The Institute for Molecules and Materials (IMM) is an interdisciplinary institute that is engaged in research in chemistry and physics at the university. Its mission is to perform fundamental research in order to better 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. Its staff actively explores and promotes interaction with industry and the application of its research results.
The IMM, which is composed of twenty-two research groups, employs around 150 PhD students and every year some 30 of them graduate. There is a strong emphasis on interdisciplinary research involving theorists and experimentalists as well as physicists and chemists. Research is focused on three themes:

1. Structure and Dynamics of Molecules
2. Chemistry and Spectroscopy of Complex Molecular Systems
3. Quantum Matter

**Structure and Dynamics of Molecules**
Achieving a detailed understanding of interactions between individual molecules is of great importance to physics and chemistry. Within this research theme the aim is to unravel the interactions of molecules by building on a fundamental understanding of molecular structures. Processes that are studied include motions within molecules and biomolecules, as well as collisions and chemical reactions. Experiments are often based on advanced spectroscopic techniques such as Nuclear Magnetic Resonance and various laser techniques.

**Chemistry and Spectroscopy of Complex Molecular Systems**
Within this theme, the researchers are inspired by the chemistry in living cells. The next challenge in chemistry is to move away from studying isolated molecules and (diluted) reactions to mastering chemical processes in cells that contain mixtures of compounds with high overall concentrations. The aim is to design and synthesise chemical reaction networks, and study the complexity and functions that emerge in systems chemistry. Industrial and catalytic processes could benefit from this research, as they often take place under high concentrations and/or temperatures.

**Quantum Matter**
The goal within this research theme is to understand and develop new materials and concepts based on collective, emergent quantum effects. The main aim is to understand how properties of materials can be manipulated by changes at the atomic scale. More specifically, there is a focus on the new quantum phases that emerge in strongly non-equilibrium phases, at material interfaces, and in lower dimensional systems such as graphene. The research includes studying the robustness of superconductivity and modifications to magnetism, as well as modifications to electronic degrees of freedom.

**Research facilities**
The national and international position of the IMM is enhanced by the availability 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 is being constructed.
- The FELIX (Free Electron Lasers for Infrared eXperiments) Laboratory. The infrared lasers (FEL-1/FEL-2/FELICE) and the Terahertz laser (FLARE) are fully tunable between 3 and 1500 microns.
- The combination of FELIX and HFML offers scientists the opportunity to study matter and materials under conditions that cannot be found anywhere else in the world.
- The Solid-State NMR Facility for advanced material science, including a wide-bore 20 T (850 MHz) NMR instrument and high-field liquid-state NMR facilities up to 800 MHz.
- A Scanning Probe Microscopy laboratory capable of a wide range of Scanning Tunnelling Microscopy and Atomic Force Microscopy techniques.
- A Trace Gas Facility for applying laser diagnostics in biology and medicine.
Collaboration
The IMM groups collaborate extensively with other groups within IMM, the university and the Radboudumc and they collaborate within national and international programmes. A few examples:
- IMM coordinates the NWO Gravitation programme ‘Research Center for Functional Molecular Systems’ in which the organic chemistry groups at IMM collaborate with the Institute for Complex Molecular Systems at Eindhoven University of Technology and the Stratingh Institute for Chemistry at the University of Groningen to construct functional life-like molecular systems.
- The large pan-European partnership focusing on innovation in ‘raw materials’ (RawMatTERS).
- Groups are involved in various EU-Horizon2020 consortia.
- The IMM is a partner in two formal collaborations with the Foundation for Fundamental Research on Matter (FOM), working on:
  - The exploitation of the free electron lasers ‘FELIX and FELICE’ in Nijmegen
  - The joint running of the HFML and promotion of materials research involving high magnetic fields.
- HFML coordinates the European Magnet Field Laboratory (EMFL), which develops and operates world-class high magnetic field facilities.
- The Engineering and Physical Sciences Research Council (UK) has an access contract for using the free electron lasers at FELIX and a distributed research grant for solid-state physics done at the University of Surrey.
- Within graphene research, the groups led by Profs. Katsnelson and Maan collaborate closely with their ex-colleagues Radboud Extraordinary Professors Geim and Novoselov (now professors at the University of Manchester).
- The SPM group led by Prof. Alex Khajetoorians is part of the VILLUM Centre of Excellence for Dirac Materials of Aarhus University.

Research results
Highlights are listed below under the Institute’s three main research themes.

Structure and Dynamics of Molecules
Prof. Bas van de Meerakker and his colleagues (Spectroscopy of Cold Molecules) measured irregular diffraction patterns for inelastic collisions between NO radicals and rare gas atoms. These patterns revealed a new type of quantum stereodynamics that has no classical analogue or interpretation (Nature Chemistry).

Prof. David Parker and his Molecular and Laser Physics group have applied velocity map imaging for the first time to study UV desorption of molecular ices (submitted). Dr Frans Harren and his group have identified Pseudomonas aeruginosa and Aspergillus fumigatus mono- and co-cultures based on volatile biomarker combinations (Journal of Breath Research).

The Molecular and Biophysics group (Dr Anouk Rijs) and her collaborators from the University of Gothenburg, have developed a new infrared spectroscopy technique, which significantly extends the scope of the molecules that can be studied in the gas phase. It is particularly suitable for neutral peptide molecules that lack an ultra-violet (UV) chromophore (Phys. Rev. Lett.).

The Molecular Structure and Dynamics (MSD) group led by Prof. Jos Oomens uses the radiation from FELIX to record IR spectra of a wide variety of ultra-low density samples in tandem mass spectrometers. The IR spectra provide detailed information on molecular structures that is not available from the mass spectra alone. The group is now able to routinely record IR spectra with the sensitivity and selectivity of mass spectrometry (Nature Communications).

The FELIX Users and Operators group, which is led by Dr Britta Redlich, has, in collaboration with groups from the UK, designed a modified pump-probe experiment to investigate coherent dynamics and demonstrated their capabilities with a measurement of the inhomogeneous dephasing time for phosphorous impurities in silicon (Phys. Rev. B).

Dr Lex van der Meer’s FELIX FEL Technology group has constructed a bridge between the optical transport systems of FLARE and FELIX. This allows the light from FEL-1 and FEL-2 to be coupled to the part of the FLARE transport system that connects the FELIX with HFML. The first successful experiments in which THz radiation from FEL-1 was used in the 33-T magnet have been performed.

Within the Theoretical Chemistry group, Prof. Gerrit Groenenboom and his colleagues have developed a theoretical method for studying collisions of electronically excited molecules (J. Chem. Phys.). Dr Herma Cuppen and her colleagues have shown that solid-to-solid phase transition in molecular crystals can indeed proceed through cooperative motion (Cryst. Eng. Comm.).
The solid-state NMR group (Prof. Arno Kentgens) and the Theoretical Chemistry group (Dr Gilles de Wijs) have performed NMR, NQR and DFT studies in order to better understand the structure and dynamics of methylammonium lead halide perovskites (J. Phys. Chem. Lett.).

**Chemistry and Spectroscopy of Complex Molecular Systems**

In collaboration with the group led by Prof. Jan van Hest, Prof. Ger Pruijn and his colleagues at Biomolecular Chemistry have developed a molecular zipper-based approach to immobilising proteins at predefined positions on a solid surface. This approach is widely applicable for analysing biomolecular interactions (Analyst). Dr Kim Bonger and her colleagues explored a novel bio-orthogonal reaction for the chemical modification of biomolecules (Angewandte Chemie Int. Ed.).

Dr Daniela Wilson and her team (Bio-organic Chemistry) developed nanorockets with a molecularly built temperature-responsive braking system consisting of brushes made of polymers, enabling the rockets to start and stop at desired locations. The brushes swell or collapse in response to temperature, thus regulating access to hydrogen peroxide, which fuels the nanorockets (Nature Chemistry).

The Huck group (Physical Organic Chemistry) developed a new method for creating monodisperse liposomes using microfluidics. These liposomes are important building blocks for the creation of artificial cells. (J. Am. Chem. Soc.).

The Synthetic Organic Chemistry group led by Prof. Floris Rutjes has discovered a new method and mechanism for the stereo-selective synthesis of beta-mannose/mannuronic acid esters. This is a highly challenging linkage to synthesise, which can lead to biologically relevant sugar-based biomolecules (Angewandte Chemie International Edition).

**KEY PUBLICATIONS**

The Biophysical Chemistry group (Dr Hans Heus) developed a new DNA-responsive hydrogel. By incorporating DNA aptamers that target cell receptors, the hydrogel can be used to control cellular behaviour from the outside in (Advanced Functional Materials).

Researchers in the Solid State Chemistry group led by Prof. Elias Vlieg designed a comprehensive classification system for multicomponent crystals. Classification may seem to be an old-fashioned topic in science, but it is highly relevant for the pharmaceutical industry because of patent issues (Cryst. Growth. Des.).

The group led by Prof. Roeland Nolte (Molecular Nanotechnology), in collaboration with a group led by Prof He Tian at the East China University of Science and Technology in Shanghai, China, has developed a new supramolecular system which displays tunable multicolour photoluminescence, including the emission of pure white light (J. Am. Chem. Soc.).

Dr Paul Kouwer and the Molecular Materials team developed new approaches to hierarchically organising functional materials on substrates. They used liquid crystal templating, found ways to create complex structures from dilute aqueous solutions and were able to manipulate their organisation by external fields. (Adv. Funct. Mater. and a patent application).
Prof. Peter Christianen and his colleagues (Soft Condensed Matter & Nanomaterials, HFML) have discovered a new polymorph of coronene which is grown at high magnetic fields (*Nature Communications*). In collaboration with Biophysical Chemistry (Prof. Jan van Hest and Dr Daniela Wilson) they have developed a novel method for fabricating polymersomes of different shapes, which are promising for application as nanocontainers and in drug delivery (*Nature Communications*).

**Quantum Matter**

The group led by Prof. Nigel Hussey (Correlated Electron Systems, HFML) has explored members of the delafossite family PdCoO$_2$ and PdCrO$_2$, revealing the presence of an anomalous magnetothermopower (*Phys. Rev. Lett.*), evidence for the chiral anomaly often associated with Weyl semi-metals (*Nature Communications*), and the loss of interlayer coherence at a magnetic transition (*Nature Communications, in press*).

New materials sometimes exhibit spectacular resistance phenomena. However, in a recent experiment in a well understood ultra-high mobility GaAs quantum well, the SCNS group led by Uli Zeitler demonstrated that a simple physical model is sufficient to explain the phenomenon of linear magnetoresistance. This showed that exotic explanations for spectacular phenomena do not always provide the right answer (*Physical Review Letters*).

The Spectroscopy of Surfaces and Interfaces group (Prof. Theo Rasing and Dr Alexey Kimel) discovered Femtosecond optical control of spin-polarised currents in magnetic nanostructures without the need for any applied voltage, which opens the way for future studies of THz spintronics (*Nature-Nano*).

Prof. Andrei Kirilyuk and his Atomic Nanostructures group, in collaboration with the Theory of Condensed Matter group, discovered novel behaviour of magnetic exchange interactions at the sub-nanometre scale. This discovery relates the magnetic interactions with the electronic structure of nanomaterials, and paves the way for creating novel magnetic materials by design (*Scientific Reports*).

Members of the Theory of Condensed Matter group (Prof. Mischa Katsnelson) studied mechanisms that limit charge carrier mobility in a novel 2D material: phosphorene, single-layer black phosphorus. Using a combination of membrane theory and first-principles computations, they found that in-plane vibrations of phosphorus atoms are the main factor determining intrinsic mobility in phosphorene. These results are practically important as they establish a fundamental limit for the performance of phosphorene-based devices (*Physical Review Letters*).

In 2016, members of the SPM department (Prof. Alex Khajetoorians) completed construction of two new state-of-the-art cryogenic scanning tunnelling microscopes, which operate in UHV and in a magnetic field, with temperatures down to 30mK. In addition, they published two prominent *Nature Communication* papers on understanding the magnetism of individual atoms and the chiral interactions between them, and they published characterisations of various 2D materials, including MoS$_2$ and TaS$_2$, in collaboration with Aarhus University.

Prof. Peter Christianen and his colleagues (Soft Condensed Matter & Nanomaterials, HFML) published three linked papers on the magneto-optical properties of excitons in the single-layer transition-metal dichalcogenide WS$_2$ (*Physical Review Letters, Nature Communications, Nano Letters*), a novel two-dimensional semiconductor that has promising properties for opto-electronic applications.

The Applied Materials Science group (led by Dr John Schermer) worked on a new deep-junction structure for high-efficiency III-V solar cells. Compared to the commonly used shallow-junction design, deep-junction
GaAs cells were shown to yield significantly reduced levels of non-radiative recombination. As a result the cell efficiency was raised from 25.8% to 26.5% (Phys. Status Solidi A).

**Awards and grants**

In 2016 Prof. Wilhelm Huck (Physical Organic Chemistry) was awarded the Spinoza Prize – the highest award in Dutch science for his research into the physical-organic, chemical and biological processes that take place in human cells.

Prof. Jan van Hest (Bio-Organic Chemistry) was awarded an ERC Advanced Grant to make artificial cells and cell components. Dr Jasmin Mcincovic (Synthetic Organic Chemistry) was awarded an ERC Starting Grant to improve understanding of genuinely important biomolecular processes in epigenetics that play essential roles in human health and disease. Dr Daniela Wilson (Bio-Organic chemistry) received an NWO Vidi award to develop nanomotors for disease detection and treatment. Dr Johan Mentink (Spectroscopy of Solids and Interfaces) received funding for a tenure track to carry out theoretical research on laser manipulation of magnets and thus increase the energy efficiency of data centres.

A FOM programme was awarded to Nigel Hussey (HFML) for research on ‘strange metals’. FOM (prof)jectgrants were awarded to Bas van de Meerakker, Alexey Kimel, Alex Khajetoorians and Shengjun Yuan. Marie Sklodowska-Curie ITN were awarded to Elias Vlieg, Hugo Meekes (both Solid State Chemistry) and Floris Rutjes (Synthetic Organic Chemistry) and to Simona Cristescu (Trace Gas Facility). Dr Frans Harren (Trace Gas Facility) received an Interreg grant and an H2020 grant and Prof. Floris Rutjes received an EFRO grant. Jeroen Jansen was awarded an ISPT grant. Both Prof. Theo Rasing (Spectroscopy of Solids and Interfaces) and Prof. Peter Christianen (Soft Condensed Matter & Nanomaterials, HFML) were awarded a FET open grant. A KWF grant was given to Hans Heus (Biophysical Chemistry) and Alan Rowan (Molecular Materials). Dr Shengjun Yuan (Theory of Condensed Matter) received a Take-Off grant from the Dutch Technology Foundation STW.

Prof. Misha Katsnelson received the Hamburg prize for Theoretical Physics. Dr Anouk Rijs (Molecular and Biophysics/FELIX) was awarded the Minerva Prize for the best physics publication. Prof. Lutgarde Buydens (Analytical Chemistry) was elected member of the Academy Europa. She also became dean of the Faculty of Science. Prof. Floris Rutjes (Synthetic Organic Chemistry) was elected as chairman of the KNCV, the Dutch chemistry association. He is a Spinoza laureate, an elected member of the KNAP and the Academia Europaea and recipient of an ERC Advanced Grant. To date, his research has yielded more than 450 publications with over 10,000 citations. He is also the initiator and coordinator of various large national and international partnerships and a member of the FOM Executive board. Prof. Rasing is keen on bridging the gap between research and society by participating in public debates and delivering popular lectures for general audiences.
The Radboud Education Prize went to Dr Steffen Wiedmann (HFML) and Dr Alix McCollam (HFML) has won the education award from the Faculty of Science at Radboud University.

**Societal impact**

IMM trains the next generation of leaders in science and entrepreneurship, thus contributing to society by providing industry, academia and other institutions with highly qualified personnel with the ability to work in interdisciplinary settings. IMM collaborates with leading companies, including AkzoNobel, ASML, Corbion, DSM, Friesland Campina, Huntsman, NXP, Philips, Shell, Solvay, Teijin, Hitachi and Unilever. In addition, IMM collaborates with (local) SMEs and the Institute has given birth to many spin-off companies. Research in the IMM focuses on societal relevant problems, such as faster and more energy-efficient ways of computing, transferring and storing data, more efficient chemical reactors and molecular quantum devices, as well as new methods for drug delivery. At IMM innovative products have been co-discovered and developed, including graphene, ultrafast switchable magnetic materials, solar cells and hydrogels for biomedical applications. High-quality equipment and state-of-the-art research facilities contribute substantially to technological and social innovation. IMM plays an important role in this respect. HFML, FELIX and the NMR facilities are part of the National Roadmap for Large-Scale Scientific Infrastructure.

**Future research**

The fact that HFML/FELIX and the NMR facilities are part of the National Roadmap for Large-Scale Scientific Infrastructure provides opportunities for future funding. The European Magnetic Field Laboratory (EMFL) – of which the Nijmegen High Field Magnet Laboratory (HFML) is part – was awarded the Landmark status by the European Strategy Forum on Research Infrastructures (ESFRI).

The NWO-BIG grant in 2006 for the Nijmegen Centre for Advanced Spectroscopy (NCAS) provided the resources IMM needs to construct both a 45 Tesla hybrid magnet for the HFML (this will be ready in 2018) and a Free Electron Laser for research using Terahertz radiation (FLARE). The coupling of the FELIX infrared and THz laser radiation to the 33 T HFML high-field magnet provides a unique experimental set up, which IMM will continue to exploit in 2017.

The NWO ‘Gravitation’ Research Centre for Functional Molecular Systems – in collaboration with partners in Eindhoven and Groningen – was positively evaluated in 2016 and the remaining funding was made available. The Radboud Nanomedicine Alliance, a joint initiative of Radboudumc, NCMLS, and IMM, focuses on developing new, more effective medicines and materials for the treatment of diseases, tailored to the needs of individual patients.

The IMM will actively pursue R&D funds that are available in the region (EFRO and Euregio) and will apply for funding from the Dutch ‘Top’ sectors. Moreover, IMM aims to acquire funding for societal challenges within the European Framework Programme and researchers will be encouraged to apply for individual grants.

**Integrity**

IMM follows ‘The Netherlands Code of Conduct for Scientific Practice’. Each new staff member is explicitly made aware of this document in the welcome letter they receive, and the code is listed on the IMM website. Implementation of this code is the task of senior researchers. Thematic afternoons on scientific integrity are organised and a course on this topic for all PhD students is being developed as part of their education programme.