the antibodies that are specifically related to rheumatoid arthritis. Dr Feiters and Okklo Life Sciences aim to make a medicine that will avoid the accumulation of harmful substances in the body, caused for instance by a genetic disorder. Profs. Rutjes and Pansynt will focus on a new class of compounds that look like very promising antibiotics. These compounds can only be produced under high pressure.

On 2 October 2014 the Radboud Research Facilities, which give mainly small and medium-sized enterprises access to state-of-the-art equipment for research and development, were officially opened. Selected research equipment from the IMM is included in these facilities and is thus made more widely available. The Radboud Research Facilities are partly funded by a ‘Robuuste Investeringsimpuls’ from the Province Gelderland worth €6 million.
Future research

A continuing challenge is provided by a €27 million grant from the national investment in large infrastructures (NWO-BIG) in 2006 for the Nijmegen Centre for Advanced Spectroscopy (NCAS). This exceptional grant provides the resources IMM needs to construct a new 45 Tesla hybrid magnet for the HFML (which will be ready in 2017) and a Free Electron Laser for research using Terahertz radiation (FLARE). HFML’s new hybrid magnet will create new research opportunities based on world-leading magnet technology. FLARE, which is part of the FELIX Laboratory, is used for studying magnetic excitations in molecules and for low-energy spectroscopy on large molecules and biomolecules. Moreover, these free electron lasers are suitable for various kinds of spectroscopy on electrons in high magnetic fields.

The national Sector Plan for Physics and Chemistry (SNS) was approved in 2010 with a very positive outcome for Radboud University. Two new initiatives in Chemical Biology and Advanced Spectroscopy of functional molecules and materials started then within IMM. This has led to exciting scientific results and, after two successful progress evaluations, the expectation is that SNS will continue as a structural source of funding after 2015.

The annual operational hours of the HFML have increased to 2,000 per year in 2014 and these will continue to increase in 2015. This growth is thanks to a partnership between Radboud University and FOM (2011) and two grants (worth €11 million and €15 million, respectively) from the National Roadmap for Large-scale Research Facilities in 2012 and 2014. A continuing challenge is the search for structural funding for the operation of the HFML at the target level of 3,000 hours per year.

The successful implementation and exploitation of the ‘Gravitation’ Research Centre for Functional Molecular Systems (FMS) – in collaboration with partners in Eindhoven and Groningen – is of the utmost importance for IMM. Many highly talented students have been hired and several meetings were organized to encourage greater scientific interaction.

The Radboud Nanomedicine Alliance, a joint initiative of Radboud UMC, NCMLS, and IMM, focuses on developing new effective medicines and materials for the treatment of diseases, tailored to the situation of individual patients. The available research facilities will be open for intense cooperation with chemical and biomedical industrial partners.

In 2015, all leading scientists at the IMM will continue to make their on-going research projects a big success and to acquire substantial new funding for future projects. In this way the IMM will continue to build on its strong national and international reputation.
prof.dr. Stuart Parkin
prof.dr. Martina Havenith
prof.dr. Claudia Felser
prof.dr. Ludwik Leibler
prof. dr. Steven de Feyter
prof.dr. Nigel Hussey
prof.dr. Khajetoorians

IMM
Colloquia 2014
IMM Colloquia 2014

18 February  
prof. dr. Stuart Parkin  
IBM Almaden Research Center, San Jose, California  
*The spin on electronics science and technology of spin currents in nano-materials and nano-devices*

Preceding presentation:  
Bas Pieters (Biomolecular Chemistry & Synthetics, Organic Chemistry)  
*The effect of trimethylated lysine 4 histone 3 (H3K4me3) peptide length, on its recognition by various reader proteins*

25 March  
prof. dr. Martina Havenith  
Physical Chemistry, Ruhr-University, Bochum  
*It is water that matters*  
*THz absorption studies - a new tool to study biomolecular hydration*

Preceding presentation:  
René Steendam (Solid State Chemistry & Synthetic Organic Chemistry)  
*Crystals: A handy solution for enantiopure synthesis*

2 March  
prof. dr. Claudia Felser  
Max Planck Institute, Chemical Physics for Solids, Dresden  
*New tetragonal Heusler compounds for spintransfer torque*

Preceding presentation:  
Sjoerd Postma (Physical Organic Chemistry)  
*Understanding the cell: how to deal with molecules that both move and react?*

24 June  
prof. dr. Ludwik Leibler  
ESPCI ParisTech/CNRS, Paris  
*Adhesion and organ repair by nano-particle solutions*

Preceding presentation:  
Eduardo Monfardini (Theoretical Chemistry)  
*Modelling the chemical evolution of molecular clouds as a function of metallicity*

23 September  
prof. dr. Steven de Feyter  
Laboratory of Photochemistry and Spectroscopy, University of Leuven  
*Nanopatterning of graphite and graphene at the liquid/solid interface via molecular self-assembly: from fundamentals to applications*

Preceding presentation:  
Peter van Rhee (High Field Magnet Laboratory)  
*Giant magnetic susceptibility of gold nanorods detected by magnetic alignment*
22 October  prof.dr. Nigel Hussey
High Field Magnet Laboratory, IMM
*High-temperature superconductivity and the Catch-22 conundrum*

Preceding presentation:
Albert Wong (Physical Organic Chemistry)
*A retrosynthetic approach to a chemical reaction network*

25 November  prof.dr. Khajetoorians
Scanning Probe Microscopy, IMM
*Spin sensing and magnetic design at the single atom level?*

Preceding presentation:
Dmytro Afanasiev (Spectroscopy of Solids and Interfaces)
*Anharmonic magneto-acoustics induced by a femtosecond larger pulse*
The Institute for Molecules and Materials announces

sIMMposium 2014

Date • 19 & 20 May
Place • Cultureel Centrum ‘de Lindenberg’ • Ridderstraat 23 • Nijmegen
Presenting • Six keynote speakers and many IMM graduate students

The Institute for Molecules and Materials (IMM) is an interdisciplinary research institute in chemistry and physics at the Radboud University Nijmegen. Its mission is to fundamentally understand, design and control the functioning of molecules and materials. The institute is a centre of excellence that trains the next generation of leaders in science and entrepreneurship.

Magnetism of organic-metal interfaces
Stefan Blügel
Theory of Solids, Peter Gruenberg Institut, Jülich, Germany

Ultrafast charge and spin control with atomically strong terahertz fields
Rupert Huber
Quantum Electronics and Photonics, University Regensburg, Germany

Bio-inspired and supramolecular approaches in transition metal catalysis
Joost Reek
VAN ‘T HOF INSTITUTE FOR MOLECULAR SCIENCES, UNIVERSITY OF AMSTERDAM

Large molecules in space
Xander Tielens
Astronomy, Leiden Observatory, Leiden University

Exploring the constancy of physical law, forces beyond the Standard Model and the dimensionality of space-time from molecular spectroscopy
Wim Ubachs
UU University Amsterdam

Bio-inspired chemistry with proline-rich peptides
Helme Weitnauer
Bio-Inspired Organic Chemistry, Swiss Federal Institute of Technology, Zurich, Switzerland

Nanosponges and polyglycidol hydrogels to customize the delivery of proteins and drugs
Eva Harsh
Vanderbilt University, Nashville, USA Radboud University Nijmegen

www.ru.nl/imm
sIMMposium 2014

The 2014 Edition of the sIMMposium was held on 19 and 20 June at the conference venue “De Lindenberg” in downtown Nijmegen. The new venue at the riverside and the weather were great! Professor Xander Thielen (Leiden Observatory) gave the ‘IMM Honorary Lecture’ at the start of the symposium. His presentation dealt with the “Large molecules in space”. The evening lecture on Monday was given by professor Wim Ubachs on his exploration of the constancy of physical laws and it was followed by the traditional dinner in the Restaurant Vlaamsch Arsenaal, also in the center of Nijmegen.

In total 7 invited lectures by renowned scientists, 19 presentations by PhD students, and 30 poster presentations were given during this edition of the sIMMposium. Because of the beautiful weather and the nice courtyard of the Lindenberg, the poster session was held outside which gave a pleasant atmosphere. The organizing committee gave the IMM Award for the Best Oral Presentation to Bas Pieters (Synthetic Organic Chemistry) and the IMM Award for the Best Poster Presentation to Merel van Wijk (Theory of Condensed Matter).

The main objective of the ‘sIMMposium’ is for all research groups to have a chance to present the progress they made during the past year. All IMM scientists and other interested staff members assemble for a two-day programme of lectures, posters, and informal discussions. The topics are as varied as the IMM itself and give the participants the opportunity to broaden their scientific horizon. Presentations are given by PhD students of the IMM and by world-class scientists that are invited to the sIMMposium.

The IMM is grateful to the organizers of the sIMMposium 2014: Kim Bonger, Alan Rowan, Alexei Kimel, Jos Oomens, Erna Gouwens, and Iwan Holleman.
GC-MS/O (Gas Chromatography coupled to Mass Spectrometry and Olfactometry) is a technique for the analysis of odour-active compounds in e.g. food products. It enables to simultaneously obtain information on both the chemical and sensory properties—the odour—of a mixture of compounds (see Figure 1). The data resulting from a GC-MS/O experiment however have a very complex nature, since it consists of data from two different but complementary or orthogonal detectors, which should be properly linked (associated). State of the art is that this analysis easily takes several weeks for a standard GC-MS/O experiment via current manual procedures. In this study, we have developed two approaches that revolutionize the interpretation and speed of the analysis of GC-MS/O data. We demonstrate these approaches here with the GC-MS/O analysis of a flavoured beverage from Heineken.

The work was carried out within the ALBERT project (Analysis of Large data sets By Enhanced Robust Techniques), which was granted during the TA-COAST1 call in 2012. The ALBERT project aims at the development of generic strategies and methods to facilitate better and more robust data analysis methods for complex analytical data. This should not only lead to a reduction in time and cost for the (industrial) data analysis step, it also boosts the value of the complex data. The project is carried out by three industrial partners (AkzoNobel, DSM and Heineken) and two academic partners (Radboud University and UMC Groningen).

**Approach 1: automated analysis of GC-MS/O data**

The basic challenges in linking GC-MS/O data are differences in elution time for identical compounds between chromatographic runs and mismatches in detection (time) between the mass spectrometer and olfactometer in the same run. Our first approach has automated the linking of the chemical and sensory data by overcoming these challenges. This approach has several advantages: 1) total data analysis time is reduced to about half an hour, which is de facto several hundreds of time faster than the state of the art analysis; 2) a less biased association of odours to compounds is obtained compared to manual data analysis and human interpretation; 3) the approach is independent of the analysed sample and can be used for the analysis of data from every GC-MS/O experiment. A paper about this approach is submitted (Gerretzen et al., submitted).

**Approach 2: modelling GC-MS/O data**

In the next step, we have taken data analysis further by modelling the data, to extract the relevant information from the data. An example of such a model can be found in Figure 2. Assessors within one rectangle perform similar: they have a similar perception of the same odour-active compounds. A path from top to bottom indicates that an assessor is associated to a specific odour description. It can therefore easily be concluded that e.g. all assessors are associated to ‘Fruity’, which is perceived due to the presence of compound D in the flavoured beverage. Assessors EB, HV and HZ need more training in detecting compounds with a ‘Vegetative’-like odour. At a glance, this model shows which odours are linked to which compounds and which assessors perceived those odours. We are currently improving this model, its visualisation and we are comparing it to well-known chemometrical tools as Principal Component Analysis. Both approaches are already implemented and in use at Heineken. They have also gained attention in the annual ‘Elements’ magazine from NWO and on the COAST website, showing that the value of this work is also recognized by other partners.
Solar cells convert sunlight into electricity. They can be made of a large range of materials. In general, the price of the cells is correlated to the performance of the cells. Cheap cells have efficiencies below 10% (organic, amorphous silicon), the immediately priced cells which are mostly applied nowadays (wafer based silicon) have efficiencies between 15 and 20% and the best cells (multi-junction III-V, material compounds of group III and V in the periodic system) can reach efficiencies above 40% but are more expensive. In order to make III-V cells commercially attractive for terrestrial application a cheap lens is used to concentrate sunlight with a concentration factor of 500-1000 on a tiny III-V cell. In such a system the 1-sun cell current is multiplied by the concentration factor and can therefore reach values up to 30 A/cm². The multi-junction configuration implies that multiple cells are deposited in one growth run in order to use the solar spectrum more efficiently. These cells are series connected with a so-called tunnel junction in between. A tunnel junction consists of a highly doped p-n-junction that behaves as a resistor at low voltages. At higher voltages the current collapses which is disastrous for the cell performance. The most important demand for a good tunnel junction is therefore that the maximum current at low voltage is significantly higher than the maximum current generated by the concentrated sunlight. In addition the tunnel junction should be optically transparent, thus photon absorption in the tunnel junction should be minimized that to avoid losses. High bandgap tunnel junction materials (e.g. InGaP) that can be grown lattice matched on GaAs can meet the requirement of low absorption, but their peak currents are far too low. Furthermore, we found that in lower bandgap materials at high doping levels our standard p-type dopant zinc diffuses into the surrounding layers which also lowers the peak current. To overcome this problem an autodoping technique was developed in which carbon builds into the growing layer under extreme conditions. Carbon doping was explored for a range of materials with the best results for AlGaAs. This p-type layer was combined with a highly doped GaAs n-type layer in the final tunnel junction. Gradual decreasing of the thickness of both layers to minimize absorption resulted in a tunnel junction with a thickness of only 13.5 nm (n-type 6 nm, p-type 7.5 nm) with an extremely high peak current of at least 600 A/cm². This tunnel junction was applied in a double junction cell (InGaP and GaAs). Due to the lower absorption compared to a standard 20/20 nm tunnel junction, the wavelength dependent response (EQE) of the underlying GaAs cell improved which lead to a 4% (relative) higher efficiency of the double junction cell.
NMR is a widespread spectroscopic technique with applications in chemistry, biology and medicine. It is often used in the analysis of complex mixtures (e.g. biofluids, food extracts, reaction mixtures), mainly due to its aspecific character and straightforward, non-destructive sample preparation. However, because of NMR low sensitivity, analysis of dilute solutions is generally precluded. One way of increasing the sensitivity of NMR is by inducing non-Boltzmann nuclear spin state populations with hyperpolarization techniques. Signal Amplification By Reversible Exchange (SABRE) is a technique in which the NMR signals of small molecules in solution are enhanced without any chemical modification. SABRE-derived hyperpolarization is based on the reversible association of both p-H₂ and a substrate molecule to a mediating Iridium complex. When such a complex is formed at low magnetic field, a transient scalar-coupling network drives the transfer of spin order from the p-H₂-derived hydrides to the nuclear spins of the substrate molecule, resulting in strongly enhanced NMR signals. Because of the reversible character of the interaction, enhanced NMR signals are also observed for substrate molecules free in solution.

SABRE works usually well at relatively high concentrations (in the millimolar range); however, the obtained hyperpolarization is strongly reduced in dilute solutions and eventually disappears at low micromolar concentrations. We have found that this problem can be circumvented with the addition of a second ligand (referred to as “co-substrate”) in large excess with respect to the Iridium catalyst. The ligand 1-methyl-1,2,3-triazole (mtz) proved to be an optimal co-substrate for SABRE hyperpolarization of several substrates. SABRE hyperpolarization in the presence of co-substrate is shown in Figure 2A, for different samples of pyridine at low micromolar concentrations. The thermal equilibrium spectrum (top trace, black) was acquired with 512 scans for the 5 µM sample. The colored spectra were acquired at concentrations between 0.5 and 5 µM with a single scan following SABRE hyperpolarization. By comparing the signal integrals at thermal equilibrium and after SABRE, an enhancement factor of 121 is obtained for the 5 µM pyridine sample. Thanks to our approach, SABRE can be successfully applied at concentrations of a few micromolar. As illustrated by the plot in Figure 2B, a linear dependence exists between SABRE signal intensity and substrate concentration in the low micromolar regime. This result is important as it indicates that hyperpolarization allows quantitative NMR analysis at much lower concentrations than routinely employed. Furthermore, by comparison with conventional NMR quantification methods, we have shown that the proposed approach results in a dramatic reduction (ca. 100-fold) of measuring time. These results support possible future applications of SABRE for quantitative determination of dilute components in complex mixtures such as natural product extracts, reaction mixtures, or biofluids.
The post-translational conversion of peptidylarginine to peptidylcitrulline, a process also known as citrullination, is catalyzed by the enzyme family of peptidylarginine deiminases (PADs). Citrullination of proteins has been demonstrated to be involved in several physiological processes, such as regulation of gene expression, and to be associated with various diseases, such as cancer, multiple sclerosis, rheumatoid arthritis and Alzheimer’s disease. Interest in this type of post-translational modification is likely to accelerate, especially with the recent development of PAD inhibitors. To elucidate the role of PAD enzymes and citrullination in both health and disease, more insight into the substrate specificity of PADs is of crucial importance.

The human genome encodes 5 PAD isotypes, hPAD1, -2, -3, -4 and -6. Since hPAD2 and hPAD4 are the isotypes expressed in inflammatory cells and protein citrullination by these PADs has been proposed to mediate pathophysiological processes in the diseases mentioned above, we performed two types of experiments to obtain more insight into the selectivity by which these PADs citrullinate substrates. Recombinant hPAD2 and hPAD4 were expressed in bacteria or mammalian cell lines and allowed to citrullinate proteins in cell lysates, as well as a series of synthetic peptides. The citrullinated residues in proteins and the efficiency of peptide citrullination were determined by mass spectrometry. In total 320 hPAD2 and 178 hPAD4 citrullination sites were characterized. Amino acid residues most commonly found in citrullination sites for both isotypes are Gly at +1 and Tyr at +3 relative to the targeted arginine. For hPAD4 several additional amino acids were observed to be preferred at various positions from –4 to +3 (see Figure). The second approach was based on a synthetic peptide (L1) that was known to be citrullinated by both hPAD2 and hPAD4. The effect of single amino acid substitutions on the efficiency of conversion by these PADs was determined and this partially confirmed the preferences derived from the citrullinated protein data (see Figure). Nevertheless peptide context dependent differences were also observed. Taken together, our data show that the enzyme specificity for cellular substrates and synthetic peptides differs for hPAD2 and hPAD4. hPAD4 shows more restrictive substrate specificity compared to hPAD2.

Consensus sequences, which can be used as the basis for the development of PAD inhibitors, were derived for the citrullination sites of both hPAD2 and hPAD4. Isotype-specific PAD inhibitors may not only be useful for studies aimed at the biochemical function of these enzymes, but may also find applications in the development of therapeutics for treatment of diseases in which citrullination plays a pathological role.
The living cell contains smaller organelle subcompartments that are used to spatially organize and separate enzymes and reagents in order for the cell to function properly. In this fashion, incompatible processes and environments can be physically separated from each other, while still being able to function in close proximity and work together in multistep processes without interference from each other.

To attain a model system to study the benefits of the natural compartmentalization process in more depth, a simple cell mimic was created based on polymer building blocks. Several different types of small compartments containing enzymes (organelles) were encapsulated together with other reagents in a cell-sized polymeric vesicle and used to carry out a model enzymatic reaction sequence (Figure 1). Three different enzymes were included in the system, Candida antarctica lipase B (CalB) and Alcohol Dehydrogenase (ADH) were each encapsulated in different semi-porous PS-b-PIAT nanoreactors that acted as organelle subcompartments, while Phenylacetone Monooxygenase (PAMO) was kept in the main compartment of the cell-sized vesicle.

A pro-fluorescent substrate, which should undergo sequential modifications by first PAMO, then CalB and finally ADH, before becoming fluorescent (Figure 1, reaction scheme), was used to study the model cascade reaction in the system using fluorescence microscopy. This showed that the fluorescent product was produced inside the cell mimic and that the reaction intermediates were capable of accessing the different subcompartments. It was also observed that the final product of the cascade reaction was locally produced and confined in an organelle subcompartment if the last enzyme (ADH) of the reaction sequence was also enclosed in the same compartment (Figure 2).

Furthermore, by substituting CalB for Alcalase, a protease that degrades other enzymes, the effect of spatial separation was studied. If Alcalase was kept in solution with PAMO and ADH, the reaction sequence was severely affected due to degradation of the other enzymes by Alcalase. But if the incompatible enzyme was separated from the other enzymes via encapsulation in one of the organelle subcompartments, the enzymes were able to work together in the reaction sequence without interfering with each other.

Further development of these concepts might lead to a better understanding of the structure and functioning of the living cell and could also lead to new ways of combining incompatible catalysts in a single reaction sequence without interference.
Magnetically frustrated materials are those in which the preferred alignment of electronic spins cannot be achieved due to the geometrical arrangement of atoms on the crystal lattice. A particularly important class of magnetically frustrated systems are triangular lattice antiferromagnets. Figure 1 illustrates the nature of the frustration: In a conventional antiferromagnet on a square lattice, the electron spins (represented by arrows in the figure) are arranged in an alternating up-down configuration. On a triangular lattice, two of the spins can obey the up-down arrangement, but the third spin cannot be anti-aligned with both of the other two. The triangular antiferromagnet is “frustrated” and this can lead to a variety of magnetic states as the spins reorganise to find their lowest-energy configuration. The study of magnetically frustrated materials is of great importance to our fundamental understanding of complex magnetic interactions, as well as uncovering new phases of matter that have many potential applications in electronics and other technologies.

In the metallic triangular antiferromagnet 2H-AgNiO₂, detailed calculations predict that one of the low-energy states will be a magnetic supersolid, as shown in the theoretical phase diagram in figure 2(b). In this context, a supersolid has an arrangement of spins that breaks both the translational symmetry of the lattice, analogous to a solid, and spin-rotational symmetry within the triangular plane, which is analogous to a superfluid. A magnetic supersolid is a quantum phase of matter which is well described theoretically but has yet to be confirmed experimentally, with much of the experimental difficulty related to the conditions of very low temperatures and very high magnetic fields needed to access the relevant region of the phase diagram. Using the facilities of the HFML, we have carried out a detailed experimental investigation of 2H-AgNiO₂, studying properties such as magnetisation, magnetic torque and electrical resistivity in the region of the supersolid phase. The measurements performed, which also include experiments in intense pulsed magnetic fields in France and the USA, were on extremely pure single crystals with dimensions of ~70 x 70 x 0.1 µm³, requiring the highest sensitivity measurement techniques that are currently available. The experimental phase diagram we have constructed is shown in figure 2(a), and bears striking similarity to the theoretical predictions. Moreover, there is evidence for intriguing additional magnetic transitions within the proposed supersolid phase, which may be related to the metallicity of the material and the interaction of mobile conduction electrons with the underlying frustrated spin system. The role of conduction electrons in frustrated materials is relatively unexplored, and will be an important topic for future work.
Topological insulators are a new state of quantum matter. In two dimensions, topological insulators are referred to as the Quantum Spin Hall effect. This state is characterized by an insulating gap in the bulk and gapless edge states, which are protected by time-reversal symmetry.

In collaboration with scientists from the University of Würzburg, we have found a temperature-driven transition from a classical semiconductor to a two-dimensional topological insulator. This transition which we predict in band structure calculations, see figure 1, is probed by temperature-dependent magneto-transport experiments up to 30 T. At room temperature, the band order reflects a conventional semiconductor [figure 1a] whereas below a critical temperature $T_c$, band structure is inverted, and the system is a two-dimensional topological insulator [figure 1c] with gapless helical edge states in the bulk band gap. The samples are inverted HgTe QWs (at low temperatures) with [001] surface orientation grown by molecular beam epitaxy on a CdTe substrate. Lithographically defined Hall-bar structures have been produced equipped with a metallic Au top-gate. At low temperature, we are in the quantum Spin Hall regime where transport is governed by helical edge states when the Fermi energy is in the bulk band gap [figure 2a between (ii) and (iii)]. If the Fermi energy is the conduction or valence band, respectively, (quantum) Hall effect for electrons and holes is observed [figure 2b]. The magneto-transport experiments at room temperature can be described by a classical two-carrier model [figures 3a,b]. In an intermediate temperature range between 100 and 205 K, we observe a peculiar and pronounced linear magneto-resistance that develops from a classical quadratic low-field magneto-resistance in the regime where the band structure is inverted [figures 3c,d]. Due to the small bulk band gap $E_g$, electrons and holes coexist in transport which is reflected in the positive (negative) Hall resistivity at low (high) magnetic field.

In summary, we demonstrate that temperature ‘tunes’ the band structure of HgTe/CdTe quantum wells from a conventional semiconductor to a two-dimensional topological insulator.

**Figure 1.** Bulk band structure calculations using an eight-band $k\cdot p$ model. (a) $E(k)$ at $T=300$ K with the conduction band E1 and the the valence band H1. The system is a conventional semiconductor (SC). (b) Temperature dependence of the subbands in a HgTe quantum well – at $T_c$, band inversion occurs. (c) $E(k)$ at $T=4.2$ K with the conduction band H1 and the the valence band H2. The system is a two-dimensional topological insulator (TI) (dashed dotted lies are the linear gapless edge states).

**Figure 2.** (a) Quantum Spin Hall regime at $B=0$ and (b) ambipolar (quantum) Hall effect at 4.2 K

**Figure 3.** Magneto-transport (a,b) at room temperature (fit: classical two-carrier model) and at 100 K (c,d). A peculiar magneto-resistance (linear at high magnetic fields) is observed below $T_c$. 
The mission of the FELIX Laboratory is to provide the scientific community with tunable radiation of high brightness in the mid-, far-infrared and THz spectral range. The leading objective for the year 2014 has been to establish user operation at an excellent level in terms of both quality and quantity of the radiation and support delivered to the internal and international users. In 2014, a major step towards a fully established user facility has been achieved by executing successfully two full calls for proposals for IR- and THz users. In addition, first light and first user experiments have been achieved with the FEL-1 laser and the commissioning of FELICE progresses well. Two semi-permanent setups from the Ruhr-University Bochum (group Havenith) and the University of Cologne (group Schlemmer; Fig. 2) have been connected successfully to the beamlines as well as temporarily one apparatus from the University of Lyon (group Compagnon) and one from Leiden University (group Linnartz). Figure 3 shows infrared spectrum of the C$_2$H$_2^+$ ion recorded at low temperature in the 22-pole ion trap from Cologne.

In parallel, first experiments are performed using the long wavelength radiation of the FLARE laser. Even with a lossy waveguide connection to direct the output of FLARE into the magnets of HFML several experiments have been performed that hold great promise for the future.

The coming year, the facility development activities will be focused on:

- further commissioning of the FLARE laser, in particular the understanding of the scanning problem of the laser presents a major challenge;
- the installation of the optical transport systems of the different lasers to all user stations;
- the commissioning of the FELICE free electron laser as well as the intra-cavity setups;
- the implementation of new experimental opportunities at the laboratory with emphasis on the combination of the FELIX laser with the DC magnets at the HFML.
Conformation selective far-infrared action spectroscopy in combination with the novel Born-Oppenheimer Molecular Dynamics (BOMD) theoretical method have proven to be a promising new tool for the detailed structural characterization of peptides in vacuo. Especially for larger peptides, where the diagnostic amide vibrations in the mid-IR spectrum may suffer from spectral congestion, low-energy vibrations in the far-IR spectrum may form an interesting alternative. These soft vibrational modes are typically delocalized over the entire molecule, and therefore expected to relate particularly to the global conformational structure of peptides. BOMD simulations are used to decipher the structural information from the far-IR spectra. Tunable, high-intensity far-IR radiation is produced by the free electron laser FELIX.

Vibrational spectroscopy provides an important probe of the three-dimensional structure of peptides. Thus far, most peptide spectroscopy studies have considered the structurally diagnostic Amide A (NH stretching), Amide I (C=O stretching and Amide II (NH bending) modes. Including the far-IR region in the structural analysis has several advantages. Where mid-IR vibrations are localized modes containing information about local electrostatic and H-bonded environments, the soft vibrations in the far-IR range are typically delocalized over the peptide and are hence expected to be highly sensitive to secondary structural motifs. Moreover, even in the environment of a supersonic molecular beam expansion, the IR spectra of larger peptides often suffer from increasing spectral congestion to an extent where only families of structures can be identified rather than a single conformation. The far-IR spectrum shows a wealth of well-resolved absorption bands, allowing for improved structural assignments, provided theoretical predictions are reliable. Predicting vibrational frequencies of small neutral and ionized gaseous peptides has become a routine application using quantum-chemical methods; the vibrational frequencies are commonly extracted from a harmonic approximation of the potential energy surface. Although the far-IR region (<500 cm⁻¹) may contain a wealth of structural information, as already recognized in the condensed phase studies, such an analysis often performs poorly for the far-IR spectra, since it ignores the intrinsic anharmonic character vibrational potentials, which is often particularly pronounced for the soft vibrations. Here, we successfully apply BOMD computations to predict the far-IR signatures of two γ-turn peptides. These BOMD simulations are not based on a harmonic approximation and provide theoretical, anharmonic vibrational spectra directly.

The far-IR action spectroscopy / BOMD combination is demonstrated for two γ-turn capped dipeptides Ac-Phe-Gly-NH₂ (FG) and Ac-Phe-Ala-NH₂ (FA). The far-IR spectrum shows well-resolved and sharp bands down to 130 cm⁻¹ with an average line width of only 3 cm⁻¹, limited by the bandwidth of the free electron laser FELIX. The far-IR vibrations are reliably reproduced by the BOMD dynamical spectra. Especially the bands below 500 cm⁻¹ are in excellent agreement, with deviations below 10 cm⁻¹. To identify the vibrational character of the far IR bands, Fourier transforms of intramolecular coordinate time correlation functions (TCF) are calculated over the trajectories. This allows us to visualize these complicated delocalized vibrations such as for example the signature resulting from the C7 (γ-turn) interactions present in both the FG and FA peptides.
Nowadays, well-established frequency comb sources offer great opportunities for broadband precise measurements in gas sensing applications. Their recent development in the mid-infrared is of great interest in this field, as most of the molecules exhibit their strongest rotational-vibrational transitions in the mid-infrared region. Dual-comb spectroscopy is evolved from traditional Fourier transform spectroscopy (FTS), taking advantages of frequency combs light sources to offer broad spectral coverage, high spectral resolution and fast acquisition time. To demonstrate mid-infrared dual-comb spectroscopy, we propose an optical parametric oscillator (OPO) based on two periodically poled lithium niobate (PPLN) crystals generating light in the 3-5 μm wavelength region.

The laser source is a two-crystal, ring cavity OPO consisting of two 5 mm-long PPLN crystals pumped by two identical Yb-fiber lasers. The innovative ideas of this work rely on the design of the OPO cavity. A schematic of the setup is depicted in Fig. 1. The pumps are delivering 80 fs optical pulses at a central wavelength of 1.04 μm with an average output power of up to 2 W. The repetition frequencies of the femtosecond pulses are phase locked to a frequency synthesizer at around 90 MHz, while the carrier-envelop offset frequencies are free-running. To compensate the light dispersion introduced by the crystals, the 3.3 m long cavity is folded with 6 chirped mirrors. The four concave mirrors around the two crystals are anti-reflective coated for the pump and idler wavelengths. The OPO generates two collinear 100 mW mid-infrared beams. A first one is used for probing the gas sample, experiencing absorption and dispersion due to the molecular interaction, the other one is a local reference measuring the optical mid-infrared frequencies of the first one. The OPO design, proposing for the first time two crystals in a ring cavity for combs generation, offers an undeniable advantage in term of stability. Moreover, the two signal beams resonating within the optical cavity are counter-propagating and do not affect the generation of the two idler beams. As a demonstration, Fig. 2 shows a measured spectrum of methane (CH₄, 1% in nitrogen, 1 bar pressure, 15 cm path length, Δν = 204 Hz). The upper panel shows the measured absorption spectrum (blue curve) recorded in only 0.1 s, which is compared to the HITRAN database (red curve). The P, Q and R branches of the ν₃ vibrational transitions of methane can be clearly observed between 2850 cm⁻¹ and 3200 cm⁻¹, giving a bandwidth of more than 350 cm⁻¹ and a spectral resolution of 0.2 cm⁻¹. The lower panel shows the dispersion information retrieved from the same measurement which is immune to the intensity fluctuations of idler powers.

In conclusion, we have demonstrated for the first time broadband mid-infrared dual-comb spectroscopy, measuring absorption and dispersion spectra in gas phase simultaneously with a bandwidth of more than 350 cm⁻¹, and a spectral resolution of 0.2 cm⁻¹ has been achieved within 0.1 s. The broad spectral coverage and the fast acquisition time associated with extreme sensitivity will enable extensive spectral studies of rarefied samples and real time monitoring of processes. The unique capabilities of our spectrometer, for measuring rapidly evolving spectral events, should make it very attractive for monitoring dynamic phenomena like chemical reactions.
Mechano-responsive gels are very common in Nature; for instance gels based on actin, collagen, fibrin, intermediate filaments and many more proteins and carbohydrates display mechanical properties that are not only dependent on their biochemical environment, but also show an immediate response to deformation. Many of these gels strain-stiffen (they become stiffer as the stress or strain in the material increases), which, for instance, aids in the protection of tissues from rupture and in long-distance cell-cell communication. Typically, these biopolymers show a universal structural design element: they are relatively stiff and assemble into bundles or fibrils of defined dimensions, which results in both a high sensitivity and a high responsiveness towards stress.

The stiffness of hydrogels is crucial for their applications. Nature’s hydrogels become stiffer as they are strained. When optimised, such strain-stiffening materials become extremely sensitive and very responsive to stress. Strain-stiffening, however, is unexplored in synthetic gels since the structural design parameters are unknown. We demonstrate, for the first time, how readily tuneable parameters such as concentration, temperature and polymer length impact the stiffening behaviour. Our work also revealed the marginal point, a well-described, but never observed, critical point in the gelation process. Around this point, we observe a transition from a low-viscous liquid to an elastic gel upon applying minute stresses, smaller than 1 Pa.

In this work we described the effect of common, easily controlable variables (concentration, polymer length and temperature) on the mechanical properties of semi-flexible polymer hydrogels. Such gels are highly strain-stiffening and we can use this property to create extremely stress-sensitive materials. We anticipate that the behaviour that we described is universal, in other words, many other strain-stiffening materials will behave similarly. Why, then, were these properties never described before? Two major reasons: (i) the majority of strain-stiffening materials have biological origins and it is often not easy to precisely define and control critical parameters such as length or connectivity, and (ii) the length scales in the materials should match in order to enter the highly responsive regime: both the length ($L$) and the stiffness of the polymer bundle or filament ($l_p$) should be of the same order of magnitude as the mesh size of the network. When the polymers are too flexible ($l_p$ is too low), linear behaviour dominates and stiffening will only be observed at high stresses where the gel is likely to break. In addition, a (significant) minimum length is required to maintain network properties (sufficient crosslinks) at low concentrations.

Typically, the persistence length of synthetic polymers is too low, even when we consider them rigid polymers. We firmly believe that bundle formation is the best way forward to increase $l_p$, but full control over such process remains a challenge to be solved. The outlook, however, is a class of materials, where the mechanical properties ($G_0$, $\alpha$, and $m$) can be readily adjusted by changing conditions ($c$, $L$, $T$, etc.) and which mechanical properties can then be dramatically changed as a function of stress or other external stimuli.

The control over the materials properties of these gels has found direct application in the biomedical field, as a synthetic extracellular matrix for stem cell growth and adaptive wound dressings. This new class of materials has also applications in other fields that use responsive soft matter applications.
The invention of the transistor at the end of the 1950’s, its implementation in the chip and the computer, and the subsequent spreading of this technology resulting in the internet have had an enormous impact on society. A great challenge for the future will be the development of computers that can perform calculations on the molecular level. The basic ideas about the working principles of a computer were developed by Alan Turing in 1936. He proposed a (hypothetical) device, now called Turing Machine, that manipulates symbols on a strip of tape according to instructions provided by a tape head. We have embarked on a project involving the construction of a Molecular Turing machine, which writes and reads data on a polymer chain using information from a ring attached to a molecular device that moves along this chain. The blueprint of this molecular machine is shown in Figure 1.

In previous studies we have developed a molecular cage compound derived from glycoluril that can thread onto a synthetic polymer and glide along it while catalytically modifying it, i.e. by placing oxygen atoms on it. The presence (binary digit 1) or absence (binary digit 0) of oxygen atoms and the locations where these oxygen atoms are present can be seen as information that is encoded on the polymer chain. In a separate project we have synthesized a cage compound that contains a ring with functional groups, which can be switched between different states and as such can act as a tape head that provides information. One of the current goals is to transfer this information to a second cage compound that takes care of the writing process (see Figure 1). One possibility to realize this is to synthesize a double cage compound in which information transfer is possible by allosteric interactions, i.e. controlled changes in the shapes of the cavities resulting in stronger or weaker binding of guest functional groups (in this case connected to the ring or to the polymer chain in Figure 1). In order to study the possibility of allosteric information transfer we have measured the threading rate and binding strength of polymeric guests in zinc cage molecules that were designed to form dimeric complexes by metal-ligand and hydrogen bonding interactions. The effects of threading and binding a polymer chain in one cavity on the threading and binding of a second polymer chain in the other cavity of the dimeric complexes were measured by fluorescent spectroscopy. It was shown that binding information indeed can be transferred from one cage to the other via allosteric interactions. Furthermore, it was found that pentameric complexes composed of two cages and two threaded polymers connected by a bidendate ligand are easily formed even at very low (10^-6 M) concentrations. Nevertheless, it was decided that in the final design the two cages will be connected by a covalent linker to eliminate any other than dimeric species in solution. As it is very important to have full control over the writing process, the movement of the writing head on the polymer chain and the actual writing process (oxidation of double bonds on the polymer) should be adequately matched. Previously, a cage compound that moved too quickly, i.e. faster than the rate of placing oxygen atoms on the chain, was used. We have synthesized a new cage compound that can wrap itself around the polymer chain and as a result its movement is slowed down. This compound will be used in the further studies on the Molecular Turing machine. Another aspect that was studied involved the actual process of threading, i.e. how the cage compound finds the end of the polymer chain and threads on it. Previous measurements had revealed that the cage compound first binds to the outside of the polymer chain and subsequently threads through the opening of the cage molecule due to the higher effective molarity effect, which is the result of the binding process. However, another mechanism, in which a folded polymer directly threads through the cage just like a folded string passes through the eye of a needle, could not be excluded. By measuring the threading rate of a large series of polymers that are blocked on one side and have an open end of varying bulkiness on the other side, it could be shown that the first mechanism was correct. Current work is focussed on the synthesis of a double cage compound that is linked by a spacer of suitable length and on the actual transfer of chemical information from the ring to the polymer chain by allosteric interactions, see Figure 1.

Figure 1. Blueprint of a Molecular Turing Machine

**Highlight 12**

**Publication:**


When first proposed in the 1980’s, the hypothesis that polycyclic aromatic hydrocarbon (PAH) molecules may occur abundantly in interstellar clouds was received with substantial skepticism. After all, was it not unlikely that such complex molecules could form under the harsh conditions of interstellar environments? However, over the years, radio astronomers detected ever more and ever more complex molecular species in the interstellar medium, so that the PAH hypothesis gained credibility and today it has become fairly widely accepted that such large molecular species may form especially in the shielded environments of (dense) clouds.

Although not a single PAH molecule has been identified individually, a set of very similar IR emission bands observed from many galactic sources, once referred to as the Unidentified Infrared Bands, is now commonly associated with PAHs. Much effort has been devoted to the study of the IR spectroscopy of neutral and ionized PAHs in the laboratory in order to provide reference data for the interstellar spectra. Matrix isolation and gas-phase spectroscopic techniques have provided a wealth of experimental data on isolated neutral and positively charged PAHs. Experimental IR spectra of negatively charged PAHs are however virtually non-existing. This is unfortunate since PAH IR spectra are known to vary substantially with charge state, while on the other hand PAHs have been suggested to become the dominant carriers of negative charge in clouds with high electron densities (high metallicity).

In this study we have presented the first experimental IR spectra of mass-selected negatively charged (i.e. anionic) PAHs. Very generally, one could produce anionic species either by attachment of an electron to a neutral PAH, forming an odd-electron radical anion, or by removal of a proton, forming a more stable even-electron anion. The former method is impeded by the relatively low electron affinities of (small) PAHs and the latter by the low acidities of PAHs. We have therefore employed a two-step process based on electrospray ionization tandem mass spectrometry (ESI-MS). First, PAH carboxylate anions are produced as precursor ions from a solution of a PAH carboxylic acid (Figure 1). Collisional activation of the carboxylate in the mass spectrometer induces loss of neutral CO₂ generating the even-electron PAH anion of interest, which is mass isolated. Wavelength-dependent IR induced electron detachment using the tunable radiation from the FELIX free electron laser then allows us to record an IR spectrum of the anionic PAH by monitoring the ion intensity as a function of IR wavelength. The experimental IR spectra provide an important benchmark for quantum-chemical calculations of the IR spectra. Comparison of experimental and theoretical spectra suggests that good agreement is obtained using the B3LYP density functional and a basis set that includes diffuse functions (Figure 2). The calculations also indicate that the charge in these deprotonated PAHs is not delocalized over the molecule’s π-system, but instead is strongly localized in the carbon lone pair orbital (Figure 2). Unlike most other (neutral and charged) PAHs, these H-deficient anionic PAHs therefore possess high permanent dipole moments. Although this may provide an interesting opportunity for the detection of individual PAHs via their radio-wave spectrum, we suspect that the extremely small rotational constants, large partition function, high abundance of ¹³C-isotopomers and possibly large sample heterogeneity may form severe obstacles in such detection attempts.

**Figure 1.** Outline of the experimental procedure to obtain experimental IR spectra of anionic PAHs.

**Figure 2.** Experimental spectrum of the naphthyl anion compared with its DFT computed spectrum. The HOMO of the anion is strongly localized generating a substantial permanent dipole moment.
Chemistry in a traditional round-bottom flask is completely different from chemistry within a living cell, where the typical diffusion times of components are of a similar magnitude as their reaction times. These so-called reaction-diffusion systems can show extremely complex behaviour and it is the aim of our research to understand and harness this complexity, for example in the development of materials with life-like characteristics. Our approach is to start from relatively simple systems, and slowly increase complexity. Two examples of our latest results are described below.

In a first project, we used a functionalized hydrogel to look at reaction-diffusion processes of calcium (Ca\textsuperscript{2+}), which has a key role in many complex signaling pathways. We synthesized a derivative of the well-known fluorescent Ca\textsuperscript{2+}-sensor Indo-1 that could be covalently coupled to a polyacrylamide hydrogel. We used hydrogels to obtain the same diffusivity as of proteins inside living cells. Another gel with well-controlled spatial features was loaded with Ca\textsuperscript{2+} and placed on top of the Ca\textsuperscript{2+}-sensing gel (See Fig. 1A). The diffusion of Ca\textsuperscript{2+} into the bottom gel was monitored with fluorescence microscopy. Next, we introduced a Ca\textsuperscript{2+}-binding protein (Calbindin, CalB) to the bottom gel, which dramatically changed the diffusion profile of Ca\textsuperscript{2+} (See Fig. 1B). We were able to simulate our results as well, showing that we fully understand the underlying processes. In future research, our Ca\textsuperscript{2+}-responsive gels can be used to visualize pattern formation in Ca\textsuperscript{2+}-dependent reaction-diffusion networks. Furthermore, the difference in signaling properties of diffusive and immobile Ca\textsuperscript{2+}-binding proteins can be investigated, potentially ending a longstanding debate within the vast Ca\textsuperscript{2+}-signaling community.

A second project focused on the development of artificial signaling pathways based on reaction-diffusion networks that carry out specific functions in hydrogels. The core enzyme in the network is trypsin, which is able to produce more trypsin by activating trypsinogen in an autocatalytic process. Importantly, trypsin can be inhibited by the protein Soybean Trypsin Inhibitor (STI). Initial experiments explored the properties of systems in which a gel with certain spatial features was loaded with trypsin and placed on top of gels loaded with either inhibitor or both trypsinogen and inhibitor. A fluorogenic substrate responsive towards trypsin provided the necessary readout. The final system was able to recognize the distribution of trypsin (See Fig. 2). A gel with a distinct pattern of dense pillars forming the letter A surrounded by randomly spread pillars was soaked in trypsin and put in contact with a gel loaded with trypsinogen and inhibitor for only a few minutes. When trypsin diffuses into this second gel, there is a competition between autocatalytic production of trypsin and inhibition by STI. Only in places where the pillars are dense, the lower perimeter-to-area ratio prevents enough “fresh” inhibitor to diffuse into the activated area and stop trypsin formation. Therefore, only below the letter A trypsin will spread into the gel, and reach the bottom readout gel with fluorogenic substrate. The system is able to recognize the pattern of the upper gel and filter out the noise of the randomly distributed pillars. Interestingly, this fairly simple setup already results in a reasonably complex system with properties that cannot be predicted based on individual components, exactly like living cells.

**Figure 1A.** The experimental setup for the Ca\textsuperscript{2+}-experiments. A gel with pillars is soaked in Ca\textsuperscript{2+} and placed on top of a gel with fluorophores which changes fluorescence upon binding Ca\textsuperscript{2+}. **B)** Time-space plot of Ca\textsuperscript{2+} in absence (top) or presence (bottom) of a Ca\textsuperscript{2+}-binding protein (CalB) with one pillar in the center of the image as seen from below.

**Figure 2A and B.** Pattern recognition and noise filtering by an enzymatic reaction-diffusion network. Only where the pillar density is high (forming the letter A), a signal is observed in the bottom readout layer. Tr = trypsin, Tg = trypsinogen, I = trypsin inhibitor, S and P are fluorogenic substrate and fluorescent product, respectively. C) The influx of diffusing inhibitor is relatively larger at low pillar density.
We have demonstrated that high magnetic fields can be used to reversibly open and close nano-sized polymer capsules. This finding makes it possible to capture and release cargo particles, which is a crucial first step towards applications in magnet-assisted drug delivery. The nanocapsules are made by deflating hollow spheres, consisting of a polymer membrane, into a bowl shaped structure (left images Figure 1). Previously it was shown that these nanovesicles can be loaded with nanoparticles using chemical methods, such as osmosis. Now it has been demonstrated that magnetic fields can do the same, but in a reversible and more controllable way.

Magneto-valves
When placed inside a strong magnet, the molecules in the membrane of the vesicle align perpendicularly to the magnetic field direction. This alignment leads to stretching of the membrane, the deformation of the capsules and the opening of their mouth (right images Figure 1). The strength of the magnetic field determines the size of the opening, resulting in a reversible process. The vesicles open in a magnetic field, but return to their original closed state once the magnetic field is removed. It is the first time that such a magneto-valve nanosystem has been realized, permitting to load and unload cargo particles in a controlled way (Figure 2).

Nanorockets
The Bio-Organic Chemistry group has recently demonstrated how to use the vesicles as nanorockets by loading them with a platinum nanoparticle. In the presence of fuel the nanoparticles create oxygen bubbles, which are ejected from the vesicle opening, propelling it forward. Future research is aimed at combining the nanorocket and magneto-valve functionalities, creating a vesicle with an opening large enough to allow propellant to be ejected, but small enough to contain the cargo. When the rockets have arrived at the right location, the cargo can be released by opening the vesicle even further.

Fine-tuning
To reach this goal the technique needs to be fine-tuned. The opening of the capsule mouth-opening at several field strengths needs to be investigated. New membrane molecules should be developed and tested; molecules that are bio-compatible and that respond to lower magnetic field strengths, paving the way for clinical applications using the magnets of a MRI-scanner.
Scanning tunneling microscopy (STM) has proven itself as a powerful technique to obtain spatial information at the atomic level. It can be used to investigate dynamics of molecules and chemical phenomena on surfaces, which is essential to explore the details of interfacial reaction processes involving single molecules. Besides using the STM to observe, an exciting possibility is to use it to locally trigger chemical reactions. In collaboration with ICMAB Barcelona (Spain) and KU Leuven (Belgium) we have succeeded in inducing a chemical reaction at the nanoscale, with manganese porphyrins adsorbed at a solid/liquid interface, by employing voltage pulses between the conductive surface and the metallic STM tip.

The manganese porphyrins depicted in Figure 1A spontaneously self-assemble into highly ordered arrays at the solid/liquid interface when a dilute solution of the compound is deposited on an atomically flat graphite surface. Upon reduction of their Mn(III) centers to Mn(II), these molecules can bind and activate O₂, generating reactive Mn(IV)=O complexes, in which a single oxygen atom is attached to the manganese center of the porphyrin. This species can react with a second Mn(II) porphyrin to yield μ-oxo manganese porphyrin dimers (Figure 1B – structure on the right), in which an oxygen atom is sandwiched between two manganese porphyrins. We were able to locally induce the formation of these μ-oxo porphyrin dimers by positioning the STM tip above the monolayer, and subsequently applying well-defined voltage pulses (~ -4.5 V, 100 μs). In the following STM scan, the monolayer contained many large, bright spots surrounding the locations of the pulses (Figure 1B). The presence of oxygen (from the air) was essential for their formation: when the pulse experiments were carried out under an argon atmosphere, no bright spots were formed. In addition, the magnitude of the pulse had an impact on the yield of the spots: at both polarities, a threshold of ~ -2.5-3 V had to be surmounted before the spots appeared. Comparison with our earlier STM work on manganese porphyrins led to the conclusion that the bright spots were the μ-oxo manganese porphyrin dimers depicted in Figure 1B (right).

The following mechanism was proposed for the generation of the μ-oxo-manganese porphyrin dimers (Figure 2): (1) ‘hot electrons’ present during the voltage pulse reduce Mn(III) porphyrins that are adsorbed close to the pulse location to Mn(II) porphyrins, which then bind O₂ and generate Mn(IV)=O species. (2) During the pulse, the inhomogeneous electric field near the tip apex attracts polarizable manganese porphyrins present in the supernatant solution, increasing their local concentration. (3) Several of these porphyrins are also reduced as a result of the pulse, and the formed Mn(II) porphyrins react with the Mn(IV)=O complexes present on the surface, yielding μ-oxo dimers. The fact that no bright spots are observed at short distances (below 15 nm) from the pulse location is attributed to an induced desorption of molecules in the monolayer in close proximity to the pulse. This work opens the way to manipulate chemical reactions locally at the nanoscale, in particular at solid/liquid interfaces.

Figure 1. (A) Molecular structure of the manganese porphyrin. (B) STM image of a monolayer of the manganese porphyrins at a graphite/1-octanoic acid interface after the application of 2 voltage pulses at the location of the yellow crosses. The yellow bar corresponds to 20 nm. Structures of the unreacted manganese(III) porphyrin (left) and of the μ-oxo manganese porphyrin dimer (right) (alkyl chains are omitted for clarity) are related to the small and the large bright spots, respectively, in the STM image.

Figure 2. Proposed mechanism of the generation of μ-oxo manganese porphyrin dimers by employing voltage pulses in an STM operating at a solid/liquid interface in air.
Single-molecular chirality from achiral reactants


Highlight 17
Publication:
René R.E. Steendam, Jorge M.M. Verkade, Tim J.B. van Benthem, Hugo Meekes, Willem J.P. van Enckevort, Jan Raap, Floris P.J.T. Rutjes & Elias Vlieg
Solid State Chemistry
Synthetic Organic Chemistry

Single chirality can be considered as a signature of life, since without nature’s selection of one chiral molecule over the other our existence would be very different, if not impossible. The synthesis of chiral molecules from achiral starting materials proceeds to give both enantiomers of the product. A fascinating question in science is therefore how molecular single handedness arose from an achiral abiotic world. To shed light on this fundamental issue, an extensively studied topic in chemistry is the formation of single-handed (enantiopure) molecules from achiral reactants under achiral conditions. Frank anticipated in 1953 that an asymmetric reaction from achiral reactants could be possible if the chiral product acts as an asymmetric catalyst for its own production (asymmetric autocatalysis). This concept of self-replication was demonstrated in solution by means of the Soai reaction. However, the Soai reaction requires chiral molecules from the beginning to reach single chirality.

We have developed a reaction in which an enantiopure product can be obtained from achiral reactants in a single reaction. With the Rutjes group we prepared a reversible reaction in solution (Figure 1) and with the Vlieg group we studied the crystallization properties of the product. By combining these two branches of science, we revisited Frank’s concept and used crystal-solution interactions as the asymmetric autocatalytic driving force to reach single chirality. Our proof of principle consists of the synthesis of chiral amine 1 from its corresponding achiral reactants. Once the reaction commences in solution, the achiral reactants rapidly react to give an equal amount of right- (R-1) and left-handed (S-1) versions of the product because no chiral bias is present (Figure 2). As the reaction progresses, the solution becomes saturated with the poorly soluble product, and both enantiomers of the product precipitate in equal amounts as racemic conglomerate crystals. The initial symmetry of this solid state is broken due to either local statistical fluctuations in enantiomeric excess or a local difference in crystal size distribution between the enantiomers. Grinding of the crystals in combination with solution-phase racemization then leads to complete deracemization of the solids through a process also known as Viedma ripening. The yield of the solid product is about 70%.

This conceptually new approach shows that a very strong asymmetric autocatalytic system can be realized through crystal-solution interactions. The facile isolation of the crystalline enantiopure product with high yield renders laborious work-up procedures obsolete and makes this an appealing method to obtain enantiopure pharmaceutically relevant building blocks. Considering the general principle that any organic reaction is reversible and that synthetic products usually are more complex and less soluble than their precursors, we envision that a wider range of chiral molecules is accessible in enantiopure form. Therefore we are currently extending this method to other pharmaceutically relevant molecules. We are also studying the parameters which control the deracemization rate as well as the final configuration of the product.

**Figure 1.** In solution both enantiomers of the product (R-1 and S-1) are obtained whereas in combination with crystals, an enantiopure product can be acquired.

**Figure 2.** The experiment starts with achiral reactants in solution. After addition of an achiral catalyst, both left- (S, blue) and right-handed (R, red) products are formed in solution. Both enantiomers precipitate and the resulting crystal-solution system undergoes deracemization through Viedma ripening.
One ultimate practical goal in the field of interaction of light with magnetic matter is to learn how to control the magnetic state of a medium on an ultrafast timescale by optical means. Despite the claimed importance of the research for magnetic recording technologies, most studies have been focused on continuous metallic films with relatively low values of magnetic anisotropy ($K_u < 10^7$ erg/cm³). On the other hand, state-of-the-art recording media are based on granular ferromagnetic compounds featuring high anisotropy values ($K_u > 10^7$ erg/cm³) in order to increase the data storage density. A possible ultrafast control of the magnetization depends crucially on whether sub-picosecond laser excitations can trigger coherent spin dynamics in such a granular compound.

The investigated material is a prototype hard disk, containing a granular film of FePt of industrial quality provided by our collaborators at Hitachi Global Storage Technologies. FePt will be the recording medium used in next generation hard disk drives as it has an exceptionally high magneto crystalline anisotropy which allows for higher data storage densities than can be achieved with current recording media.

The sample is placed in an external magnetic field and irradiated by 100 fs laser pulses in a pump-probe scheme: An intense 100 fs laser pulse (pump) excites the sample while a low-power pulse (probe) is used at different time-delays to probe the effect of the pump on the magnetic state of the system. Figure 1 (a) shows a typical measurement at room temperature and an applied magnetic field of 7 T. The laser pulse excitation leads to an initial ultrafast reduction of the magnetization within 1.5 ps. Following this demagnetization, the magnetization recovers while also starting to oscillate at a certain frequency which increases with applied magnetic field (Figure 2). This is typical for ferromagnetic resonance (FMR) oscillations. Thus, sub-picosecond laser pulses can indeed trigger coherent spin precession in this granular medium. Furthermore, we can analyze the frequency and lifetimes of the oscillations at different applied magnetic fields to determine important parameters such as the anisotropy field and the damping parameter of the magnetic system. For example, the unusually high FMR frequencies in the THz regime found in this sample yield huge anisotropy fields up to over 10 T (Figure 2).

We could thus show that ultra-short laser pulses apart from being a valuable analytical tool, can cause coherent magnetic excitations in granular high anisotropy materials. This is a first step towards all optical control of magnetism in technologically relevant media. To continue and expand this research, high magnetic fields are needed, especially at low temperatures where the anisotropy further increases. We therefore have just finished building in the HFML the first ever pump probe setup allowing to investigate spin dynamics on a subpicosecond timescale in fields up to 37.5 T.
The challenge to develop a material, the magnetic state of which could be controlled with the help of light, has long intrigued people in very different research areas ranging from the physics of semiconductors and dielectrics to organic chemistry. The tremendous developments of lasers which are able to generate sub-100 fs optical pulses has made optical control of magnetism especially appealing as it may potentially revolutionize magnetic recording and information processing technologies, pushing their operational frequencies into the THz-range. Our team has revealed a very effective way to control magnetization with light. Instead of a direct coupling between light and magnetism, we generate a high-amplitude sound wave which triggers high-anharmonic large amplitude magnetization oscillations. Here we show that optically triggered lattice vibrations of atoms in a micrometer slab of the transparent magnetic dielectric FeBO$_3$ establish a long-living ($\leq 1$µs) standing sound wave at a frequency $f$. This acoustic wave drags the magnetization along [see Fig. 1]. Physically this becomes possible because the mechanical strain causes periodic changes of the magneto-crystalline anisotropy, which the magnetization has to follow. Such acoustically driven spin dynamics has a rather large amplitude of $\sim$10 degrees and relatively easily enters the anharmonic regime where the spectrum of the magnetization dynamics reveals not only the fundamental frequency $f$ but also contains higher harmonics with the frequencies $2f$, $3f$ etc. [see Fig. 2].

The fact that the laser-induced oscillations of the magnetization are anharmonic is very intriguing. It means that the energy transfer from light to spins might be done very effectively and we are getting close to the ultimate goal – to record magnetic information with the help of light.

Note that this phenomenon of the lattice-driven magnetization dynamics is not limited to the case of FeBO$_3$, but could be observed in a large class of magnetic dielectrics including hematite - one the cheapest magnets and widely spread minerals.

**Figure 1.** Artist representation of sound wave triggered in a medium with the help of a femtosecond laser pulse. The sound wave at the frequency $f$ causes a very anharmonic response of the magnetization that oscillates at the frequencies $f$, $2f$ and $3f$.

**Figure 2.** (a) Laser-induced dynamics of the magneto-optical response in FeBO$_3$ measured for different optical pump fluences. (b) FFT spectrum for different pump fluence. (c) Pump fluence dependence of the observed harmonics.
Despite the great strides that have been made in the determination of the structure of large (bio)molecules by solid state NMR, the lack of solution-state like proton spectra in solids is one of the biggest hurdles for unleashing its full potential. Protons have a small chemical shift range compared to other nuclei and often the resolution is limited by strong dipolar couplings. Nonetheless it is desirable to study protons in the solid state because they are highly NMR receptive and give important information about the structure. Proton resolution can be obtained in the solid state either by fast magic angle spinning (MAS) or by averaging the dipolar coupling among spins in spin-space (so called homonuclear decoupling). The best results are obtained when both techniques are combined at moderate spinning speeds. We have shown that micro setups are beneficial for homonuclear decoupling due to the very homogeneous radio-frequency fields.

Recently we developed a novel three-channel high field (20 T) micro magic angle spinning (μMAS) probe. The sample volume is only 50 nL but most proton experiments can be recorded using only a single scan. The proton resolution achieved in this micro-setup exceeds the resolution achievable so far using a conventional probe. In glycine the dipolar couplings of the CH₂-protons are among the strongest known and therefore glycine is often used for a benchmark for proton resolution. The spectrum in figure 1 is obtained using a single crystal of natural abundant glycine (~40 nL). All three resonances are well resolved and the two different environments of the CH₂ protons in the crystal structure are clearly resolved. To our knowledge this is the highest resolved proton spectrum of glycine in the solid state, improving the resolution over recently published approaches by more than a factor 2.

By miniaturizing the detection coil the mass sensitivity increases and partly compensates for the reduced detection volume. The triple-tuned setup allows the study of minute quantities of molecules by conventional 2D-correlation experiments (e.g.: ¹H-¹³C, ¹³C-¹³C, ¹³C-¹⁵N etc.) with highest resolution and sensitivity. When homonuclear decoupling is combined with correlation spectroscopy and inverse detection we can obtain very information rich spectra of nL/μg sample amounts. We have shown that by inverse detection, i.e. detecting the proton signals, a sensitivity gain of a factor 5 can be obtained. In figure 2 a ¹H-¹³C heteronuclear correlation spectrum of glycine, using homonuclear decoupling and inverse detection, is shown. The top trace shows that the carbon in the CH₂ group is in contact with all protons while the carbonyl (bottom trace) sees only the amine protons.

The new probe allows studying selected and mass-limited samples with the highest sensitivity and resolution. The achievable resolution allows exploiting the proton chemical shifts for structural assignments in the solid-state. We will use this setup to study specific regions of polymers and aligned polymer fibers to get new insights into their local physical properties. These experiments are supported by DFT calculations of structural models of the polymer by Gilles de Wijs.

The fruitful collaboration with Pegah Zolfaghari and Gilles de Wijs (TC) is gratefully acknowledged.
Background
Floris van Delft (Synthetic Organic Chemistry) and Matthias Bickelhaupt (Theoretical Chemistry) have joined forces in an interdisciplinary IMM team. The purpose of this team was to develop and unveil the nature of a new type of ultrafast, bio-orthogonal click reactions. The famous click reaction developed in 2002 has gained tremendous popularity across the scientific disciplines, due to its ease of access and operation, versatility, clean reaction and high yields. However, the indispensable copper(I), used up to 20 mol% to catalyze the reaction, is toxic and may lead to undesired oxidative side-reactions. Strain-promoted azide–alkyne cycloaddition (SPAAC) is a promising alternative to copper-catalyzed chemistry and has found application in material sciences, chemical biology and even in vivo use.

Problem and Solution
Despite its versatility, SPAAC is rather slow, while attempts to increase reaction rates by tailoring of cyclooctyne structure have suffered from a poor trade-off between cyclooctyne reactivity and stability. Now, IMM scientists Floris van Delft and Matthias Bickelhaupt and their colleagues have developed and quantum chemically analyzed a tremendous acceleration of strain-promoted cycloaddition of an aliphatic cyclooctyne (bicyclo[6.1.0]non-4-yn, BCN: see Figure 1, lower left) with electron-deficient aryl azides (for example, phenyl azide: see Figure 1, lower right). A remarkable difference in rate constants of aliphatic cyclooctynes versus benzoannulated cyclooctynes is noted, enabling a next level of orthogonality by a judicious choice of azide–cyclooctyne combination, which is inter alia applied in one-pot three-component protein labeling. The pivotal role of azide electronegativity is explained by density-functional theory calculations and electronic-structure analyses. Unexpectedly, the latter reveal that an inverse electron-demand mechanism is operative (see red orbital-mixing lines in Figure 2, upper) which explains the experimentally observed reactivity trend.

Outlook
The results of the successful IMM collaboration have been published in Nature Communications. Importantly, they can find immediate application as a general tool involving copper-free click chemistry, spanning from fundamental research to commercial use, as for example in Floris van Delft’s biotechnology start-up SynAffix, which has specialized in the development of targeted cancer therapies with site-specific antibody-drug conjugates (ADCs). The therapeutic approach involves the chemical connection (with click chemistry) of a highly cytotoxic drug to a monoclonal antibody (see Figure 2). The antibody ensures selective delivery of the toxic payload to cancer cells by specific receptor-binding.

Further quantum chemical studies are under way, in which activation strain analyses of the reactions are carried out for a more detailed understanding of the relationship between azide and octyne geometrical and electronic structure on one hand and the height of the cycloaddition barrier on the other hand. Also, a broader range of reactants will be explored to obtain a more general overview of the scope of this type of click reactions.

Figure 1. The ultrafast azide–cyclooctyne click reactions have an inverse-electron-demand nature (see red orbital-mixing lines).

Figure 2. Formation of site-specific antibody-drug conjugates (upper) through a metal-free click reaction between an azide and a cyclooctyne functional group (lower).
In 2014, the Theoretical Chemistry group and the Electronic Structure of Materials group merged. New collaborations are initiated by this merger and in this highlight we will describe the work of our first joint publication, on the interactions of adsorbed CO$_2$ on water ice. The background of the research lies in astrochemistry. In the cold and dense regions of the interstellar medium molecules adsorb, diffuse, and react on the surface of icy dust grain mantles, composed mainly of H$_2$O, CO, and CO$_2$. Interstellar water ice is thought to be the precursor of cometary ices and even water on Earth, since interstellar dust grains are the building blocks for comets and planets. Whether, how, and in what form interstellar ices survive during the evolution of a dense molecular cloud into a planetary system, is far from understood. Astronomical infrared observations of solid CO$_2$ show that it is initially intimately mixed with water ice, but as the temperature in a collapsing molecular cloud increases towards a young protostar, the spectral component associated with pure, unmixed, CO$_2$ increases, at the expense of the mixed features. We aim to understand these physico-chemical processes occurring in these ices.

A recent experimental paper argued that CO$_2$ forms islands on water ice, which means that the CO$_2$-CO$_2$ interactions are stronger than CO$_2$-H$_2$O. In our purely theoretical study, we see no indication for this. We constructed a new pair potential for H$_2$O–CO$_2$ interactions based on ab initio CCSD(T) calculations on the gas phase H$_2$O:CO$_2$ complex (see Figure 1). In the gas phase, the binding energy of the CO$_2$:H$_2$O complex is about twice as strong as that of the CO$_2$:CO$_2$ dimer. Hence, one would expect CO$_2$ to show full wetting behavior on a H$_2$O surface, instead of forming islands.

Using our new potential, we find that on a water ice surface, the water molecules will not easily accommodate the CO$_2$ adsorbants, leading to an effective weakening of the CO$_2$–H$_2$O interactions, but not to such an extent that island formation is preferred. From dynamical simulations of the deposition of CO$_2$ molecules we arrive at the same conclusion. Under typical laboratory conditions, in terms of substrate temperature and deposition method, we observe no formation of CO$_2$ islands as can be seen in Figure 2. From additional Density Functional Theory calculations, we showed that induced electrostatic interactions, which are not included in the pair potential model, do not alter this behavior.

We conclude that the signal complexity, on which the experimentalists based their conclusion, are rather caused by the substrate morphology of the water ice, and not by the intrinsic wetting behavior of CO$_2$ on water surfaces. This was confirmed by similar experiments at University College London of CO$_2$ on water ice where this signal complexity was absent. We therefore conclude that CO$_2$ wets a water ice surface, which means that CO$_2$:H$_2$O segregation is driven by water clustering and not by CO$_2$ which would rather remain mixed with H$_2$O.
The superposition of crystalline layers, with either slightly different lattice constants or different orientations, creates moiré patterns. One such case where a moiré pattern occurs is graphene on hexagonal boron nitride (h-BN). h-BN has the same honeycomb lattice as graphene but with a slightly larger lattice constant and alternating B and N atoms. Graphene on h-BN is an interesting interface as h-BN has become the standard substrate for graphene growth. It is also an example of a van der Waals heterostructure, in which 2D layers of different materials are combined to form a new material. The van der Waals interactions between different layers are weak and difficult to probe.

Strain distributions in graphene on h-BN have been recently observed by scanning probe microscopy. The different interatomic distances originate from a competition between maintaining the equilibrium structure and stretching to the most favourable stacking on the substrate. The resulting distortions can affect properties that are important for both applications and fundamental physics. Usually, moiré patterns are only considered from a purely geometrical point of view, as rigid surfaces. In order to obtain bond lengths and compare to experiments, however, it is necessary to relax to a minimal energy configuration.

We have used a fully atomistic model to compute atomic displacements. It turns out that in-plane and out-of-plane distortions are very sensitive to the interplanar interactions. We first studied the adaptation of a graphene layer to a substrate of stretched graphene meant to represent h-BN, since no empirical potential that describes the interaction between graphene and h-BN is available. It turns out that the asymmetry in C-N and C-B interactions is crucial to reproduce the observed strain distribution. We obtained a strain distribution similar to experiment only if we reduce the strength of the C-B interactions. Unexpectedly, as shown in fig. 2, the distortion pattern resembles the potential energy surface. In a sense, the moiré patterns take the role of a magnifying glass which projects the interatomic interactions at a larger length scale.

Comparison of our strain distribution to the experiment indicates that the C-N interaction is two to three times stronger than the C-B interaction. We suggest that the strain distribution and out-of-plane displacement in moiré patterns give direct information on the interplanar interactions in van der Waals heterostructures. This presents a new way to get information about these weak interactions that is otherwise hard to obtain.
J.S. Willemsen • M.M.E. Delville • A.M.C. Segbers-Lokate • A.E.M. Wammes • S.A.M.W. van den Broek • R. Medapalli • A.M. van Buul • R.P. Sanders-Temming • J. Jalink • D.M. Jupin • G.M.M.W. Bissels • V.K. Guduru • A. Adawyn Hassan • A.S. Stodolna • M.B. van Eldijk • N.L. Afanador • K. Koch • S. Jaeqx • J. Grzetic • B. Koene

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31 January  
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FELIX User Publications without RU co-author: 11

Molecular and Laser Physics


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Molecular Materials


Molecular Nanotechnology


Molecular Organic Chemistry


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Solid State NMR


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** Active emeritus professor
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IMM in numbers

On this page some statistics of the composition of the Institute for Molecules and Materials are given. This may help to understand the complexity and nature of the research institute.
Spin-offs from IMM

Chiralix
Focuses on the development and supply of chiral ‘drug-like’ building blocks on research-scale for drug discovery and early development.

Encapson
Performs custom synthesis of functional polymers and develops encapsulation technology based on block co-polymers.

FutureChemistry
Offers Lab-on-a-chip technology for chemical and pharmaceutical applications.

Mercachem
Produces on-demand, small-scale chemicals, has grown to 124 employees: 95 moved to an industrial park in Nijmegen and a small part of the company is housed in Mercator III.

ModiQuest
Concentrates on the development of novel diagnostics and therapeutics for autoimmune diseases. Its primary line of business is the discovery and marketing of new antibodies, technologies and targets for autoimmune diagnostic and therapeutic applications.

ReRa Systems
ReRa has many years of experience in the development of PhotoVoltaic measurement systems. This resulted in two state of the art measurement software applications: Tracer and Photor. Besides software, ReRa offers consultancy, software and measurement equipment design for your laboratory. This unique combination results in excellent measurement systems which finally improves the efficiency of your solar cells.

Sensor Sense
Development and production of traces gas detectors and measurement solutions.

SolarSwing
Development and production of daylight regulation systems that at the same time generate energy by smart integration of high-efficiency photovoltaic cells.
**Sphere Fluidics**  
Sphere Fluidics is a new company targeting a combined market of 27 billion euro in the Drug Discovery and Development, Biofuels and Chemical Sciences industries.

**Spinnovation**  
Offers IMM Instrument-time, and performs specific service-measurements and data-analysis for industry.

**SynAffix**  
SynAffix’ aim is to develop technology to make covalent bonds between molecules and apply this technology in life sciences research, medical imaging, material sciences or other areas of interest that require clean and efficient conjugation reactions.

**Synthon**  
Produces pharmaceuticals and is by far the largest spin-off company of the IMM, now employing over 1250 people worldwide. Research is still being done in Nijmegen.

**TeraOptronics**  
Research and development a terahertz camera, the TeraCam, will operate like a conventional camera, producing images which can be analyzed by a computer via an UBS port.

**tfz Devices**  
Development and production of *thin-film three-five devices* in particular high-efficiency solar cells for concentrator and space applications.

**NovioTech**  
NovioTech is a fully privately held corporation committed to bringing new technological solutions to the market. NovioTech collaborates with the Radboud University Nijmegen to valorize a number of technologies developed in the organic chemistry cluster of the Institute for Molecules and Materials.

**NovioSense**  
NovioSense is a spin out company from Fraunhofer IMS in Duisburg, NovioTech BV and Radboud University in Nijmegen. The NovioSense technology is a wireless platform for non-invasive monitoring of disease biomarkers in tear fluids.
IMM Barbecue 2014

In 2014 it was not possible to organize an IMM Sportsday due to interference with the RU Sportsday, which was held early June. Therefore it was decided to organize an IMM Barbecue. The BBQ was held after the IMM colloquium of professor Steven de Feyter (University of Leuven) on Tuesday 23 September. The weather was very good and about 150 IMM colleagues enjoyed the BBQ at the back terrace of the Huygens building. It was a great social event!

The IMM Sportsday, the so-called ‘OIlIMmpiad’, is a binding factor of the institute and, of course, great fun! Therefore it has been decided by the IMM board that the OIlIMmpiad will return on Wednesday 16 September 2015.