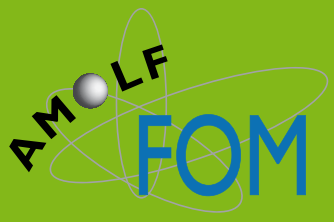
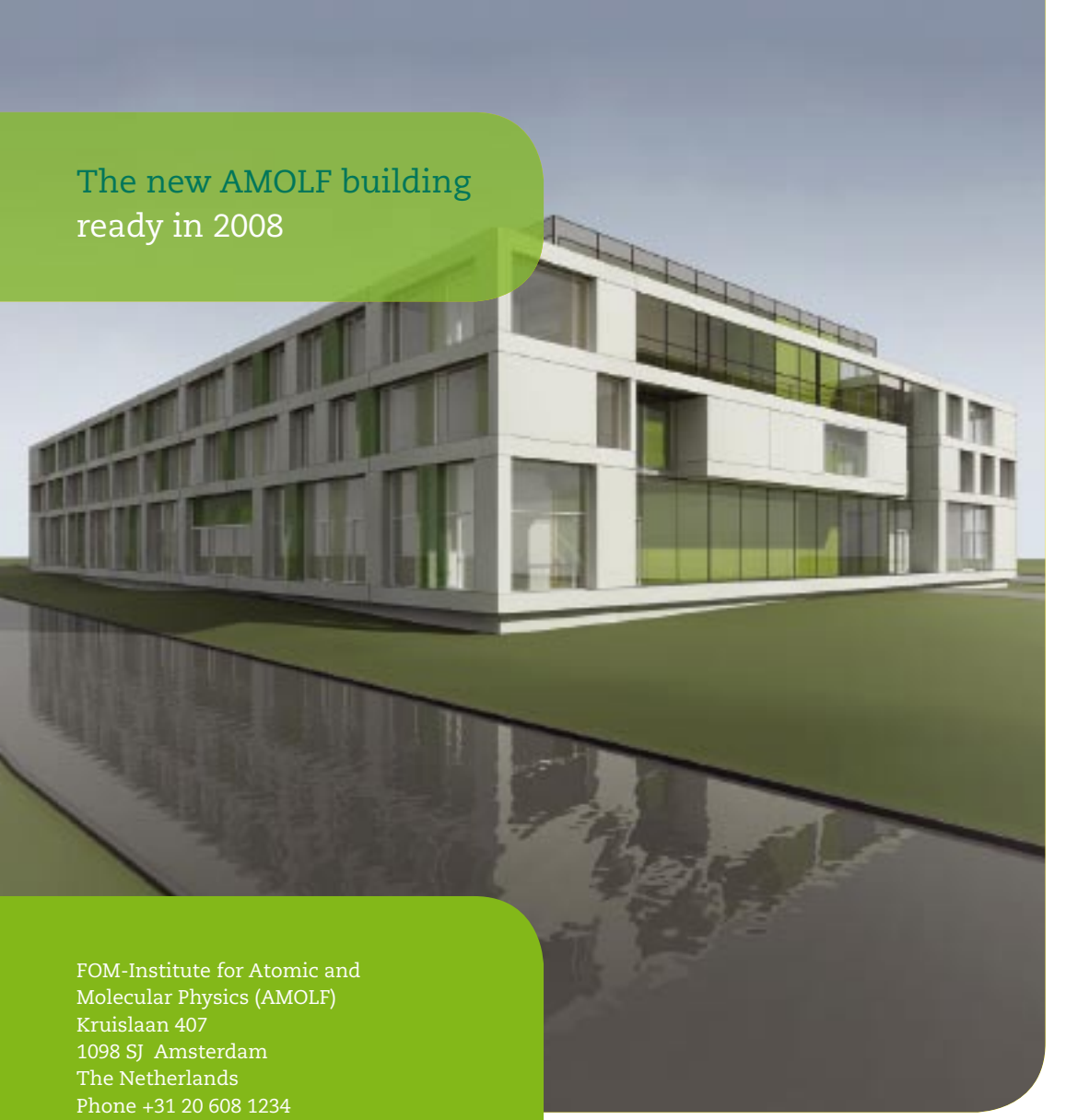


Visitor's guide



The new AMOLF building ready in 2008

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Welcome to AMOLF!

This guide provides an introduction to the FOM-Institute for Atomic and Molecular Physics (AMOLF) for visitors and for those considering joining AMOLF. In the first part of this booklet, AMOLF's mission and organization is introduced. Next, the research groups and their research programmes are presented with descriptions of their work over the past six years and a brief outline of future research directions. In subsequent chapters the support groups are introduced, and further practical information is given. For the most recent information please visit our website at www.amolf.nl. We hope you will enjoy reading this visitors' guide and look forward to seeing you at AMOLF.

Albert Polman
Director

Contents

1 Introduction

The Institute for Atomic and Molecular Physics (AMOLF), located in the Science Park Amsterdam, is one of the research laboratories of the Foundation for Fundamental Research on Matter (FOM), the physics division of the Dutch National Science Foundation (NWO). AMOLF employs about 130 research staff and 50 support staff. AMOLF's yearly budget is 12 million euro.

The mission of AMOLF is:
To perform leading fundamental research on strategically important complex atomic and molecular systems with key potential for technological innovations, and to transfer knowledge to industry and society.

Quality, **ambition**, and **multidisciplinary inspiration** are AMOLF's guiding principles in carrying out its mission. We aspire to deliver scientific output of the highest possible quality and impact, as measured by e.g., citation analyses. We are ambitious in that we want to achieve national leadership in our two research programmes, striving towards international leadership as well. Multidisciplinarity determines the research directions that we choose and inspires the innovations that lead to knowledge transfer to industry and society that is a key element of our mission.

AMOLF's research programme focusses on two main themes:

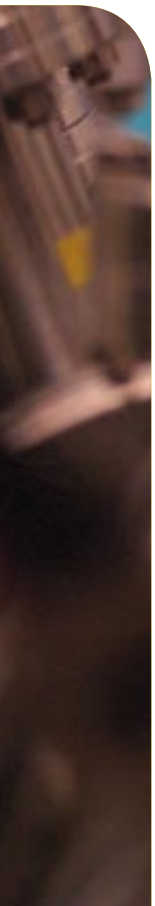
- **Physics of Biomolecular Systems**, focusing on the study of collective and active mechanisms in the spatial and temporal organization of the "hardware" (biomolecular structures) and "software" (biochemical networks) of cells. Fundamental research on the physical basis of these mechanisms will inspire the design of new functional materials, and will contribute to the "systems-level" understanding of biological systems needed for future breakthroughs in medicine and healthcare. This research programme explores existing strengths in soft matter- and biophysics, femtophysics, mass spectrometry and computational physics. It is organised in three coherent themes, each benefiting from the concerted effort of four to six research groups with complementary experimental and theoretical expertise:
  - Biomolecular dynamics and interactions,
  - Supramolecular structures and active biomaterials,
  - Spatio-temporal design of biomolecular networks.

  The total staff of this programme is 70 researchers.

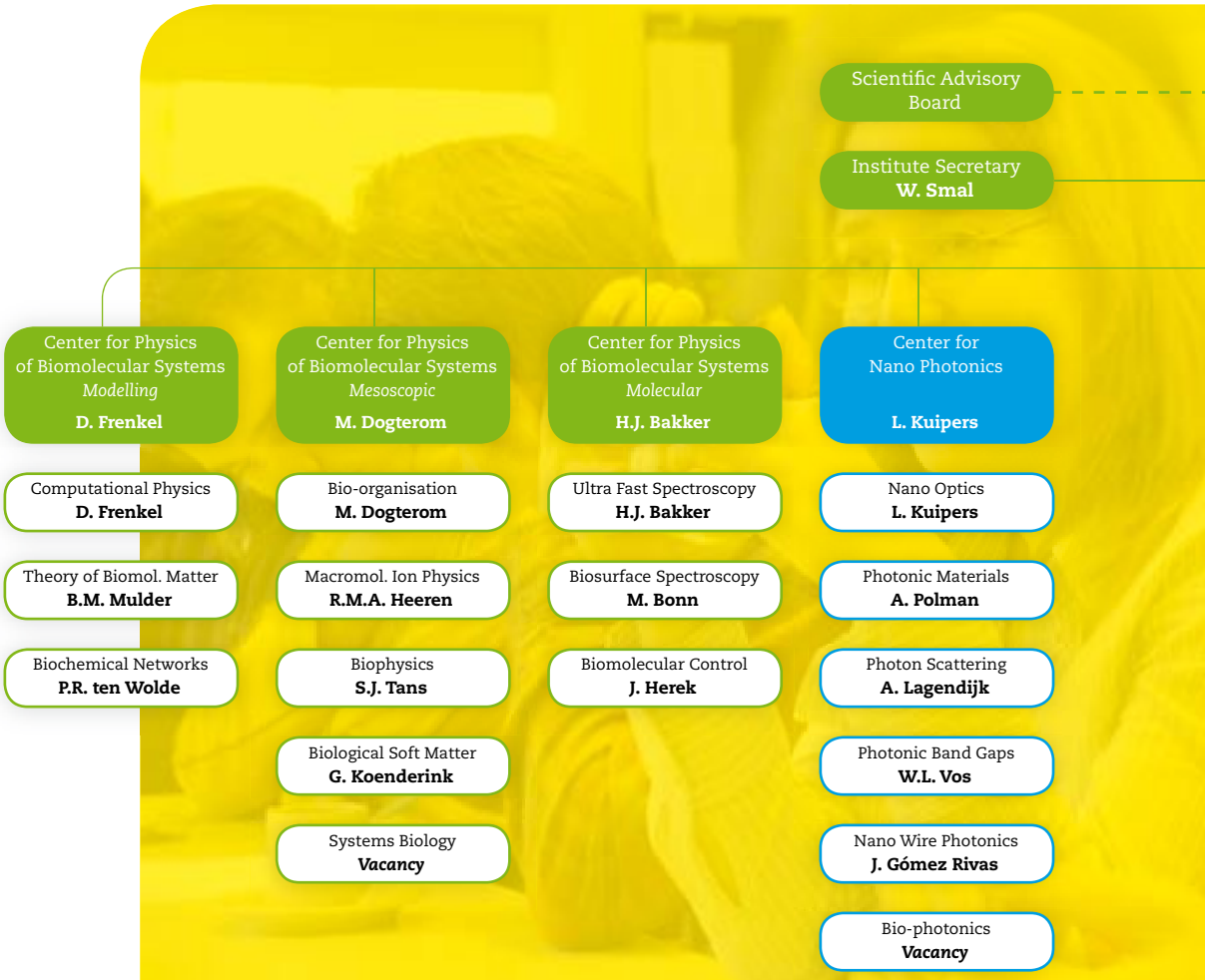
- **Nanophotonics**, focusing on the manipulation of light in artificially engineered nanostructures, with the aim of controlling and understanding emission, concentration and propagation of light. Fundamental research on the generation, manipulation, confinement, scattering and amplification of light at length scales smaller than the wavelength of light may lead to novel functional devices that are applied in communication, information and medical technology. The programme is organised in three coherent themes, each benefiting from the concerted effort of three to five research groups with complementary experimental and theoretical expertise:
  - Photonic and plasmonic light sources,
  - Dispersion control and nanoscale confinement of light,
  - Photonic integrated circuits.

  The total staff of this programme is 45 researchers.

In addition to the two main programmes, AMOLF carries out an **Exploratory Research Programme**. This programme serves to identify new strategically important research directions, and is used to start small-scale research projects that may later grow into new main directions of AMOLF's research programme. It also includes projects that do not naturally fit in either of the two main research programmes, but operate between them or play an important role in providing technology and infrastructure important to both.

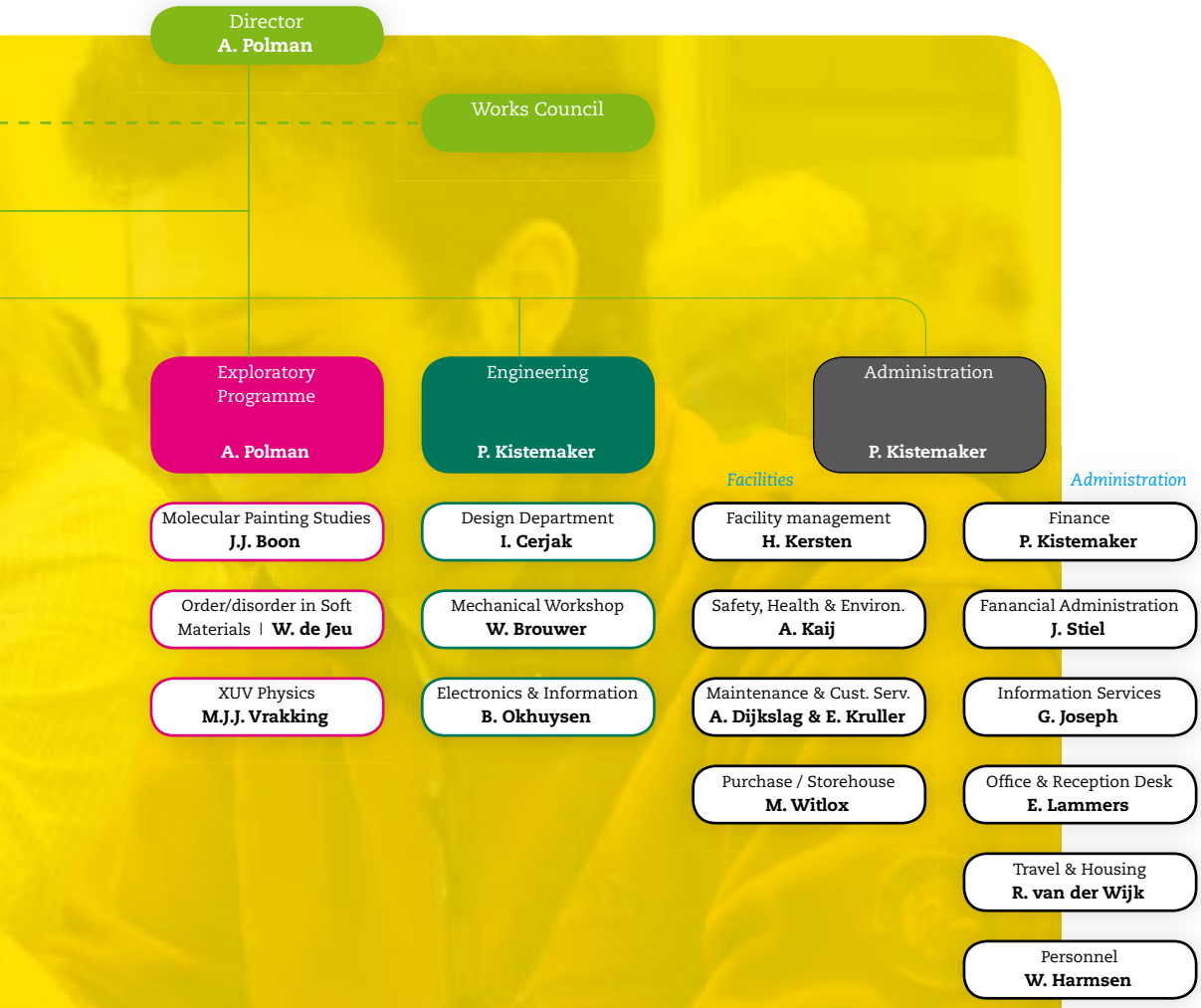


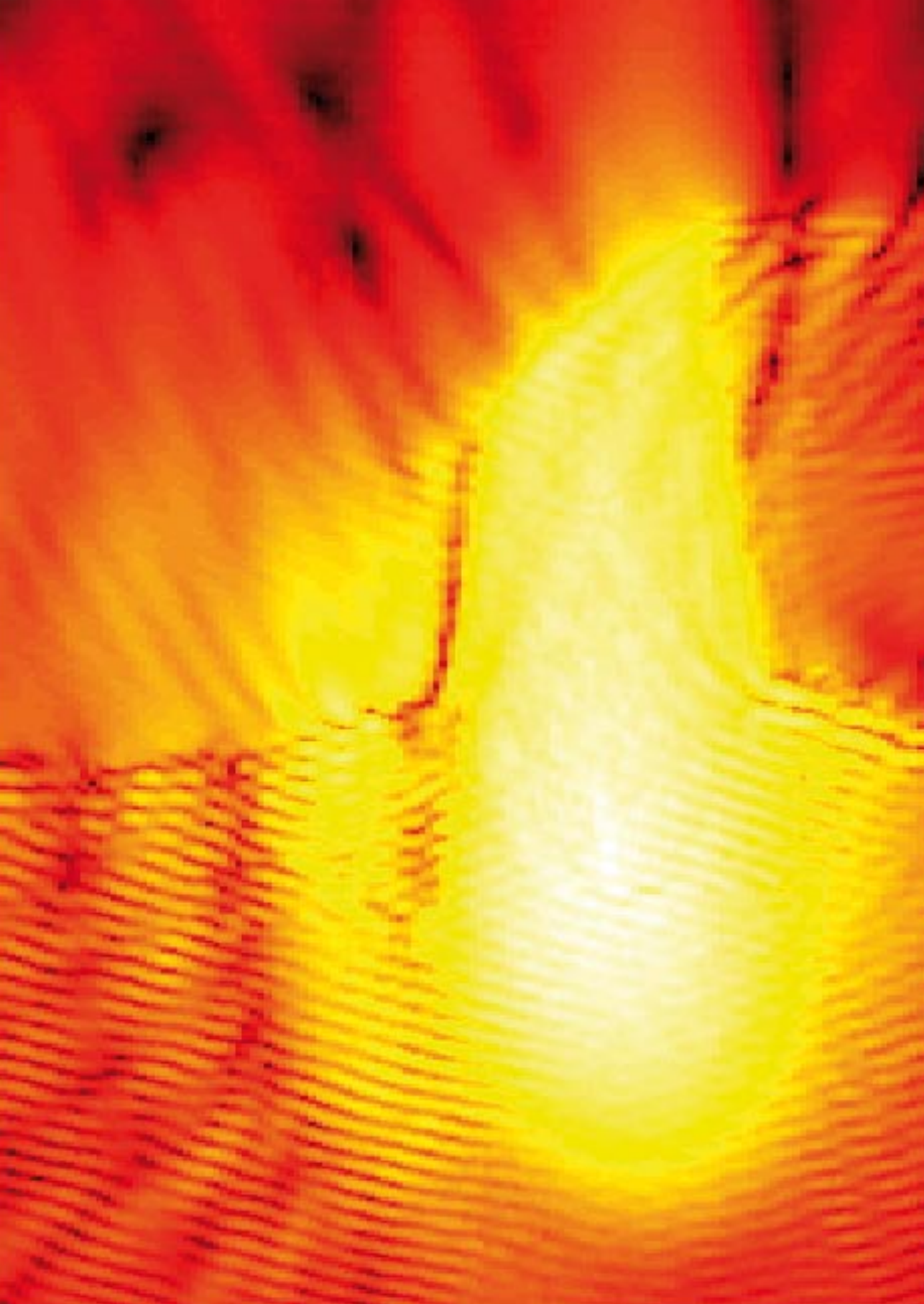
The two main themes are organised within the Center for Physics of Biomolecular Systems (eleven research groups organised with three departments: Modelling, Mesoscopic, and Molecular), and the Center for Nanophotonics (six research groups, organised within one department). Three research groups are organised within the Explorative Research programme. Support groups are organised within Engineering and Administration Departments. The director, heads of departments and the institute secretary serve as members of AMOLF's management team, which discusses and decides upon strategy and management issues regarding the Institute. Scientific staff and engineering support group leaders form the scientific staff meeting to coordinate activities, discuss the general strategy of the Institute, and to provide advice to the director.

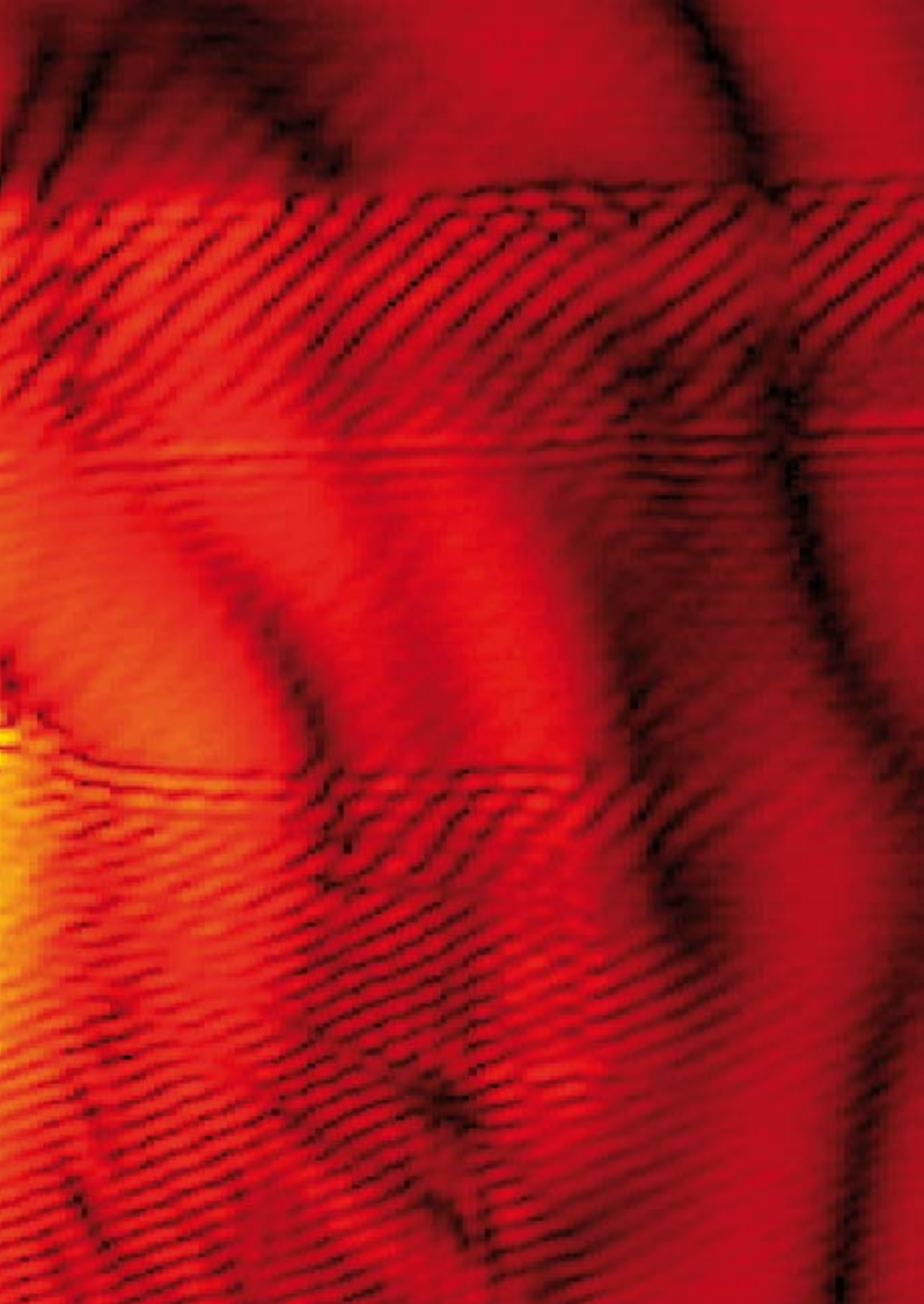


AMOLF's Scientific Advisory Board, with members from academia and industry, provides advice to the director of AMOLF on the development of the Institute's strategy, budget, investments, and on personnel decisions. AMOLF personnel is represented by the Works Council, which is elected every two years. The Council had regular meetings with the director and formally consults him in cases where this is prescribed by law.

Each scientific research group is lead by a group leader or project leader. Group members are PhD students, post docs, undergraduate students and guests, to a total of 5-10 per group. The group/project leader bears full responsibility for running the group and attracting external funds to carry out research projects. Fifteen of AMOLF's group leaders are associated to one of the Dutch universities as a professor; the graduation of AMOLF's PhD students takes place at these universities. AMOLF's organisation chart is shown below.







2 Center for Physics of Biomolecular Systems **Mesoscopic**

2.1 Bio-Assembly and Organization

GROUP LEADER
Prof. dr M. Dogterom

RESEARCH GOAL
The assembly, force generation and organization of cytoskeletal polymers lies at the basis of many essential cellular processes. The research objective of this group is to gain a quantitative understanding of the physics behind these cytoskeleton-based processes. This is achieved through a combination of *in vitro* experiments in simplified physically and biochemically controlled microfabricated environments, theoretical modelling and, increasingly, experiments in living cells.

RESEARCH HIGHLIGHTS

Force generation by individual cytoskeletal polymers

During the past six years, we developed a unique set of *in vitro* experimental techniques that allow us to measure, quantitatively, the growth process of individual microtubules when generating force in contact with a microfabricated barrier. The most recent tool is based on a newly designed 'keyhole' optical tweezers set-up, whereby the dynamics of a microtubule that is pushing against a barrier can be followed at nanometer (i.e. molecular) resolution. The experiments performed thus far have provided us with unique knowledge about the intrinsic force-generating capabilities of microtubules. We have shown that microtubule dynamic instability is accelerated under the influence of force and that force generation is consistent with a Brownian ratchet mechanism. We are now in a position that we can ask direct questions about the molecular mechanism and the (regulatory) effect of microtubule (end-)binding proteins. Using the nanometer resolution provided by the optical tweezers set-up, we have, for example, shown that XMAP215, which accelerates the growth of microtubules, facilitates the addition of long tubulin oligomers to the growing MT end. The expertise developed in quantitative studies of microtubule-based force generation can be considered unique in the world. In collaboration with Theriot (Stanford University), we recently also began to apply our techniques to growing actin filaments. Preliminary results show that measurements of force generation by single actin filaments are now within reach for the first time.

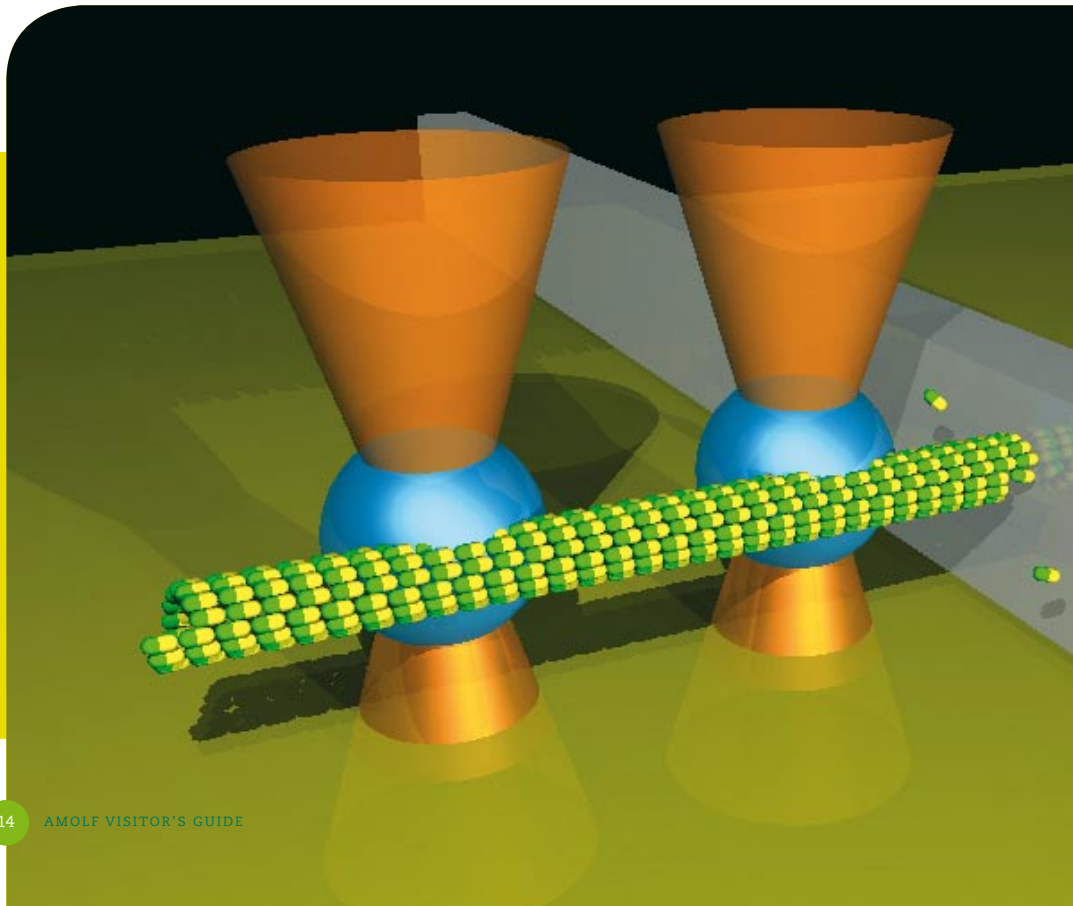
Organization of cytoskeletal networks in confined geometries

We used microfabrication techniques to create microchambers that mimic the size and shape of cells, and applied these techniques to study the intrinsic ability of microtubule-organizing centres to position themselves in response to microtubule forces generated in interaction with rigid barriers. This has enabled us to show that catastrophes are essential for efficient positioning of microtubule organizing centres. Recently, we managed to locally introduce motor proteins at the sidewalls of these chambers, so that we can now study the positioning of asters in response to both pushing and pulling forces (as is observed in living cells). In collaboration with plant cell biologists (Emons, Wageningen University) and theory groups (Mulder, AMOLF, and Juelicher, MPI PKS Dresden), we

also studied ring formation in motor-filament systems, which has relevance for the organization of microtubules in plant cells.

Highlights of other projects

In a separate project, we worked on the *in vitro* reconstitution of motor-driven tubulation of membranes and showed that, while individual motor proteins are not sufficiently strong to deform lipid bilayers, they do have the ability to dynamically associate into clusters of motors that together can generate the required force. We have also shown that the force barrier for tube formation is heavily affected by the way the forces applied to the membrane are distributed. In collaboration with Van Blaaderen (Utrecht University), we further worked on developing new ways of using optical tweezers techniques in biophysics and colloid science. We recently started a project to unravel the molecular mechanism of the contractile apparatus in dividing bacterial cells (in collaboration with Den Blaauwen, University of Amsterdam).

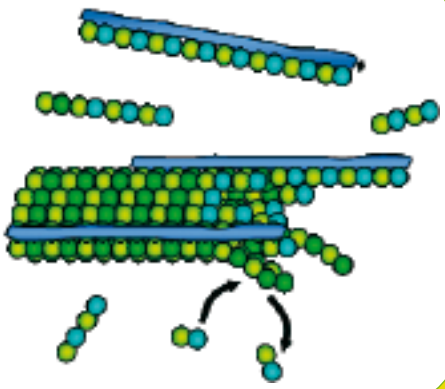


FUTURE DIRECTIONS

As well as continuing the *in vitro* experiments related to (the regulation of) force generation by cytoskeletal polymers, we plan to investigate the role of cytoskeletal-based force generation and linear transport in the design of biochemical networks.

Cellular components involved in biochemical pathways often travel through the cell in a linear fashion. For example, the transport of polarity markers in fission yeast cells occurs at the tips of highly dynamic microtubules. In this system, the correct spatial distribution of cell-end markers depends on feedback circuitry between the position of the microtubule-organizing centre, the spatial organization of microtubules, the linear transport of proteins at microtubule ends, and the regulation of microtubule dynamics and force generation when microtubules reach the cell ends.

The goals of our future research programme will be to understand how microtubule end-binding proteins interfere, at the molecular level, with microtubule assembly and force generation; how regulation of microtubule dynamics and forces is used to control positioning of microtubule-organizing centres in cells, and how linear transport of regulatory proteins and force generation are involved in the feedback circuitry that assures the correct spatial distribution of proteins in cells. In general, we aim to understand what the 'design advantages' are of feedback circuitry that relies on linear instead of diffusive transport. This research will involve experiments with living yeast cells at AMOLF (with Brunner, EMBL, Heidelberg).



Microtubules are self-assembling force-generating biopolymers. Optical tweezers techniques allow us to follow the assembly dynamics, as well as the effect of regulatory proteins, at molecular resolution.

2.2 Macromolecular Ion Physics

GROUP LEADER
Prof. dr R.M.A. Heeren

RESEARCH GOAL
The research of the macromolecular ion physics group focuses on the investigation of the spatial and molecular structures of macromolecules in or from complex systems in order to find a link between molecular structure and biological or chemical function.

RESEARCH HIGHLIGHTS
The realisation of the Mass Microscope in the context of the NWO large facility investment project has opened up new possibilities for rapid high-resolution analysis of biomolecules in cells and tissue. We demonstrated that 1-micrometer-resolution single-shot mass-resolved images can be acquired using both ultraviolet and infrared lasers, breaking the diffraction limit in the latter case. Many new studies were initiated based on this project. Using Matrix Assisted Laser Desorption and Ionisation (MALDI) imaging mass spectrometry (MS), we were able to profile neuropeptides at the single-cell level, in parallel for all cells present in a tissue section. This novel approach can significantly speed-up neuropeptide discovery and localization. Two models are used: the cerebral ganglion of the pond snail *Lymnaea stagnalis* and the rat brain. In collaboration with neurobiologists from theFree University Amsterdam and Utrecht University, nervous tissue is studied that revealed the location as well as the type of neuropeptide processing involved in the regulation of, e.g., food intake.

Whole rat brain image as an example of high-resolution imaging using microscope-mode MALDI-IMS with a pixel size of 600 nm. In gray the microscope mode total-ion-count image overlain of a rat brain with the distributions of three peptides (blue, red, green).

Matrix-Enhanced Secondary Ion Mass spectrometry was shown to drastically increase the yield of intact pseudomolecular ions from cells and tissue. In addition, a novel methodology was developed that allowed the semi-quantitative recording of the topography of a sample, using high-resolution arrival time measurements in the imaging time-of-flight mass spectrometer. Through mapping the topography-related mass shifts of the matrix ions, the analogous mass shifts of higher mass ions can be deconvoluted and higher resolution and greater sensitivity obtained.

The functionality of macromolecules in a biological environment depends heavily on the three-dimensional molecular structure. Changes in the conformation will dramatically alter intramolecular binding energies. We established a methodology to determine the amount of internal energy deposited in macromolecules. A combination of thermal activation and gas-phase collisions was employed to assess the internal energy deposition during desorption and ionisation techniques required for biomolecular studies, including biomolecular imaging. The rates of gas-phase internal energy deposition and loss were determined on an absolute scale and related to structural changes in biomolecules. This was achieved by manipulating the Boltzmann temperature of a protein ion population trapped in our novel Fourier Transform Ion Cyclotron Resonance-MS cell. For this purpose, the new thermostated ICR cell was used and operated in the temperature range 77-500 K. In addition, Electron Capture Dissociation (ECD) was used to locate and identify sulphur-based posttranslational structural modifications such as mono and di-sulfide bridges in lanthibiotics and neuropeptides. Fundamental studies on conformational manipulation of small peptides in the gas phase demonstrated that ECD can be used as a tool to probe conformational changes. Studies at 77 K showed that a strong decrease in conformational heterogeneity leads to selective dissociation along the peptide backbone.

Our studies on noncovalently-bound protein complexes, in collaboration with Utrecht University and the Free University Amsterdam, revealed that it is possible to follow chaperone-assisted protein folding with high-resolution mass spectrometry. The correct folding of two proteins, Rubisco and a Bacteriophage capsid protein (Gp23), into their biologically active conformation depends on a specific, structurally very similar, molecular chaperone complex (GroEL.GroES and GroEL.Gp31 respectively). Since there is structural similarity between the two chaperone complexes, the question arises what physical mechanism ensures the exquisite selectivity in the correct folding of the substrate protein. To answer this question, we adopted a novel mass spectrometric approach designed to reveal the interactions of the substrate protein with the chaperone complex, its association energy, the intermediate conformations of the protein to be folded and the energy required to make a transition from one folded state to another. Studies were performed and compared in the solution as well as gas phase.

The large amount of data, together with the associated storage and handling problems, were tackled in collaboration with the BSIK project

'Virtual laboratory for e-sciences' (VL-e). In that project, a new collaborative framework is being developed which will benefit all present and future collaborative research projects.

FUTURE DIRECTIONS

The future research of this group will focus on new fundamental questions arising in biomedicine and the associated development of nanomedicine. Heavy emphasis will be placed on the further development of imaging mass spectrometric strategies directed at improving speed and resolution to the sub-micron level. Part of this research will be carried out in the recently approved EU consortium COMPUTIS , which focuses on imaging technology development for biomedicine. The action and functioning of nanoparticle-based drug-delivery systems is one of a number of new applied studies that we intend to pursue in our research. For this purpose, new desorption and ionisation techniques will be investigated, aimed at the desorption of elements and molecules from areas on biological and macromolecular surfaces at a resolution below 100 nm.

We will continue our research on the structural examination of biomolecules with trapped ion mass spectrometry in support of the imaging studies. The emphasis will shift towards structural analysis using dissociation techniques in combination with gas-phase vibrational spectroscopy. In these studies, we intend to investigate the determining role of water in protein folding and to expand our research on non-covalently-bound protein systems. The research in the VL-e Dutch telescience laboratory will be continued to further strengthen our capabilities for both molecular structural analysis and high-resolution molecular imaging.

2.3 Biophysics

GROUP LEADER
Dr ir S.J. Tans

RESEARCH GOAL
The aim of the research of the Biophysics group is to reveal the design principles of biological systems. To this end, we use an approach that integrates biophysical experiments of simple biological model systems with numerical simulations, employing molecular cloning, microbiology and single-molecule and single-cell techniques.

RESEARCH HIGHLIGHTS
Pathway simulations in evolutionary energy landscapes
In an evolutionary process, mutations are accumulated in a stepwise manner that can be seen as a trajectory in an 'energy landscape'. Here the energy represents the performance of the network, which in turn influences the speed of growth of the cell. What these landscapes with large degrees of freedom actually look like has remained unknown until now because of our inability to predict protein-DNA-binding energies from sequence. With a novel simulation approach that uses existing measured data, we have been able to take a first look at the fitness landscape of a small model network. We have shown that this method can be used to trace evolutionary pathways that are possible in real cells. Importantly, we have demonstrated that networks have a surprisingly rapid ability to change: each step along the path can be accompanied by an energy increase, which radically improves the probability of success.

Experimental evolution of genetic networks
We studied similar evolutionary processes experimentally. Here, network components such as regulatory proteins and DNA binding sites were designed and constructed into DNA strands using molecular biology techniques. After their introduction into live bacterial cells, these components perform an elementary function such as turning on the expression of a gene when an external molecule is applied. We set out to investigate how difficult it is to change this function and to create an 'inverter', whereby the gene expression is now turned off when the external molecule is applied. It was found that even such a radical change can be obtained surprisingly rapidly by just one or two rounds of point mutations and selection, thus mirroring the findings of our theoretical results. The results indicate that experimental evolution can be powerful in obtaining changes that would have been impossible to achieve through rational design.

Internal diffusion of supercoiled DNA
For recombination events to occur, many molecular partners must find each other in the cell and form a complex: two DNA sites and four recombination proteins. In this project, we aim to measure the statistics of co-localization, which is central to many other cellular processes. Our first focus has been on the two DNA sites, which are situated in circular and supercoiled (twisted around the long axis) strands of DNA. These two

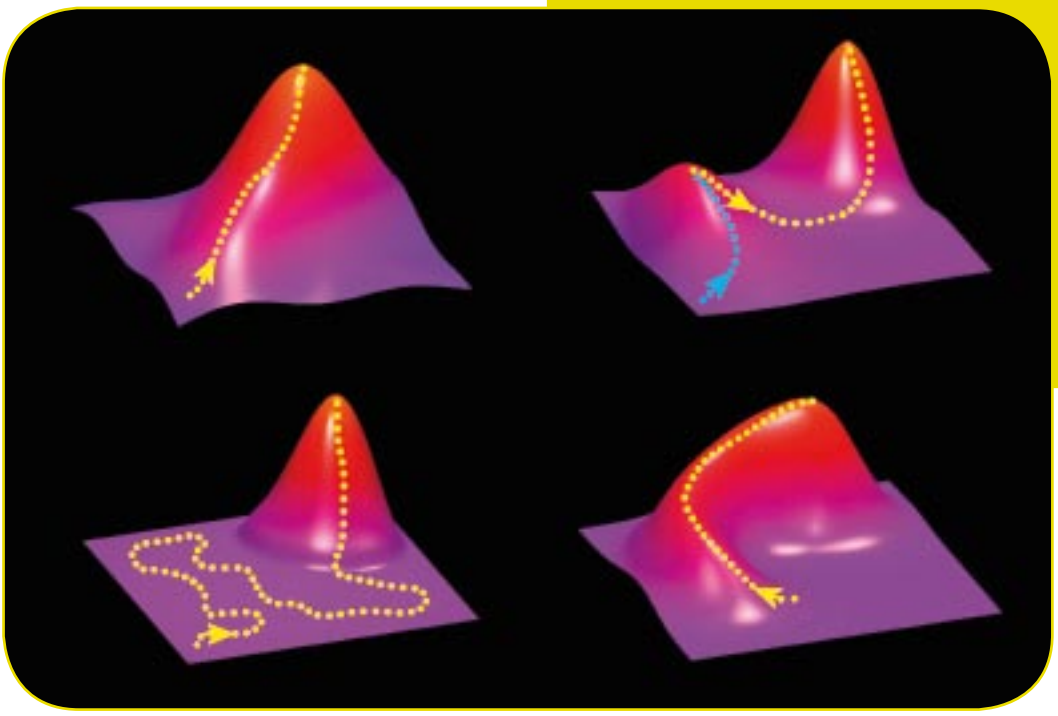
sites then meet through internal diffusive motion of this twisted molecule. The idea is that these rapid fluctuations in co-localization can be measured by the FRET technique. We have shown that such measurements are indeed feasible in test samples.

Pulling on proteins

Cellular membranes perform the intriguing task of grabbing folded proteins, unfolding them and translocating them across the membrane. Using bulk experiments on engineered proteins with multiple repeats, we were able to show that this translocation machinery acts as a processive motor. We also made protein constructs that allowed us to specifically attach different linkers at either end. With these constructs, we were able to measure the unfolding dynamics of individual proteins using optical tweezers.

FUTURE DIRECTIONS

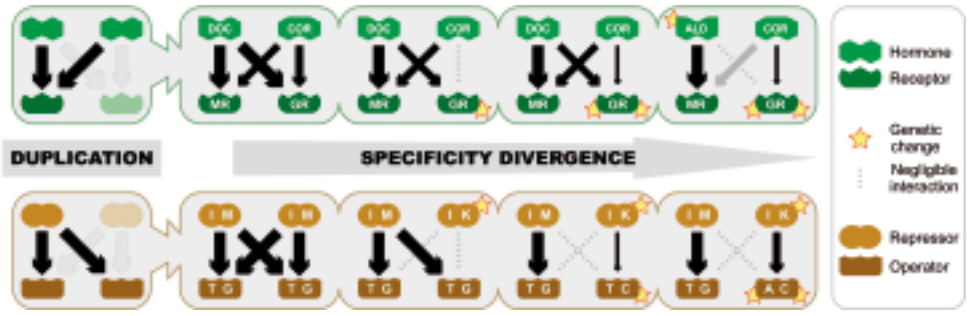
The evolutionary remodelling of gene networks in bacteria will be continued by applying it to more complex networks in order to build logic



gates. In new related work, bacteria will be evolved by letting them adapt to varying environments, mimicking natural evolution. At the theoretical level, we will build on the approach we developed, and investigate the architectural ingredients of regulatory interactions that are important for evolvability. Furthermore, we will develop time-lapse microscopy experiments to observe growing bacterial cells. We will use this technique to improve our understanding of the dynamics of site-specific recombination as well as their statistics. In this research line, we will also exploit micro-patterned surfaces in order to manipulate and direct the movement of cells. The behaviour of cells in these confined geometries will be studied. The first (un)folding measurements now open the door to characterize the folding and unfolding properties, and importantly, to understand how these characteristics are altered when the chaperone secB is added, which is known to bind this protein and keep it in a state whereby it can easily be translocated. We will expand our first measurements on the inter-molecular diffusion dynamics of super-coiled plasmids, and study its dependence on plasmid size and secondary molecules.

Left schematic representations of fitness landscape features. Fitness is shown as a function of DNA sequence; the dotted lines are mutational paths to higher fitness. In case of a single smooth peak, all direct paths to the top are increasing in fitness (top left). In rugged landscape with multiple peaks (top right), paths to the top might have to go through a valley which drastically lowers their evolutionary probability (yellow path), or paths might lead in the wrong direction to an evolutionary trap (blue path). If there are regions without fitness increases (neutral landscape, bottom left), or if detours are necessary (bottom right), the evolutionary process will be markedly affected.

Bottom: Evolution of molecular interactions based on reconstructed intermediates. Top: pathway towards independent steroid receptors after duplication, via intermediate receptors that remained sensitive to their ligands. A changed mutation order produced a non-sensitive intermediate, making that path inaccessible. Bottom: pathway towards independent repressor-operator pairs following duplication. Many paths could be compared in a landscape based on over 1000 mutants.



2.4 Biological Soft Matter

PROJECT LEADER
Dr G.H. Koenderink

RESEARCH GOAL
We use experimental methods and theoretical concepts of soft condensed matter physics to elucidate physical principles of the self-organization and mechanics of living materials, in particular cells. We investigate both simplified biomimetic protein networks of controlled complexity and cells that are embedded in biomimetic polymer scaffolds.

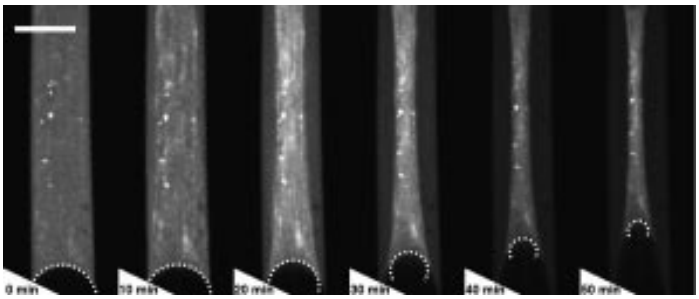
RESEARCH HIGHLIGHTS (WORK AT HARVARD UNIVERSITY)
Biological materials such as living cells are unlike any conventional synthetic materials. They are generally constructed from stiff polymers and soft membranes, which self-organise into complex, hierarchical structures that are often far out of chemical equilibrium. They have unusual mechanical properties, such as a high elasticity at rather small polymer volume fractions and a strongly non-linear, stiffening response to an imposed deformation. We wish to elucidate the design principles leading to these unique features, and to obtain quantitative measurements of the material properties to facilitate theoretical modeling. Since living materials are highly complex, being built of a staggering number of components, we investigate model systems of a limited number of purified components. These model systems allow us to identify fundamental physical principles that govern the structure and dynamics of living materials. At the same time, they inspire the design of new classes of materials with novel functionalities.
So far, we have focused on the actin cortex, a highly cross-linked network of stiff actin polymers that largely controls the mechanical and motile properties of cells. We demonstrated that a model system of only three proteins (actin filaments, filamin A cross-linkers, and myosin II motors) captures many essential features of the actin cortex. This system displays active motor-driven contractility, stiffening, and microscopic, non-thermal fluctuations. We showed that this behavior is caused by active directional sliding of actin filaments mediated by the myosin motors, coupled with stress build-up facilitated by the presence of cross-linkers that obstruct actin filament sliding.

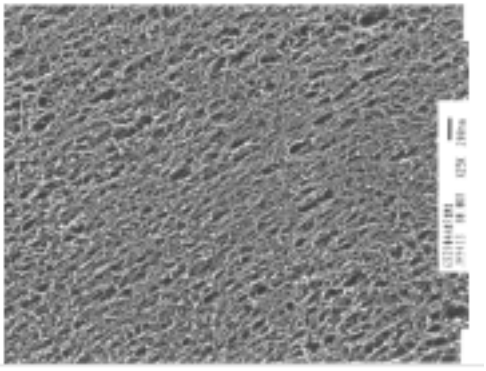
FUTURE DIRECTIONS
Biomimetic cytoskeletal protein networks
Even in the absence of active processes, cytoskeletal assemblies have a complicated equilibrium phase behavior and dynamics. They are composed of multiple filament types with distinct backbone rigidities, which are interconnected by a variety of cross-linking proteins with distinct molecular architectures and binding kinetics. We will study composite model systems of actin filaments, microtubules, and intermediate filaments that are gradually made more complex. Controlled interactions between the filaments will be created by adding physiological cross-linking proteins, depletion agents, and multivalent cations. Spatial confinement of networks in vesicles will be compared with confinement

in microfluidic channels engineered using soft lithography. To drive the networks out of equilibrium, we will incorporate force-generating motor proteins such as myosin. Active motor-driven pattern formation, motility, and contractility will be studied from a single protein level up to the network level using fluorescence microscopy. Network mechanics will be measured using rheometry and (laser tweezer) microrheology.

Mechanochemical interactions of cells in biomimetic polymer matrices

Living cells in the body are embedded in an extracellular matrix (ECM) composed of stiff polymers. Cells remodel their surrounding matrix by active contractile forces and biochemical interactions. Conversely, the ECM transmits mechanical forces and chemical signals to the cells. We will examine this bi-directional cell/matrix cross-talk by embedding cells in biomimetic ECM scaffolds. Model ECM matrices based on collagen and fibrin will be designed with controlled molecular composition and porosity, as well as spatial gradients in stiffness (durotaxis) and chemical guidance cues (chemotaxis). We will examine how cells actively remodel and contract the matrices with confocal microscopy and rheometry. Cell motility through the networks will be measured using fluorescence microscopy and particle tracking.





(a) Myosin motor molecules actively contract an initially homogeneous network of cross-linked actin filaments. The contracting gel exerts a contractile force that deforms the gel surface, as indicated by the white dotted line. Bar, 400 µm. (b) Electron microscopy shows the microstructure of the reconstituted actin network. Bar, 200 nm.

3 Center for Physics of Biomolecular Systems
Modelling

3.1 Computational Physics

GROUP LEADER
Prof. dr D. Frenkel

RESEARCH GOAL
Computational physics research at the AMOLF focuses on the study of the phase behaviour, dynamics of colloidal and (bio)polymeric systems and the kinetics of first-order phase transformations in such systems. Our holy grail is to develop hierarchical models for active and bio-molecular organization.

RESEARCH HIGHLIGHTS
During the past six years, we made significant progress in the numerical simulation of crystal nucleation. In particular, we developed a technique to compute the absolute rate of crystal nucleation of 'hard' colloids. This calculation is significant because it is the first example of a truly parameter-free prediction of a nucleation rate under realistic conditions of supersturation. We subsequently extended the method to other systems, such as simple ionic crystals (NaCl). At the moment, there is still a great scarcity of reliable experimental data for comparison.

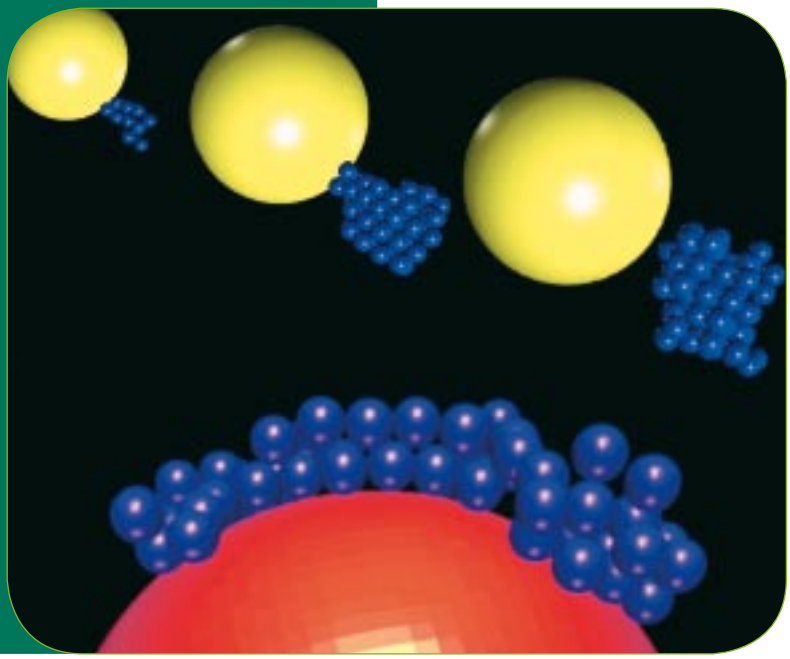
It has been known for many years that polydispersity can suppress crystal nucleation in colloidal systems. The explanation for this observation used to be that the polydisperse colloidal system forms a glass before it can crystallize. Our simulations suggest something totally different: in strongly polydisperse colloidal dispersions, the nucleation barrier does not decrease monotonically with increasing supersaturation. Rather, the barrier goes to a minimum. This prediction has observable consequences for the size distribution of colloidal crystals.

Suspensions of colloidal particles with a short-ranged attraction usually undergo structural arrest close to the point where they would undergo liquid-liquid demixing. We performed the first direct simulations in order to locate the critical point of the canonical model for colloids with short-ranged attraction, namely Baxter's 'adhesive sphere' model. We were able to show that in this system the critical point is inside the gel phase. Hence, in this system, liquid-liquid demixing is kinetically inhibited.

We performed extensive studies on the competition between crystallization and liquid-liquid demixing in polymer systems. Our simulations (of a lattice model) showed that the kinetics of crystallization is strongly influenced by the proximity of the liquid-liquid spinodal. Moreover, we studied the effect of polymer pre-alignment of the resulting crystal morphology. To our surprise, we found that a single aligned polymer is enough to induce the formation of the so-called 'shish-kebab' morphology observed in many experiments.

The easy accessibility of 'made-to-order' DNA sequences is changing materials science. We performed a theoretical analysis of the phase behaviour of colloidal particles coated with single-stranded DNA that can

Snapshot sequence of colloidal crystal nucleation on spherical seeds. Crystallites first form on the surface of the large sphere and then detach to relieve the stress induced by the curved substrate.



be linked by complementary single-stranded DNA molecules. Our analysis showed that the 'freezing' that is observed in experiments is, in fact, a liquid-liquid demixing followed by structural arrest. This work has resulted in one patent.

As microfluidic devices become nanofluidic devices, the problem of fluid transport on a chip becomes acute: the viscous drag in narrow channels is enormous and hence pumping may not be the best way to transport liquids. An alternative is to use electric fields to drive the flow of electrolyte solutions. We developed a Lattice-Boltzmann method to model such flows for arbitrary geometries. With this method, we are able to predict electrokinetic phenomena under experimentally relevant conditions.

Even though computing power continues to grow according to Moore's law, there are many problems that cannot be addressed without dramatic improvements in simulation algorithms. We proposed a method that allows us to change the strategy of Monte Carlo simulations, in such a way that information about rejected trial moves is not discarded. This scheme is particularly powerful in parallel simulations (where it can lead to exponential speed-up). We have applied this new method with success to the calculation of the folding pathway of simple model proteins.

FUTURE DIRECTIONS

The focal point of the Computational Physics group's research will shift towards coarse-grained simulations of organization and transport of biomolecules and materials containing bio-molecular building blocks.

One key line of research has been and is the study of novel DNA-coated colloids. During the past year, we obtained funding for a joint experimental-numerical project to study such materials. In the longer term, we aim to couple this with the study of active (i.e. energy-consuming) assembly of complex materials. This research is linked to parallel activities within the AMOLF nanophotonics programme, and at the University of Amsterdam, the Free University in Amsterdam and Leiden University.

We aim to gain a better understanding of the role of charge on the crystallization of proteins and (nano)colloidal salts. Recent experiments show that these systems can form surprisingly complex binary crystal structures, some of which have no simple molecular counterpart. We aim to study the factors that control the kinetics of the formation of complex binary structures and to explore the limits of 'spontaneous' self-assembly in multicomponent systems of charged (nano)colloids.

A third line of research is the study of substrate-induced conformational changes in simple models for proteins. We hope this will lead to an understanding of how to 'design' artificial binding sites with ultrahigh specificity.

3.2 Theory of Biomolecular Matter

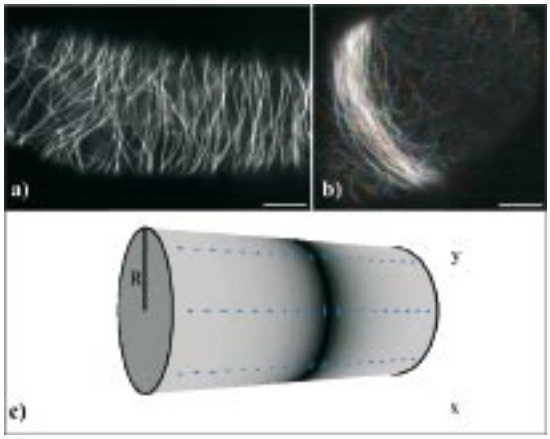
GROUP LEADER
Prof. dr B.M. Mulder

RESEARCH GOAL
The aim of our group is to understand the individual and collective behaviour of biomacromolecules and their aggregates, using the techniques of statistical mechanics and continuum mechanics. The work is inspired by concrete questions regarding the structure and function of actual components of the living cell, with a special focus on plant systems.

RESEARCH HIGHLIGHTS
In the past six years, this completed its transformation from the 'complex fluids' theme to the 'biomolecular matter' theme.

The major milestones in this period were:
- The completion of the final project in the field of soft condensed matter on the phase behaviour of semi-flexible liquid crystalline polymers. This technically very complex work opens up the possibility of rationalizing the phase diagram of complex molecules, such as side-chain liquid crystalline polymeres, on the basis of coarse-grained molecular parameters, such as connection topology and geometry, spacer flexibility and component stoichiometry.
- The full elaboration of the dynamical geometrical model for the generation of cell walls of higher plants, which serves as the basis for

The cortical transverse array (a) and the preprophase band (b) are two of the important microtubule cytoskeleton structures in higher plants (scale bar 10 μm). Here they are visualized in Tabacco BY2 cells by a constitutively expressed GFP microtubule binding domain construct. Our course-grained theory of active gels is able to generate transverse orientationally ordered ringlike structures in cylindrical geometries (c) and provides a framework for studying these structures in general.



several ongoing collaborative research projects. This is the first fully quantitative model that can explain the architecture of cellulose fibril scaffold, which determines the cell wall architecture on the basis of cellular parameters that can, in principle, be measured and manipulated. The significance of this work is its close connection to industrially important questions regarding the quality and processing of fibre-based plant products (wood, paper, flax, etc.).

Three new research topics were started, all of which are just reaching early maturity:

- In collaboration with Dogterom's experimental group at AMOLF and colleagues from the Max Planck Institute for Physics of Complex Systems at Dresden, a coarse-grained theoretical description was developed of non-equilibrium active gels of filamentous particles, in an attempt to model the dynamics and architecture of the cytoskeleton of eukaryotes. This work formed the basis of the first biological physics thesis produced in the group and provides the framework for ongoing research in understanding the functional microtubule arrays and the transitions between them in higher plant cells.

- Inspired by experimental observations from the Plant Cell Biology laboratory at Wageningen University (Esseling, Ketelaar, Emons), we are developing physico-mechanical models of tip growth in cells. Tip growth is a prime and as yet poorly understood example of self-regulated morphogenesis of cells. In some plant species, it plays an important role in mediating symbiotic interactions with soil-living bacteria, a topic of great current interest. We have shown that the diffusive delivery of exocytotic vesicles containing cell-wall building materials provides a physically realistic and consistent basis for the growth mechanism.

- Together with Woldringh of the Molecular Cytology department of the University of Amsterdam, we are exploring the physical aspects of DNA segregation in prokaryotes. In contrast to eukaryotes, the mechanism by which the duplicated genetic material of bacteria is divided over the daughter cells upon division has thus far remained elusive. The purely physical effects due to the fact that the replicating bacterial chromosome consists of a highly confined polymer of non-trivial topology have so far been overlooked. We have shown that purely entropic effects can not only explain the segregation per se, but also account for the details of the process as observed in recent experiments.

FUTURE DIRECTIONS

Although most of the group's current research topics are at the beginning of their scientific life cycle, there are a few topics likely to become important in the near future:

- The statics and dynamics of strongly confined biopolymers and their interaction with proteins, with an emphasis on understanding the bacterial nucleoid. We will attack this new field, which combines both interesting and largely unexplored physics with high potential for cell biological applications, both through analytical and computational approaches.
- Understanding the concepts of property design in complex multi-component systems. Initial target systems are the cytoskeleton *in vivo* and DNA-linked particles *in vitro*. This direction will involve the development of novel techniques for dealing with the computational exploration of high-dimensional state spaces (using, e.g., biologically inspired optimization algorithms).
- The study of the spatial architecture versus the mechanical property relationships in hierarchically structured materials like the plant cell wall. This will require a heavier emphasis on materials science concepts and techniques. This work will also increasingly evolve towards integration with plant cell biological models, functional genomics and live cell observations in a systems biological approach, for which an interdisciplinary EU-NEST network-type project was recently awarded.

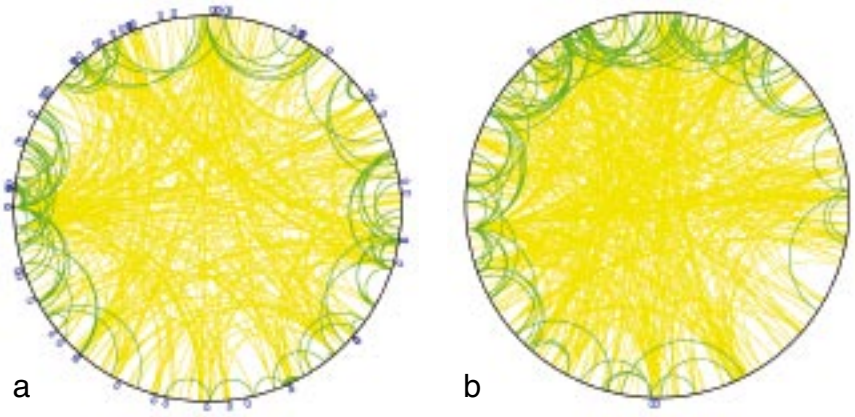
3.3 Biochemical Networks

GROUP LEADER

Dr P.R. ten Wolde

RESEARCH GOAL

Biochemical networks are the central processing units of life. They can perform a variety of computational tasks analogous to electronic circuits. Their design principles, however, are markedly different: in a biochemical network, computations are performed by molecules that chemically and physically interact with each other. The aim of the Biochemical Networks group is to unravel their design principles using a combination of database analyses, theory and computer simulation.



The gene regulatory network of E. coli shown as links between operons on the genome. Maps are shown for (a) the real network of E. coli and (b) a representative 'randomised' network with the same topology but a random permutation of the indentities of the operons. The color code is: dark: distances less than 10 kbp; medium dark: 10 kbp-500 kbp; light: greater than 500 kbp. Note the much greater prevalence of the 'short' distances in the E. coli map (a) compared to the randomised map (b).

RESEARCH HIGHLIGHTS

Development of new numerical techniques

We developed a numerical technique called Forward Flux Sampling, which makes it possible to simulate rare events in equilibrium and non-equilibrium systems. While the conventional techniques to simulate rare events are only applicable to equilibrium systems, our technique also allows the simulation of rare events in a wide variety of non-equilibrium systems, such as crystal nucleation under shear, polymer collapse under flow and bistable switches in biochemical networks.

We also developed a numerical technique called Green's Function Reaction Dynamics (GFRD), which allows the simulation of biochemical networks at the particle level and in both time and space. The main idea of GFRD is to exploit the exact solution of the Smoluchoswki equation to set up an event-driven algorithm, which combines in one step the propagation of the particles in space with the reactions between them. Under biologically relevant conditions, GFRD is up to five orders of magnitude faster than conventional particle-based techniques for simulating biochemical networks in time and space.

Spatial distributions of genes and operons

We performed a combination of database analyses, theory and computer simulations to study the spatial distribution of genes and operons along the DNA in the bacterium *Escherichia coli*. The database analyses allow us

to identify motifs, i.e. over-represented patterns of interactions between components of the network, while the theoretical analyses and computer simulations allow us to address their functional significance.

The statistical analyses revealed that co-regulated pairs of genes and pairs that regulate each other tend to be much closer to each other than can be expected for a random network and that they tend to be transcribed in diverging directions. This spatial arrangement of genes allows the regulatory domains on the DNA to overlap with each other, which, in turn, allows for *correlated* or *anti-correlated* expression of pairs of genes.

Our theoretical and numerical analyses revealed that overlapping operons can both enhance the sharpness of the network response and make biochemical networks much more robust against biochemical noise.

Spatial patterns of gene expression
We developed a model for the reliable formation of spatial patterns of gene expression in embryonic development. This model can explain recent experimental observations in *Drosophila,* which show that the centre of the embryo is accurately identified even in a noisy environment.

FUTURE DIRECTIONS

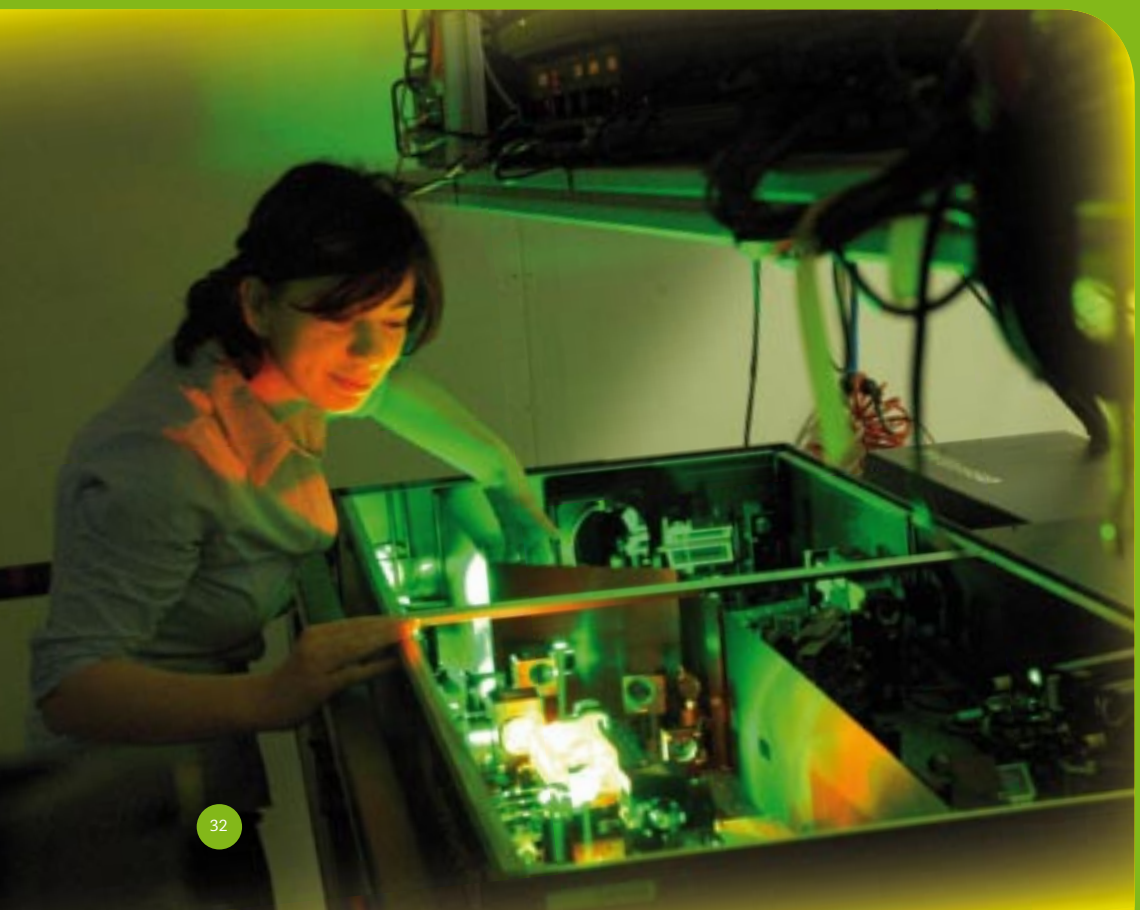
Over the past four years, our focus has been mainly on individual and prokaryotic cells. In the coming years, we plan to study higher organisms and the population of cells.

Extending current directions
In collaboration with Bastiaens's experimental group (EMBL, Heidelberg), we will study the transmission of signals in eukaryotic signal transduction pathways in time and space. Together with Howard (Imperial College, London) and Ma's experimental biology group (University of Cincinnati), we will investigate the robust formation of spatial patterns of gene expression during embryonic development. We will use our recently developed GFRD algorithm to study the robustness of gene expression patterns against biochemical noise. In collaboration with Teichmann (MRC Laboratory of Molecular Biology, Cambridge, UK), we will extend our database analyses to study the spatial organization of the genomes of higher organisms. Together with Tans (AMOLF), we will study the evolution of small network motif, such as transcriptional logic gates, bistable switches and oscillators.

New directions: game theory and cost-benefit analysis biochemical networks
Cells can respond to changes in the environment by sensing the changes or by switching their phenotypes stochastically. To understand the effectiveness of these strategies, one has to study the population of cells. Concepts of game theory and cost-benefit analyses are also required, as well as an understanding of noise properties of biochemical networks. We intend to exploit our expertise in the latter to investigate the computational strategies of prokaryotes.

4 Center for Physics of Biomolecular Systems

Molecular



4.1 Ultrafast Spectroscopy

GROUP LEADER
Prof. dr H.J. Bakker

RESEARCH GOAL
The goal of this group is the elucidation of the structure and dynamics of complex hydrogen-bonded systems, in particular of (bio)molecular systems involving liquid water. The research is carried out using advanced femtosecond nonlinear and single-molecule spectroscopic techniques.

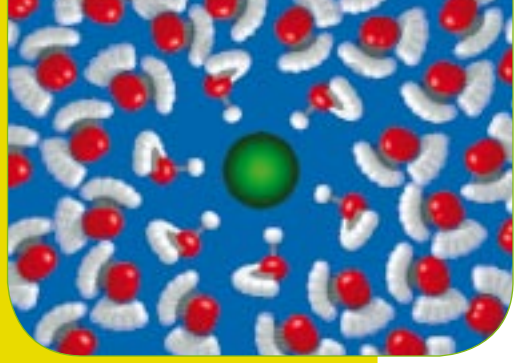
RESEARCH HIGHLIGHTS

Structure and dynamics of aqueous solvation shells
We discovered that the dynamics of water molecules in aqueous solvation shells of ions can be studied with unprecedented selectivity using nonlinear femtosecond mid-IR spectroscopy. With this technique we observed that the hydrogen bonds between water molecules and halogenic anions fluctuate with a characteristic time constant of 10-25 ps (depending on the ion), which is 20-50 times slower than the hydrogen-bond fluctuations in bulk liquid water. We also found that the water molecules in the solvation shells reorient on a time-scale that is ~3 times slower than in bulk. This reorientation is not due to rotation of the water molecules within the shell, but to orientational diffusion of the complete solvation structure. These results show that the first solvation shell of ions forms a surprisingly rigid and stable structure. In contrast, we have observed that the water dynamics *outside the first solvation shell of the ion* are only negligibly affected by the presence of ions. This result shows that ions do not act as structure breakers or makers of the hydrogen-bond structure of liquid water.

Anomalous temperature dependence of the vibrational relaxation of water
We found that the OH stretch vibrations of water show a very rapid relaxation with a time constant of 260 femtoseconds at 300 K. With increasing temperature, this relaxation becomes slower, a phenomenon which is now being acknowledged as one of the 41 anomalous properties of liquid water.

Energy dynamics of single embedded water molecules
We observed that a single water molecule embedded by acetone forms two fluctuating hydrogen bonds with the C=O groups of two neighbouring acetone molecules. We found that these hydrogen-bond fluctuations can tune the O-H vibrations of the water molecule into resonance, thereby enabling energy transfer between the two OH groups.

Dynamics of water in nanodroplets
We studied the dynamics of water in nanodroplets with a diameter of 1-10 nanometers (10-10.000 molecules). For a droplet with a diameter of ~1 nm, the OH-vibrational lifetime increases by a factor of 4 to ~1 picosecond compared to the bulk. We also found that the water layer at the surface of the nanodroplet forms a very rigid structure, whereas the water in the core of even a small nanodroplet shows the same



Artist's impression of an iodide ion solvated by water molecules in liquid solution. Femtosecond mid-infrared spectroscopic experiments showed that the water molecules in the first solvation shell of the ion have much slower dynamics than the water molecules outside this shell. The water molecules in the shell show translational (hydrogen-bond stretching) and reorientation dynamics with time constants of 18 and 10 picoseconds, respectively. Outside the shell these time constants are only 0.5 and 2.6 picoseconds.

orientational mobility as bulk liquid water. This result shows that the centre of a nanodroplet of water does not show an ice-like structure, as was commonly believed.

Proton-transfer reactions in liquid water

We studied the mechanism of acid-base reactions in water with femtosecond visible-pump mid-IR probe spectroscopy on an aqueous system of a photoacid and an accepting base. The conventional view of this reaction is that the acid and the base have to diffuse into direct contact to enable proton transfer. However, we found that proton transfer occurs primarily via Grotthuss conduction, through a hydrogen-bonded 'water wire' of 2-4 water molecules which connects the photoacid with the base.

We also found that the excitation of the second excited state of the OH stretch vibration leads to a strong delocalization of the hydrogen atom along the O-H···O hydrogen bond between two water molecules.
An important implication of this finding is that this second excited vibrational state forms, energetically, the most favourable transition state for the autodissociation of water, i.e. the process in which two water molecules split spontaneously into H_3O^+ and OH^-.

FUTURE DIRECTIONS

Water near surfaces and biomolecules

We intend to investigate the translational and orientational dynamics of water-solvating (bio)molecules and near surfaces. This study will clarify the role of water in determining the spatial structure of other molecular systems.

Aqueous proton transfer reactions

We will investigate the mechanism of proton transfer in water both for equilibrium systems, such as protons dissolved in nanodroplets of water and in ice lattices, and for non-equilibrium systems, in which the release of a proton is triggered by light.

Direct detection of low-frequency dynamics

In the past the dynamics of low-frequency vibrations such as hydrogen bonds and conformational motions have mostly been studied by probing

the response of high-frequency vibrational and/or electronic excitations. We intend to probe the low-frequency dynamics of aqueous (bio)molecular systems directly in the far-infrared (THz) region of the spectrum. For this purpose we will develop a sub-picosecond mid-infrared/far-infrared pump-probe technique that allows the direct probing of hydrogen-bond and conformational vibrations.

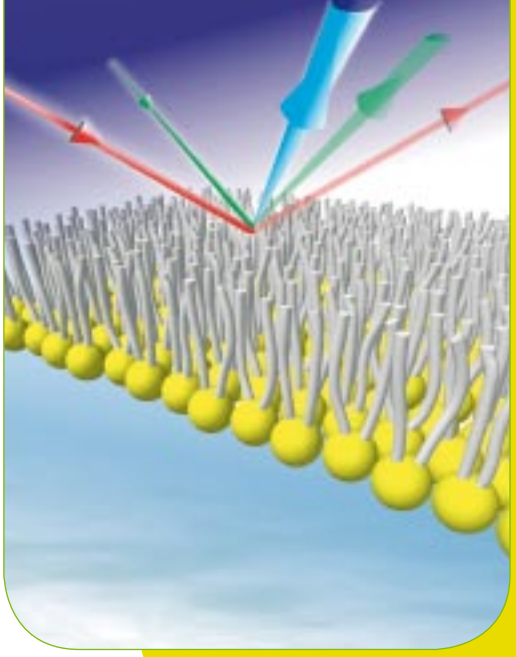
Time-resolved single-molecule spectroscopy
We propose to identify the dynamics of O-H and C=O vibrations at the single-molecule level using a new visible/mid-infrared double-excitation scheme. The technique will provide information on the vibrational frequency fluctuations of (bio)molecules, thus enabling the study of molecular dynamics at the single-molecule level.

4.2 Biosurface Spectroscopy

GROUP LEADER
Prof. dr M. Bonn

RESEARCH GOAL
The aim of the Biosurface Spectroscopy group is to elucidate ultrafast dynamics of energy and charge transfer and elementary chemical transformations with particular emphasis on surfaces. Specific efforts are aimed at unravelling interactions between the different molecular constituents of model biological membranes. In a second line of research, we are attempting to characterize and control optical properties and charge carrier dynamics in semi-conductor nanostructures using ultrafast TeraHertz spectroscopy.

RESEARCH HIGHLIGHTS
Biosurface spectroscopy
Membranes constitute the highly active partition between living cells and the outside world. They regulate molecular transport, cell adhesion and intercellular signalling. A detailed understanding – and control – of the many biological processes that occur at the membrane surface, such as viral infection and targeted drug delivery, requires insights at the molecular level. Recent developments in experimental techniques have opened avenues for the study of intermolecular interactions and chemical processes at surfaces and interfaces with unprecedented time and spatial resolution. We employ these methods, including Sum-Frequency Generation (SFG) and Coherent Anti-Stokes Raman (CARS) microscopy, to address important issues in biological (model) membranes.
The impact of these techniques may be exemplified by our recent discovery of a new phase transition of phospholipids at the air-water interface whereby we can now look at the molecular structural order of the lipid molecules. This is of biological relevance as the structure of phospholipid molecules at water surfaces determines important properties of membranes. We have also revealed the stabilizing effect of cholesterol – the second most important membrane constituent after



Lipids, consisting of polar headgroups (depicted here as spheres) and apolar tails (wiggly lines), self-assemble when put in contact with water (light blue). The monolayer model system depicted here is a good model for bilayer biological membranes. We investigate intermolecular interactions between membrane biomolecules using non-invasive, optical techniques. In the experiments, two laser pulses intersect at the surface (red: infrared and green: visible), whereupon a third colour (blue) is generated by frequency mixing, allowing the determination of the molecular conformation and orientation of membrane biomolecules.

phospholipids – on the structure of the lipid layer. In addition, we are the first to demonstrate the possibility of using surface-specific SFG spectroscopy to probe the surface molecular properties of (cell-size) colloids and vesicles, paving the way for investigating the structures of membranes in living systems.

Time-domain terahertz (THz) spectroscopy

It is challenging to characterize charge carrier movement in semi-conductor structures, partly because of the complications of attaching contacts to the sample. This is even more evident for nanostructures. Moreover, conductivity measurements at low frequencies are inherently limited in the information content. These drawbacks can be circumvented using freely propagating THz pulses. The rapidly varying electric field contained in these pulses with durations of ~1 picosecond allows for the investigation of key electronic properties of materials such as the electron mean-free path, exciton properties and confinement effects in nano-structured materials. Furthermore, the high time resolution of this technique allows the study of dynamic processes and/or systems far from equilibrium using a pump-probe experimental approach.
Using THz spectroscopy, we have investigated charge dynamics in conjugated polymers. After optical excitation, excitons or free charges may be formed. We have been able to unambiguously determine the quantum yield for the formation of the two species individually. In a parallel effort, we investigate electron dynamics in nanostructured semi-conductors of CdSe and TiO_2. For the former, we have revealed the mechanism for electron cooling for the first time, with major implications for solar cell design using semi-conductor nanoparticles.

Ultrafast surface dynamics (carried out at Leiden University)

Using femtosecond laser-based surface-specific spectroscopic techniques,

we have investigated the chemical reaction dynamics of simple molecules on single-crystal metal surfaces. We have gained unprecedented insights into the dynamics of energy flow and chemical transformation. We have, for example, time-resolved the motion of simple molecules over the surface for the first time. The ultrafast sub-picosecond motion demonstrated that, in contrast to the widely accepted view that hopping occurs by moving parallel to that surface, with the molecular axis perpendicular to the surface, excitation of the rotational mode is crucial for diffusion.

FUTURE DIRECTIONS

Membranes separate the inside of the living cells from the outside and actively regulate molecular transport, cell adhesion and intercellular signalling. Since 80% of all biomolecular interactions occur at the membrane surface, many efforts have been made to reveal these biomolecular interactions. This research has remained limited, however, to investigations of the composition and static structure of membranes, whereas information on their dynamics is lagging, owing to the lack of appropriate experimental tools. It has been widely acknowledged that detailed information on the time-scales on which these biomolecular interactions occur is essential for a detailed understanding of these processes.

In the coming years, we aim to combine our knowledge in the field of membrane (static) spectroscopy with our expertise in ultrafast surface spectroscopy, to monitor the dynamics of membrane molecules in real time, from ~100 femtoseconds to seconds. We will investigate the dynamics of three key components of a biological membrane: the lipid molecules constituting the lipid bilayer, the proteins embedded in the bilayer and the associated 'biological' water. The wide time window will be covered by combining femtosecond infrared laser spectroscopy (time window: 10^{-13} s to 10^{-9} s) with stepscan Fourier transform infrared spectroscopy (time window: 10^{-9} s to 10 s). By 'looking directly inside' the lipids, the proteins and the water by means of their molecular vibrations, this novel approach circumvents the conventional usage of probe molecules (e.g. fluorescent probes) and is thus completely non-invasive.

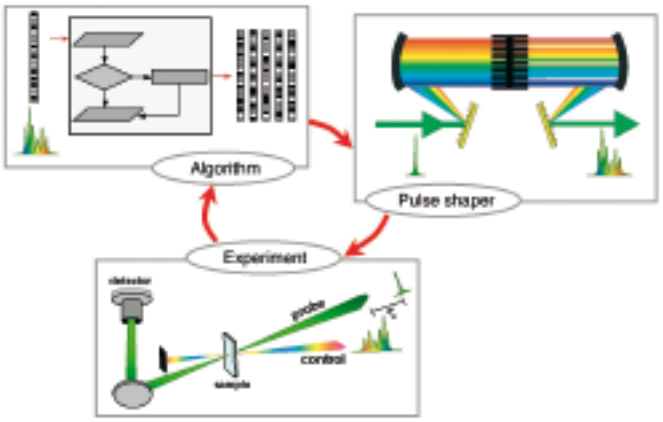
4.3 Biomolecular Control

PROJECT LEADER

Prof. dr J.L. Herek

RESEARCH GOAL

The goal of our research is to develop a new strategy to explore molecular dynamics in complex (bio)molecular systems, based on the control of reaction pathways and energy flow using tailored femtosecond laser pulses. Analysis of optimal pulse shapes will yield insight into reaction mechanisms, features of potential energy surfaces and the role of specific vibrational motions on function.



Schematic design of the learning loop for coherent control. A shaped, ultrashort laser pulse excites the sample, and a probe pulse monitors its effect. The detected signal serves as input to the learning algorithm that suggests improved pulse shapes, for repeated excursions around the loop until the objective is achieved.

RESEARCH HIGHLIGHTS

Our research focuses on controlling the dynamics and function of complex (bio)molecular systems by active manipulation of the light-matter interactions via the driving excitation field. To this end, we designed and developed a new set-up for feedback-driven optimization experiments of complex (bio)molecular systems based on adaptive femtosecond pulse shaping. Integration of an amplified femtosecond laser, two nonlinear optical parametric amplifiers, programmable pulse shaper, diode array detection, pulse characterization, sample handling and custom software has afforded a state-of-the-art system with many unique aspects, in particular:

- a home-built diode array detector with bi-line operation capable of a 1-kHz readout of 512 diode channels over two parallel arrays for simultaneous signal and reference spectra acquisition,
- a rotating sample holder for use at low temperatures (down to 4 K) within a helium cryostat, and
- a high-resolution liquid crystal spatial light modulator with phase and amplitude control over 640 individual spectral components in an excitation pulse.

Our first experiments with this set-up explored the ultrafast dynamics of a biomimetic analogue of the LH2 light-harvesting antenna. The natural photosynthetic pigment-protein complex was previously explored by adaptive femtosecond pulse shaping. It was shown that the pathways of energy flow could be manipulated by a complex excitation pulse that exploited molecular coherence. The caroteno-porphyrin dyad is an ideal model system that mimics the salient features of the natural photo-synthetic light-harvesting complex. Understanding the competing energy flow pathways in this system and the relevance of various vibrational

modes in promoting or hindering these pathways is crucial to exploring the mechanisms of control in complex systems.

We performed detailed transient absorption measurements to map out the pathways and efficiencies of energy flow in the dyad. The spectral evolution was analysed globally to extract the many overlapping contributions to the signal, and to determine regions suitable to use as feedback in the optimization experiments. In this donor-acceptor complex, energy transfer is limited by a competing ultrafast loss pathway, analogous to the dynamics in LH2. Our first experiments with shaped pulses indicate that both the functional and loss pathways can be manipulated, such that the efficiency of energy transfer may be enhanced or diminished. By analysis of the optimal pulse shapes, we hope to extract features of the potential energy surfaces that dictate the pathways of energy flow in this system, and ultimately to shed light on the active mechanisms in the natural photosynthetic complex.

FUTURE DIRECTIONS

Beyond the novelty of allowing active controlling of biological function through tailored excitation light, coherent control strategies offer a new spectroscopic tool for exploring complex systems, thus providing insight into potential energy surfaces and relevant vibrational modes. In the coming years, we will apply these techniques to a variety of systems, among which the following:

Photosensitizer efficiency

Porphyrin derivatives have been successfully applied as photosensitizer molecules in photodynamic therapy for cancerous tumors. The efficiency of this technique depends on competition between intramolecular deactivation channels. We will target specific reaction pathways with the goal of enhancing energy transfer and minimizing loss channels.

Energy localization in biological aggregates and nanostructures

By controlling the pathways of energy flow in strongly coupled biological aggregates, we will show that it is possible to spatially localize excitation energy at a given position and time due to interferences between excitonic wavefunctions.
Analogous experiments will explore energy localization in nanostructures, in cooperation with Kuipers. Sub-wavelength metallic structures exhibit many interesting phenomena at optical frequencies, including strong local field enhancement at 'hotspots'. With tailored excitation pulses, we will manipulate the positions of these hotspots by exploiting interference and dispersion effects.

Molecular switches

Diarylethene derivatives are a promising group of molecular switches for a wide variety of device applications. The stability, spectral properties, switching rates and quantum yields can be passively controlled by the choice of substituents. Our goal is to actively control the switching dynamics using shaped laser pulses.

5 Center for Nanophotonics

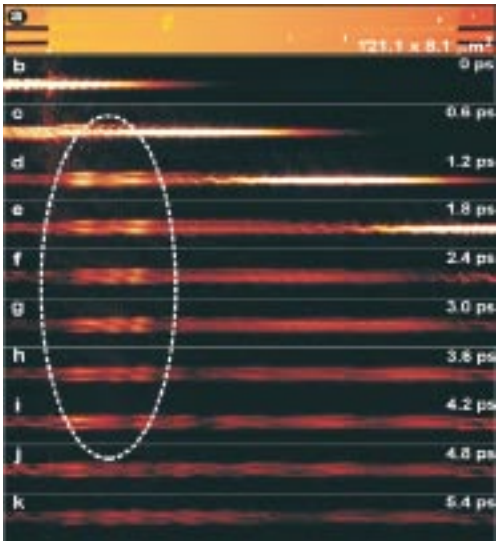
5.1 Nano-Optics

GROUP LEADER
Prof. dr L. Kuipers

RESEARCH GOAL
The aim of the Nano-Optics group is to investigate and control the propagation of light at length scales at or below its wavelength and on femtosecond time-scales. Control is achieved with individual metallic nanostructures and with plasmonic or photonic crystals, through the use of plasmonic or photonic bandgaps. Slow light propagation and local field enhancement are used to increase light-matter interactions.

RESEARCH HIGHLIGHTS
The research in the past six years can be divided into two closely related topics: light propagation in (nano)photonic structures and the influence of the nanoenvironment on the emission of single emitters.

Light emission by single molecules (carried out at University of Twente)
The environment around light emitters on nanometer-length scales affects their optical properties. Fluctuations in the nano-environment thus influence the properties of, e.g., chromophores at the single-molecule level. This notion was expanded upon, following our direct observation that the triplet lifetime of single molecules varies in time due to time-dependent changes of their nano-environment. We found that the temporal variations obey ergodicity. The time-dependent variation of the fluorescence lifetime of molecules embedded in a polymer matrix just above and below the glass transition were shown to reflect the segmental dynamics of the polymer on the nanoscale. We also confirmed the influence of layer thickness on the polymer dynamics. We took active



Snapshots of ultraslow light in a two dimentional photonic crystal waveguide. a) Measured topography of the photonic structure. b-k) Consecutive images that show an ultrashort pulse propagating through a photonic crystal waveguide. The time step between images is 600 fs. The series of images shows a relatively fast pulse moving through the structure in the first 2 ps. In its wake a light field is observed (highlighted region) that is seemingly stationary and localized to the start of the waveguide. An upper boundary of the speed of this field is c/1000.

control of the emission of a single molecule by nanopositioning a metallic object in its vicinity. Thus, the directionality of the emitted light was controllable in a reversible manner. In another line of experiments, the first pump-probe investigation of single molecules was performed. It revealed the internal vibronic relaxation of the excited molecules. The relaxation was found to slow down when two molecules were within ~2 nm of each other, which led to a significant dipole-dipole coupling.

Light propagation in nanophotonic structures (AMOLF and Twente)
A unique phase-sensitive time-resolved near-field optical microscope was developed that allows the direct visualization of ultrafast pulse propagating through photonic structures in space and time. The instrument was used to show for the first time how the co-propagation of different modes in a single waveguide can lead to the formation of phase singularities with topological charges of ±1. The Bloch nature of modes in photonic crystal waveguides was revealed, and the most comprehensive measurement of their band structure to date was performed. We observed Bloch harmonics that make up the Bloch modes in up to 4 Brillouin zones. We pioneered the visualisation of femtosecond pulses as they propagate through photonic structures in both space and time, allowing an unambiguous determination of their phase and group velocity separately. The measurement of the bandstructure in a photonic crystal waveguide led to the identification of a flat part of the dispersion. For the corresponding frequency, a seemingly stationary and localized light field was observed; the upper limit of its speed was c/1000. Recently, the first observations of slow surface plasmon polaritons were made.
We also used the fluorescence of single molecules with a fixed dipole orientation to map the vectorial nature of the electric field near metallic nanostructures.
The world's largest two-dimensional photonic crystal for visible light was realized using a new hybrid, holographic method for the fabrication of large two-dimensional photonic crystal slabs with light-guiding defects. We were the first to show that hole shape can play a crucial role in extraordinary transmission through sub-λ holes arrays. At the time, this highlighted that the prevalent understanding of this phenomenon was incomplete. Hole shape and hole size modify the height and position of the transmission peaks. Thus, the properties of hole arrays can be controlled by engineering the geometry of the unit cell.

FUTURE DIRECTIONS

We will explore novel routes to combine nonlinear optics and nanophotonics at relatively low light intensities. The nonlinear optical response generally scales with the inverse of the group velocity. We will therefore exploit slow-light propagation in plasmonic and photonic crystals to enhance the nonlinear response of nanostructures. The geometry of the unit cell of, particularly, the plasmonic crystals, can be used to increase the nonlinear interactions even further through local field enhancements. As the nonlinear phenomena are hard to predict theoretically, local time-resolved measurements are essential to unravel the nonlinear light flow at the nanoscale.
The sensitivity of the novel nanostructures to slight distortions will also

be exploited by actively using a near-field probe to reversibly create a high-Q localized photon state in its vicinity. Its high local optical field will be exploited to induce nonlinear behaviour that is tuneable with the probe position.
Ultimately, we aim to create a highly unusual optical object: a polaritonic light bullet that should have properties alien to normal wave optics, being stable against both diffraction and dispersion broadening. At present, the existence of such an object is uncertain, although its cousin – the 'light (only) bullet' – has been predicted to exist in nonlinear photonic crystals. The results obtained are expected to impact applications such as optical storage and integrated optics, and potentially, to renew interest in all-optical computing.

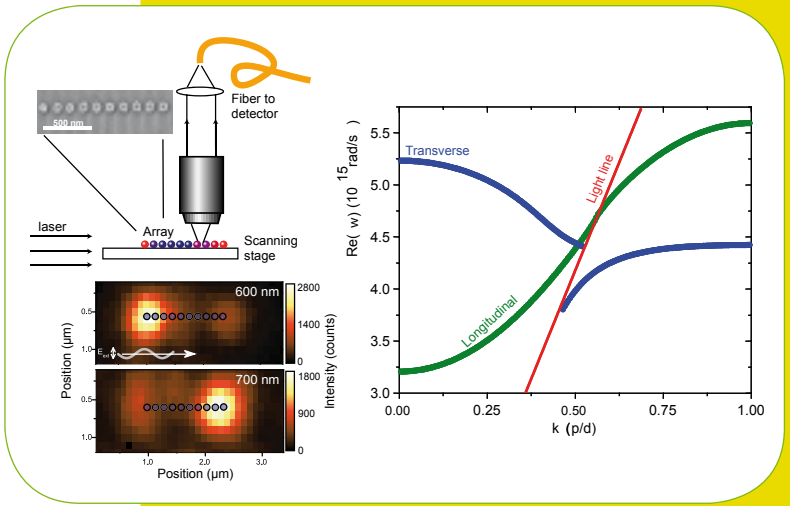
5.2 Photonic Materials

GROUP LEADER

Prof. dr A. Polman

RESEARCH GOAL

The goal of the Photonic Materials group is to study optical interactions in photonic nanomaterials with the aim of understanding and controlling energy transfer and optical emission processes. The focus is on energy transfer in metallo-dielectric plasmonic structures, optical confinement and spontaneous emission in photonic crystals and microresonators and light emission from (rare-earth doped) silicon-based nanostructures.



A chain of ten Ag nanoparticles, made using electron beam lithography, is excited with a laser. Confocal scanning microscopy shows that the field distribution along the array is a strong function of excitation frequency. The data are corroborated by calculations of the dispersion diagram of the metal nanoparticle waveguide modes, that show a polariton splitting into two anticrossing branches.

RESEARCH HIGHLIGHTS

Control of spontaneous emission is a key element in our research programme. Fermi's Golden Rule says that the emission rate from an optical emitter is determined by the local optical density of states (LDOS). By modulating the LDOS near a dielectric interface in a range of geometries (planar interfaces, thin films, colloids), we were able to control the radiative decay rate of rare-earth ions, transition metals and, most recently, Si quantum dots (with Atwater, CALTECH). Non-radiative decay processes in these transitions were also identified. We determined, both theoretically (with Tip, AMOLF, and Knoester, RUG) and experimentally, that the LDOS does not affect nanoscale Förster energy transfer between dipolar units.
We studied the coupling of optical emitters (Er ions, Si quantum dots) to surface plasmon polaritons (SPPs) on silver, by investigating polarization-dependent spectral changes and fluorescence-decay data. Using tailored metallo-dielectric nanostructures made using electron-beam lithography and colloidal synthesis, we were able to tune the plasmon resonance wavelength in the range from 400-1800 nm, and obtain control over the spontaneous emission wavelength and polarization of Si quantum dots. We subsequently developed design criteria for SPP-enhanced LEDs. In collaboration with Fleming (Sandia), we demonstrated modified spontaneous emission from defect-related optical transitions in Si, using a three-dimensional Si photonic woodpile crystal with a full photonic bandgap.

Together with Vahala (CALTECH), we developed the world's smallest Er-implanted microcavity laser on silicon, based on an ultra-high Q, Er-implanted, toroidal silica, whispering-gallery-mode cavity. The effects of cavity Q, cavity loading and Er concentration on lasing wavelength, threshold power and efficiency were measured and agreed with a lasing model developed for this geometry. Most recently, we developed a planar microdisk laser on Si, entirely made using CMOS technology, which, through proper mode engineering along the cavity's outer taper facet, has an extremely low lasing threshold.

Cooperative upconversion effects were studied in highly concentrated rare earth doped materials, and we determined how they affect the performance of erbium-doped planar optical amplifiers. Subsequently, we studied rare earth polymer waveguide films doped with rare earth complexes (with Van Veggel, Twente University). Together with Friend (Cambridge), this lead to the development of the first infrared polymer LED, based on energy transfer from a specifically engineered lissamine sensitizer that mediated energy transfer between the polymer electronic states and the Er 4*f* ligands.

To achieve control over the ion implantation technique, which, as we have proven, has great potential in the preparation of novel photonic materials, we studied several fundamental aspects of ion-solid interactions. We developed the concept of the 'mechanical stress map', which predicts the saturation stress in thin film for any irradiation condition. It takes into account the effects of radiation-induced Newtonian viscous flow and

anisotropic deformation. We also identified, for the first time, the role of capillary forces in shape changes of nanoscale objects under ion irradiation.

With Atwater (CALTECH), we calculated dispersion characteristics of planar and 'slot' SPP waveguides, which have great potential in optical structures with dimensions smaller than the wavelength. We developed a confocal optical microscopy imaging technique to study the propagation of long-range SPPs, and a cathodoluminescence imaging technique to characterize short-range near-resonance SPPs. Linear arrays of metal nanoparticles were synthesized and serve as nanoscale optical waveguides. We found an unexpected polariton splitting in the dispersion diagram resulting from radiation damping and retardation along the array.

FUTURE DIRECTIONS

The future research programme of the group will focus on plasmonics and Si-based photonics. We will study the propagation and dispersion of long-range SPPS and explore them to enhance the infrared response of silicon solar cells (with Kuipers). At high frequency, near the SPP resonance, we will try to answer the question: 'How small can a photon be shrunk?', by measuring SPP wavelength, field concentration and plasmon group velocity as the frequency is tuned up towards resonance. Using our cathodoluminescence plasmon microscope, we will investigate local modes in SPP planar and metallic nanostructures with the aim of achieving confinement of light at mode volumes as small as 10^{-6} $(\lambda/n)^3$, thus enabling ultrasensitive (bio-)sensing, non-linear switching, spontaneous emission enhancement and many other functionalities on a Si chip. By integrating Si quantum dots with plasmonic microstructures, we plan to fabricate an electrically pumped SPP source.
Using suitably engineered metallic nanopatterns, partly made using DNA-assisted assembly, we plan to demonstrate the world's smallest optical waveguide, and explore a novel two-dimensional sub-wavelength nanolithography concept that exploits retardation in coupled nanoparticle assemblies. We will also explore the use of colloidal metal nanoshells as nanocavities for light. By integrating our knowledge on SPPs, optically active Er ions and Si quantum dots as well as Si-based microcavities on Si, it is our goal to fabricate a true Si-based laser.

5.3 Photon Scattering

GROUP LEADER

Prof. dr A. Lagendijk

RESEARCH GOAL

We investigate highly disordered nanostructures with a spectacularly strong coupling to light. Our research goal is to observe deviations in and, ultimately, the collapse of, paradigmatic transport theory. We aim at inducing conditions in our complex media that will bring about quantum aspects of light transport. This group started at AMOLF in 2005.

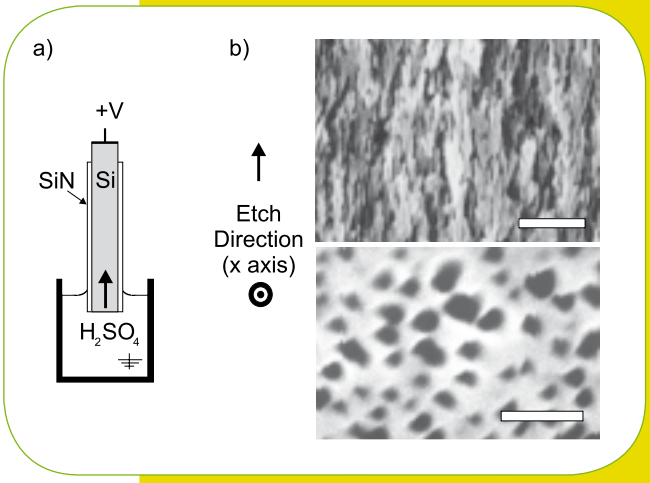
RESEARCH HIGHLIGHTS (RESEARCH CARRIED OUT AT UNIVERSITY OF AMSTERDAM AND TWENTE UNIVERSITY)

We performed the first successful experimental study ever on the propagation of quantum noise in a multiple-scattering random medium. The quantum theory of multiple light scattering is largely virgin territory, from both the theoretical and experimental point of view. Both static and dynamic scattering measurements are performed. The quantum noise observables were found to scale markedly differently, with scattering parameters compared to classical noise observables.
We predict a new spatial quantum correlation in light propagation through a multiple scattering random medium. The correlation depends on the quantum state of the light illuminating the medium, is infinite in range and dominates over mesoscopic intensity correlations.

Spatial correlations are important properties in transport theory. Usually they are inferred from far-field measurements. We observed the first near-field spatial correlations in a scattering material.

We continuously develop, generalize and extend multiple scattering theories. The general insight and progress resulting from the growing expertise underlies all our new experiments.

The ability to perform multiple scattering experiments with gain has opened up a whole new field of research, including the random laser, a combination of multiple scattering, lasing and quantum optics.
We measured laser emission in optically trapped dye-doped polystyrene microspheres and compared the results to Mie theory with gain in the sphere. We noted for the first time that Mie theory with gain produces nonphysical results above a certain gain, which we identify as the laser gain.



a) Etching setup for making Gallium Phosfide (index of refraction 3.3) samples, with the highest anisotropy in strong multiple scattering, out of wafers. Because the silicon nitride layer prevents etching at the polished surface of the wafer, pores grow from the bottom edge up.
b) SEM image of the pores. Both parallel (top image, scale bar = 1 μm) and perpendicular (bottom image, scale bar = 1 μm) cross sections with respect to the etch direction (the x axis) give a sense of the three dimensional pore structure.

On the theoretical side, we developed an exact theory for lasing dipoles. This is the first theory of lasing at a purely microscopic level. All results were compared with conventional multiple-scattering techniques.

We applied a pulsed-light interferometer to measure both the intensity and phase of light that is transmitted through a strongly scattering disordered material. From a single set of measurements, we obtained the time-resolved intensity, frequency correlations and statistical phase information simultaneously. In a detailed study, we compared a large number of independent techniques for measuring the diffusion constant for diffuse propagation of light. By comparing these independent measurements, we obtained experimental proof of the consistency of the diffusion model.

In order to arrive at the observation of light localization in the visible, we produced samples of a material that exhibited extremely anisotropic scattering. In these samples the strongest anisotropy in transport parameters ever has been observed. In addition, enhanced backscattering from these anisotropic samples was measured. The material used was a macroporous semi-conductor, gallium phosphide, in which pores are etched in a disordered position but with a preferential direction. We developed a fully anisotropic (scalar) transport theory and will, in the future, incorporate light localization.

Together with Vos's Photonic Bandgaps group, we developed new techniques for making and characterizing photonic materials. We combine, among other things, lithographic techniques, focussed ion beams and dry and wet (electrochemical) etching.

FUTURE DIRECTIONS

In many complex media, especially in the optical regime, there is a worldwide focus on local dynamic fluctuations. From fully periodic photonic crystals to completely random systems, a concentration can be found on, for instance, the (local) density of states, on account of the latter concept being introduced by us to the world of photonic crystals.

We envisage a strong focus on the quantum nature of the scattering of waves in complex media. Trying to understand decoherence plays an ever-increasing role in physics.

Our unique interferometric techniques, allowing for measuring light phase and amplitude (and their fluctuations) directly, will play a key role in observing new states of light in nanomaterials.

A major obstacle limiting the widespread application of any photonic device is the scattering of light by unavoidable variations in size and position of the crystals' building blocks. Using our theoretical and experimental expertise, we expect to be able to produce indispensable insight into this matter and may possibly come up with solutions on how to circumvent these barriers.

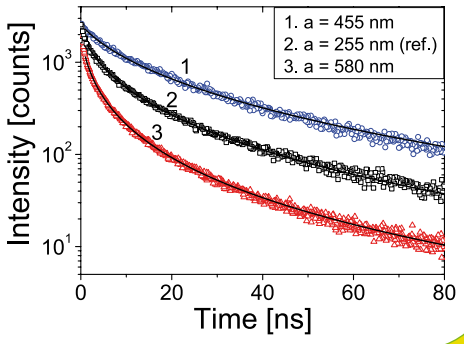
5.4 Photonic Bandgaps

GROUP LEADER
Prof. dr W.L. Vos

RESEARCH GOAL
We investigate photonic crystals, which are systems characterized by a strong interaction between light and matter. This interaction is realized with samples wherein the refractive index strongly varies periodically over length scales comparable to the wavelength of light. Ultimate control over propagation and emission of light is achieved with photonic bandgaps, a frequency range in which the density of states vanishes. This group started at AMOLF in 2005.

RESEARCH HIGHLIGHTS (RESEARCH CARRIED OUT AT UNIVERSITY OF AMSTERDAM AND TWENTE UNIVERSITY)
The *raison-d'être* for photonic crystals is their anticipated role in cavity quantum electrodynamics, in particular in the control of spontaneous emission. We obtained the first experimental evidence ever of the inhibition and enhancement of vacuum fluctuations by photonic crystals. The results were obtained by measuring spontaneous emission rates from semi-conductor quantum dots or organic dyes embedded inside the crystals. We made these observations in dynamic lifetime experiments, as well as in continuous-wave experiments. Our results verify the original prediction by Yablonovitch that started the exciting field of photonic crystals.

The spontaneous emission rate of a light source in any photonic structure depends not only on its optical frequency, but also on its spatial position. To date, the positional dependence of sources in photonic crystals



Time-resolved spontaneous emission curves from ZnSe-capped CdSe quantum dots inside titania inverse opal photonic crystals. The data were recorded at a wavelength λ = 610 nm for photonic crystals with lattice parameters a = 455 nm (1), a = 255 nm (2), and a = 580 nm (3). By varying the lattice parameter, we effectively vary the reduced frequency a/λ. The 255 nm crystal is in the long-wavelength limit and serves as a reference. Compared to the reference, the emission rate in the 455 nm crystal is inhibited due to a lower local density of states. The emission rate in the 580 nm crystal is enhanced by an increased local density of states. The decay curves deviate from single exponential decay and are well described by a distribution of decay rates (solid curves). The distribution of rates is caused by the widely pursued spatial variation of the local density of states that is probed by quantum dots at different locations in the unit cell of the photonic crystal.

remains an open question. It was therefore exhilarating when we recently obtained the first experimental evidence for the spatial variation of the emission rate.

A promising new class of light sources are semi-conductor quantum dots, which are increasingly finding applications not only in photonics but also in biology. We identified how fast such quantum dots emit light as a function of the size of the dots and their emission frequency. The results are corroborated by *ab initio* calculations.

Tremendous progress has been made in the fabrication of photonic crystals with low point and plane-defect densities. Structural variations in size and positions of the building blocks, however, are intrinsic to all photonic crystals. These deviations from perfect periodicity cause scattering of light and attenuation of coherent beams propagated by photonic crystals. We probed this light scattering using enhanced backscattering measurements for the first time on photonic crystals. We discovered a generally valid scaling relation between the attenuation of light and the magnitude of structural disorder in photonic crystals. A consequence of our analysis is that applications of large crystals, such as in proposed photonic integrated circuits, are impeded. We also managed to identify how photons that are emitted inside photonic crystals are transported to the outside world. This result is crucial to the interpretation of spontaneous emission spectra. Many such data were reported before in literature without interpretation.

We initiated original synchrotron X-ray scattering experiments to probe the structure order of photonic crystals and colloids, using, among other things, intricate correlation spectroscopy with coherent X-rays. The results demonstrate that photonic crystals made from colloids are unexpectedly well ordered.

We pioneered the development of inverse opal photonic crystals. Our seminal paper in *Science* spawned an explosion of activity, since it brought an understanding of strongly interacting photonic crystals within reach of many groups. Meanwhile, a complementary approach is being pursued using advanced industrial nanofabrication methods.

FUTURE DIRECTIONS

A new research direction is the study of point defects in 3D photonic crystals that act as tiny cavities with mode volumes much less than a wavelength cubed, so-called 'nanoboxes for light'. We are developing new techniques to produce appropriately controlled defects in self-assembled opals. Our goal is to isolate one optical mode in a nanobox and have it interact with one elementary light source, with the ultimate goal of achieving strong quantum-optical coupling.
The *raison d'être* of photonic crystals is the control of emission of internal light sources. We recently introduced efficient semi-conductor nano-crystals, or quantum dots, which allow time-resolved control of emission from inside photonic crystals. Since energy levels of such nanocrystals are quantized, the crystals can be made to behave as elementary light sources

at two levels. Our goal is to investigate the physics of quantum dots to such an extent that the dots can serve as optical probes for photonic crystals and photonic crystal cavities.
A new research direction is the ultrafast all-optical switching of photonic bandgap crystals. We recently set up a new instrument to excite charge carriers in the photonic crystal backbone. Our goal is to be able to quickly switch the photonic density of states and thereby the emission rate of embedded light sources, as well as to quickly switch cavities and thereby entrap or release photons at will.

5.5 Nanowire Photonics

PROJECT LEADER
Dr J. Gómez Rivas

RESEARCH GOAL
We study the optical emission of single semi-conductor nanowires and the interaction of light with complex nanowire structures, such as ensembles of nanowires, 2D photonic crystals and nanowire-plasmonic nanostructures. These investigations should lead to nanowires with larger internal emission efficiency and to ensembles of nanowires with larger external efficiency and controllable directionality and polarized emission for lighting and sensing applications. This group started in 2005; to achieve efficient knowledge transfer it is located at Philips Research.

RESEARCH HIGHLIGHTS
Semi-conductor nanowires have promising prospects in a broad range of technological applications. However, little is known at this time about the characteristics of light emitted by nanowires and propagation of light through ensembles of nanowires. Semi-conductor nanowires are quasi-one-dimensional structures with a large geometrical anisotropy. They are expected to exhibit an extreme optical anisotropy, i.e. polarized and directional emission, large birefringence and anysotropic scattering. Most of these phenomena are still unexplored. Without a deeper understanding of the optical anisotropy of nanowires and their emission characteristics, the development of nanowire-based optical devices with an optimum performance will be impossible. In the nine months since the initiation of the group, we demonstrated:

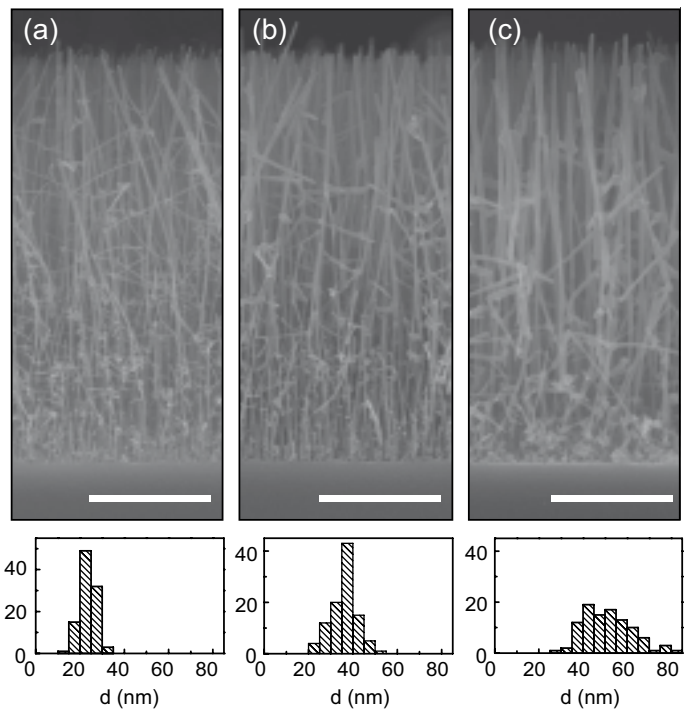
- synthesis of high-density samples of GaP nanowires by deposition of thin films of gold. We investigated the influence of film thickness on the average wire diameter and on wire density. High-density samples are important for applications in which the optical response of a large ensemble is relevant.
- large form-birefringence in ensembles of nanowires.
- state-of-the-art fabrication of bow-tie nano-antennae by e-beam lithography and their characterization using dark-field spectroscopic imaging.
- Enhancement of the photoluminescence of dye molecules close to bow-tie nano-antennae.

FUTURE DIRECTIONS

We will study the emission and scattering of light by individual semiconductor (InP, GaAs, GaP, GaN, ZnO) nanowires and by ensembles of nanowires with different wire radius, length and volume fraction. We will investigate the radiative and non-radiative characteristics and the light emission and scattering, using (micro-) photoluminescence spectroscopy, near-field spectroscopy, cathodoluminescence spectroscopy and angle-resolved transmission and reflection.

Our investigations should lead to single nanowires with optimized internal emission efficiency and to ensembles of nanowires with large external emission efficiency and controlled directionality and polarization emission. To further optimize the emission characteristics of nanowire LEDs, we will embed them in two- and three-dimensional photonic crystals, in which the emission rate can be decreased at certain frequencies (photonic stop gap) and enhanced at others (Purcell effect). We will also investigate the possibility of optimizing emission characteristics of nanowires by coupling them to plasmonic nanostructures.

The large surface-to-volume ratio of nanowires and the strong sensitivity of their optical properties to the surroundings encourage the use of nanowires as sensors. Based on our investigations of the emission and scattering characteristics of nanowires, we will define new concepts for sensitive optical (bio-)sensing.



Scanning electron microscope side view images of epitaxially grown GaP nanowire arrays for (a) 40s, (b) 200s, and (c) 300s diameter growth time. Scale bars correspond to 1 μm. Histograms of the wire diameters are displayed at the bottom of the images. The average wire diameter is proportional to the growth time.

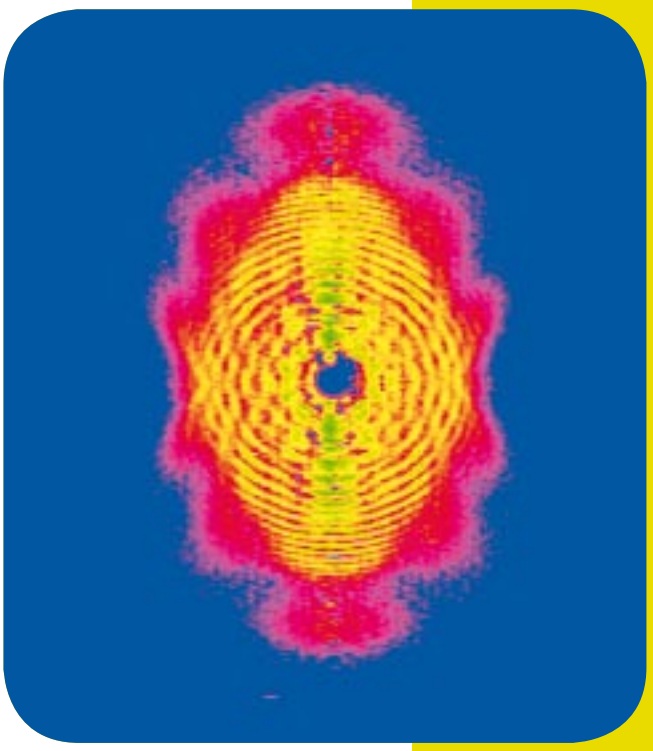
6 Exploratory and Transition Programme

6.1 Extreme-Ultraviolet (XUV) Physics

GROUP LEADER
Prof. dr ir M.J.J. Vrakking

RESEARCH GOAL
Our group studies how intense, shaped, femtosecond laser pulses can be used to control the properties of atoms, molecules and clusters. Our main focus is on time-resolved electron dynamics in atomic and molecular physics using recently developed attosecond laser pulses based on high-harmonic generation.

RESEARCH HIGHLIGHTS
The main themes of our research during the past six years have been coherent control of atomic and molecular properties and the generation, characterization and application of high harmonic radiation, particularly in the time domain, where this technique provides a means to generate attosecond laser pulses. A constant theme throughout this work, which links to many of the projects we have completed, is the response of



2D velocity map photo-electron image for the ionization of Xe atoms by an intense 6 fs long Ti:Sapphire laser pulse. The image represents a cut through the 3D velocity and angular distribution that is obtained by applying an inverse Abel transform to an experimentally obtained 2D momentum map. The image shows a number of concentric rings, that are indicative of the number of photons involved in the ionization process, as well as interferences that are thought to be due to the way that the laser accelerates the electrons after ionization has taken place.

electrons to strong (time-varying) electric fields. Our main research highlights during the past five years have been:

1 The first observation of field-free molecular alignment following impulsive excitation by an intense laser pulse: we demonstrated that excitation of molecules with an intense, short (compared to the rotational period of the molecule) laser pulse leads to the excitation of a rotational wave packet that transiently aligns itself along the laser polarization axis after the laser has been turned off. We subsequently embarked on an effort to apply optimal control techniques to this problem and have developed a technique for single-shot characterization of molecular alignment.

2 The first observation of semiclassical interferences in photoelectron imaging near an ionization threshold: we observed how electron wave packets produced during an ionization event interfere constructively or destructively, depending on the quantum mechanical pathlength difference between the associated trajectories. In related work, we observed a nondipolar photoelectron emission that displays a strong asymmetry along the propagation axis of the laser.

3 The first characterization of attosecond laser pulses using angle-resolved photoelectron spectroscopy: we demonstrated that in a RABBITT (Reconstruction of Attosecond Beats By Interfering Two-photon Transitions) experiment, attosecond pulses can be characterized on the basis of both the energy spectrum and the angular distribution of the photoelectrons. This is important for the characterization of isolated attosecond pulses.

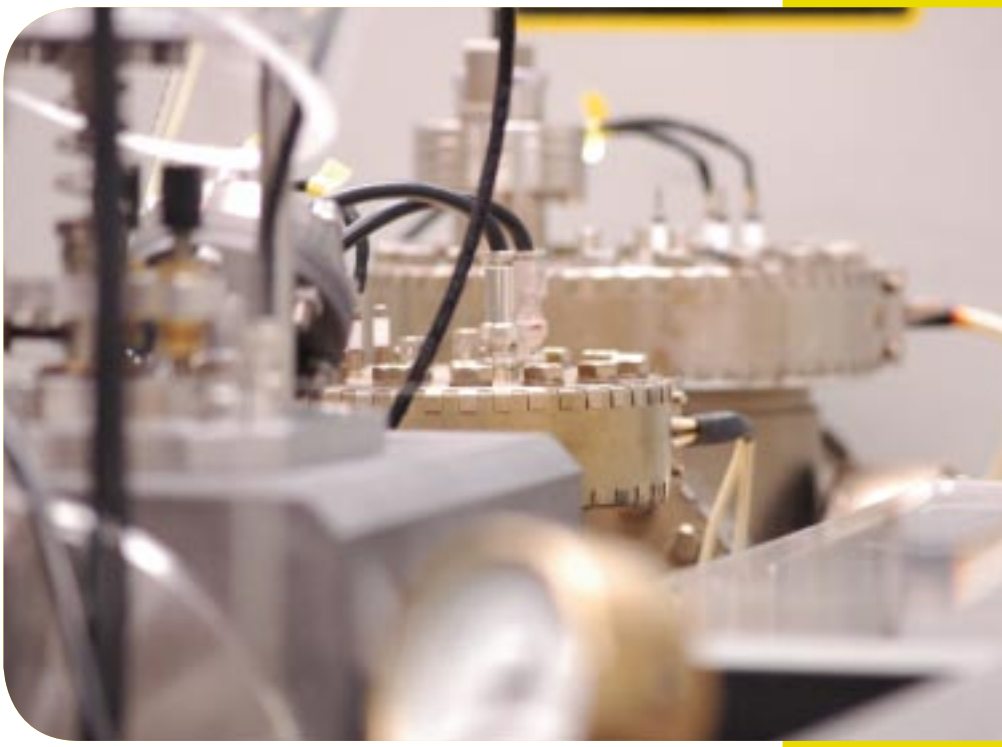
4 The first application of attosecond pulse trains to studies of atomic and molecular dynamics (with L'Huillier, University of Lund): we have performed a two-colour XUV+IR ionization experiment, that – depending on the time delay between the XUV and the IR pulses – provides information on the laser pulses and the momentum space electronic wavefunction.

5 The first observation of a carrier-envelope phase dependence to control a molecular dissociation (with Krausz, Max-Planck Institut für Quanten-optik in Garching): we demonstrated that the localization of an electron in the dissociative ionization of hydrogen molecules can be controlled using the carrier-envelope phase. This is the first demonstration of carrier-phase control in molecules. Prior to this measurement, we performed experiments on carrier-phase control in the radio-frequency ionization of high Rydberg states.

6 The first application of optimal control techniques to control the explosion of large clusters irradiated by intense femtosecond laser pulses: we experimentally observed and numerically confirmed that the cluster explosions are optimized by sequences of pulses that exploit the occurrence of enhanced ionization and/or plasma resonances in the cluster.

FUTURE DIRECTIONS

In the coming years our research will focus on the study of the motion of electrons in atoms and molecules, using laser pulses with a duration of several hundred attoseconds. In strong laser fields, we will induce electron motion using an intense infrared laser, and investigate the motion of bound electrons (in molecules undergoing dynamic alignment) and continuum electrons (in molecules undergoing ionization). Next, we plan to study photo-absorption processes in weak laser fields, where we will probe how the electronic excitation couples to other degrees of freedom, i.e., other electrons, and the rotational and vibrational degrees of the nuclei. We plan to study electron transfer and dissociation in large molecules, as well as the excitation and decay of giant plasmon resonances in clusters and large molecules such as C_{60}. As experimental tools, we intend to use techniques for measuring the emission of electrons with both angular and kinetic energy resolution, including fully coincident ion and electron detection schemes. This work will provide a deeper insight into the motions of electrons in molecules and pave the way for the exploitation of attosecond laser pulses in physics, chemistry and photobiology.



6.2 Molecular Painting Research

GROUP LEADER
Prof. dr J.J. Boon

RESEARCH GOAL
The aim of this group is to study the build-up, structure and composition of paint and paint materials in Old Master paintings in a historical perspective, with a special focus on the molecular aspects of ageing paints and the reactivity of their pigments and binding media.

RESEARCH HIGHLIGHTS
The material history of paintings is frozen in the paint layers. Over the centuries, paints undergo a slow but steady chemical change caused by inadequacies in the material used and environmental effects. The molecular orientation of our research approach, using mass spectrometry and advanced chemical microscopy, has revolutionized the field of art-technical studies of paintings and conservation. Intimate collaboration with the Royal Picture Gallery the Mauritshuis, through an Open Laboratory agreement with AMOLF, made it possible to work on paintings by Rembrandt, Rubens, Vermeer and other famous Dutch masters. A joint project with the Van Gogh Museum in Amsterdam is developing new methods for the quantitative comparison of paint layers in Van Gogh paintings, using element and molecular maps obtained by Secondary Ion Mass Spectrometry (SIMS), in combination with image-analysing

The grey brush strokes on the painting are discoloured highlights where the vermilion (HgS) has changed by chlorine induced photoinduced reactions into elemental mercury nanoparticles (black) and mercury chloride (white). SIMS detects the chloride in the intact vermilion which is a precondition for this chemical change. The sulfidic sulfur is dimishing as the photo-oxidation progresses in the blackened areas.

techniques to study the texture of the paints and grounds. The group has played a pivotal role in the fully integrated paint-analytical studies of an ensemble of 43 paintings in the Oranjezaal of the Royal Palace Huis ten Bosch in The Hague, a 17th-century art-historical icon of great significance.

Our ability to determine binding medium composition with good lateral resolution through SIMS is novel to the field and unique at present. Innovative improvements in the preparation of embedded cross-sections have led to new and spectacular results on the interaction between binding media and pigments. Through the correlation of data from the imaging analytical tools of imaging light microscopy, imaging FTIR microscopy, imaging SIMS for molecular mapping and scanning electron microscopy linked with energy-dispersive X-ray analytical mapping, it has been possible to reconstruct the materials used and their ageing history. As a consequence, we discovered a serious deterioration phenomenon in numerous paintings dating from the 16th to the 20th centuries, in which metal soap aggregates develop into lead- and zinc-containing paint layers that protrude through the surface of the painting. Our studies of oil paint and metal soaps have cast new light on the composition of oil paints in ageing paintings. The fundamental changes that take place – a viscous medium that develops through the oxidation of plant oils in the early stages of the drying of the paint into a fully hydrolyzed paint over the course of a century – appeared to be a recipe for complete disaster. Fortunately, a self-repair mechanism exists in the paint that employs the omnipresent lead ions to bind the released free acid groups to create a metal-coordinated network of high stability. This scenario not only explains the oil paints' stability, but also its defects in such phenomena as blooming, efflorescence, dissolution of lead white pigments by free acids, metal soap aggregation, protrusion and extrusion. Our studies have contributed significantly to the recognition of metal soap-related oil paint defects that are now estimated to affect at least 100,000 paintings worldwide, posing new challenges for conservation.
Imaging studies of the spatial distribution of the organic binding media and pigments in paint cross-sections have also increased awareness of the chemical reactivity of many pigments in oil paints. Our approach of imaging paint layers, using complementary microscopic-spectroscopic and microscopic-mass spectrometric techniques, is seen as novel in the analytical chemistry of paintings. Our studies on the lead-catalysed bleaching of bone black, the destabilization of CdS pigments by zinc, the discoloration of the blue cobalt glass pigment smalt, the light-induced destabilization of vermilion by chlorides that change the bandgap in HgS and the reactivity of lead-tin yellow paints towards free fatty acids, are prime examples.

FUTURE DEVELOPMENTS

The Molecular Painting Research programme will be discontinued at AMOLF. A new home is presently being sought for the acquired expertise that will be closely linked to museums in and outside the Netherlands. Boon is exploring a new research direction that focuses on biologically guided mineralisation in animals, using his expertise in chemical and electron microscopy and organic mass spectrometry.

6.3 Order/Disorder in Soft Matter

GROUP LEADER
Prof. dr ir W.H. de Jeu

RESEARCH GOAL
The research of the Order/Disorder in Soft Matter group focuses on the study and control of the ordering of soft materials, especially – but not only – at surfaces. X-ray methods (in-house and at synchrotrons) complemented by optical and atomic force microscopy are used to investigate nanostructures in (bio-)block co-polymer films, ordering and crystallisation of polymers under shear and low-dimensional order and disorder in smectic elastomers.

RESEARCH HIGHLIGHTS
To direct the self-organization of block copolymer films into nanostructures, a second ordering principle was introduced by taking comb-shaped smectic liquid crystalline polymers as one of the blocks. X-ray reflectivity of thin films of a material with a cylindrical morphology (with the smectic polymer as majority compound) indicated smectic layers parallel to the substrate. No evidence of the block period was seen. This points to cylinders perpendicular to the substrate and (see figure) still orthogonal to the smectic layers as observed in the bulk. This structure has been confirmed by grazing-incidence small-angle X-ray diffraction at ESRF. However, the observed liquid-like peak indicates that the cylinder ordering is not long range. Selective etching can give structures of either nanoholes or nanopillars with diameters of around 20 nm.

An apparatus for small-angle x-ray scattering (SAXS) with a two-dimensional detector, extended with facilities for access at wider angles (WAXS), enables simultaneous time-dependent SAXS/WAXS measurements at 30 s/frame. These results are augmented by measurements at synchrotron sources. Present work focuses on the role of nucleation agents both at quiescent and shear-induced crystallization of isotactic polypropylene (iPP). Though it is well known that in this way the speed of polymer crystallization can be enhanced, the underlying mechanisms are still poorly understood. Some first results confirm for pure iPP a clear effect of shear on the crystallization. Addition of an isotropic nucleation agent increases the speed of crystallization strongly, but now the effect of additional effect of shear is minor. These experiments are being extended to anisotropic nucleation agents (needle-like and platelets) that behave qualitatively different.

Smectic liquid crystals consist of stacks of liquid layers, formed by elongated molecules with their long axis perpendicular to the layers. In these low-dimensional systems, the layer fluctuations increase with system size, preventing the formation of long-range order (Landau-Peierls instability).

This behaviour is well established for smectic monomer systems and for

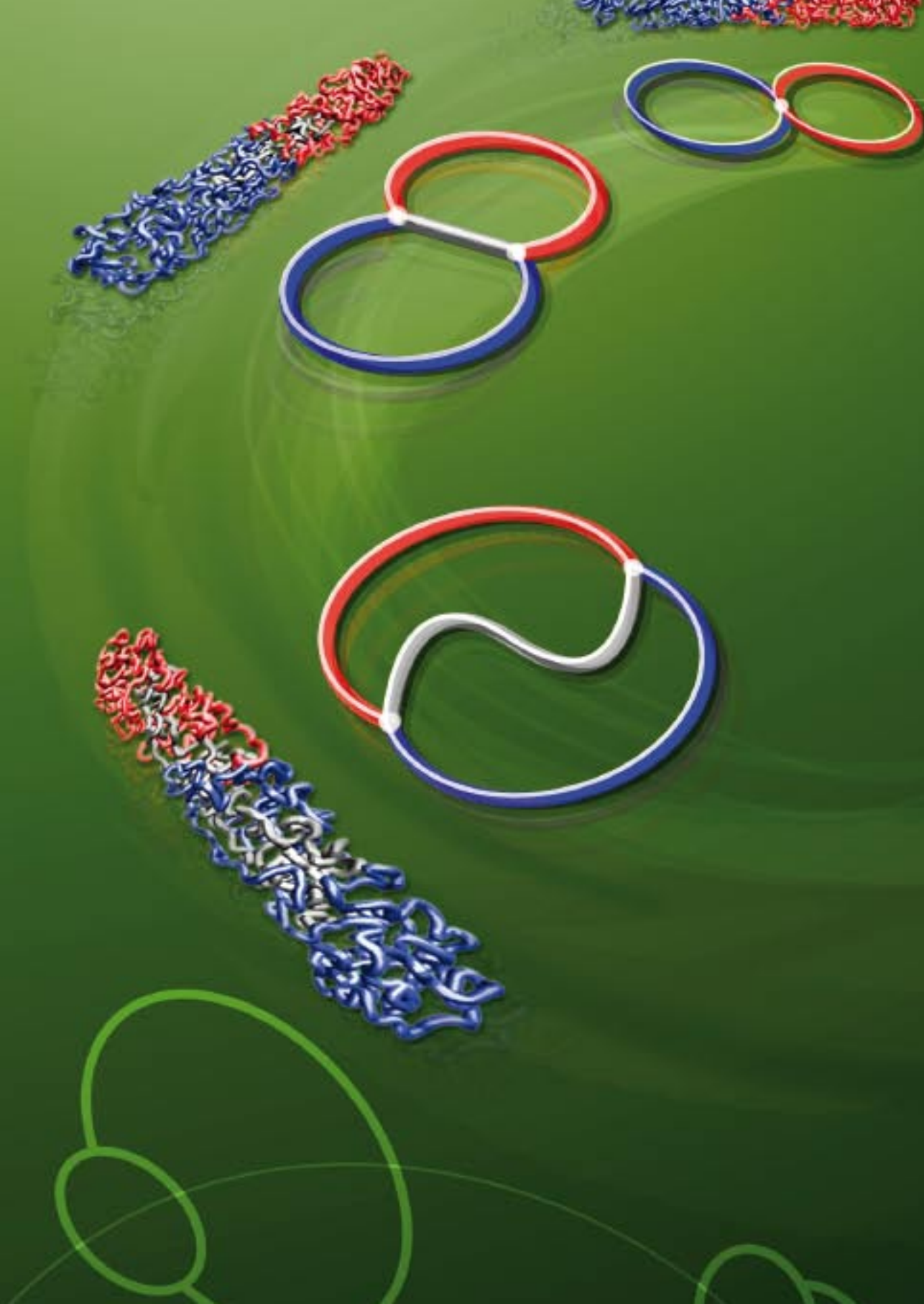
side-chain smectic polymers. If the polymer chain is crosslinked to form an elastomer, the macroscopic rubber elasticity introduced via the percolating network interacts with the smectic ordering field. We used high-resolution X-ray scattering to determine the positional correlations with increasing crosslink density. The quasi-longrange order survives in domains of decreasing size up to a relatively large concentration of about 15%. However, at a density of 20%, the random field of the crosslinks destroys the smectic density wave. This is signalled by a Lorentzian lineshape typical of short-range correlations. These results challenge existing theories of disorder associated with random fields that disorder occurs with very small distortions.

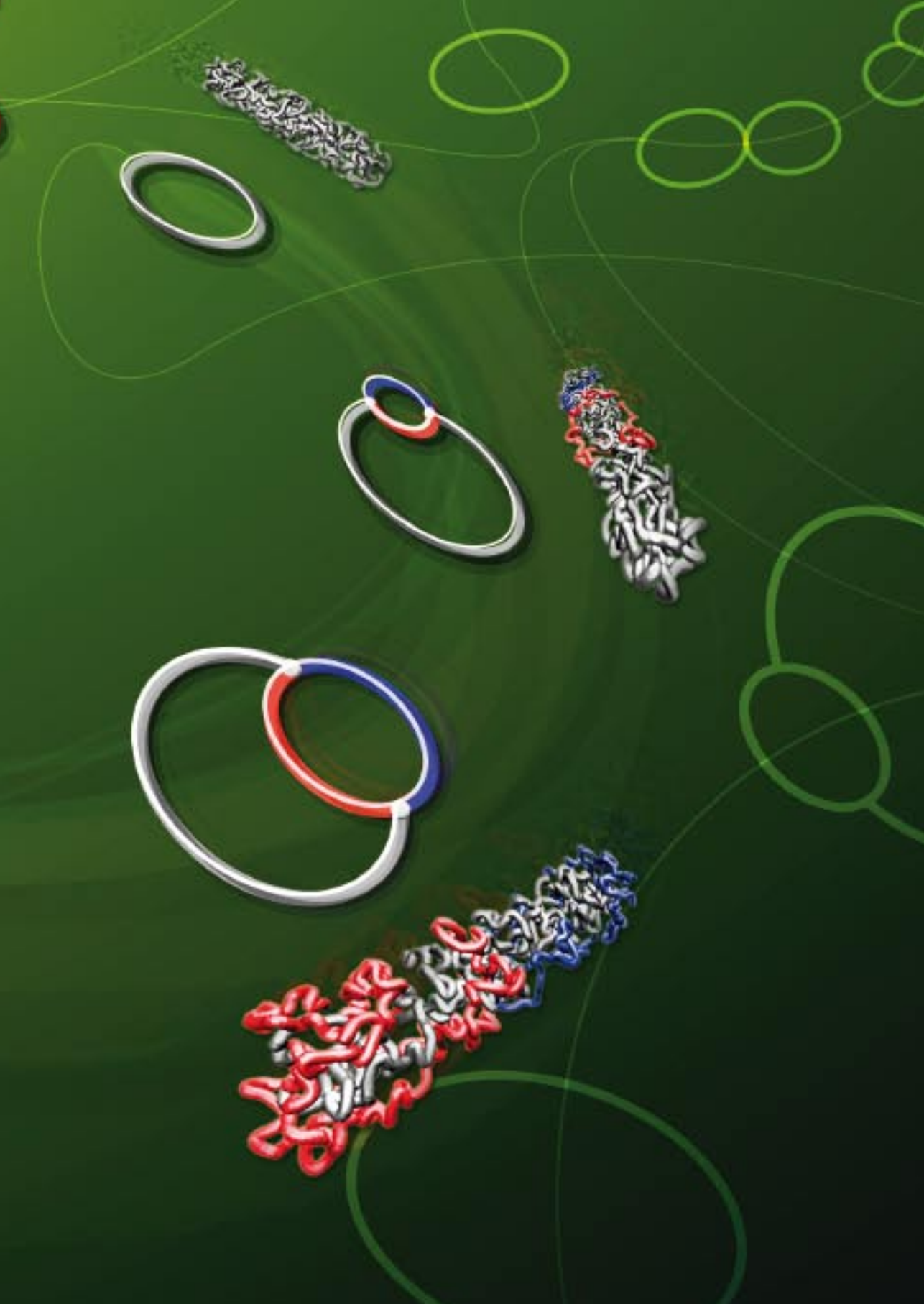
FUTURE DIRECTIONS

The group will concentrate on the following subjects:

- Nanostructuring thin polymer films is being extended to block copolymers incorporating biofunctional elements. This allows the creation of new self-assembling stimuli-responsive surfaces, with a high level of control over the lateral spatial arrangement of the active peptide or protein compound.
- The exciting results obtained during the past year made us decide to continue investigating order and disorder in smectic elastomers (in cooperation with the Macromolecular Chemistry group, Freiburg).
- The work on flow-induced crystallisation in isotatactic polypropylene will be continued in cooperation with Sabic Europe and Borealis. This research is financed by the Dutch Polymer Institute at the Eindhoven University of Technology.

AFM image of a thin diblock copolymer film with one block as cylinders oriented perpendicular to the substrate. (a) AFM phase image, (b) model, (c) grazing-incidence small-angle x-ray peak showing that the cylinders penetrate through the whole film.





7 Support Groups
Technical support

7.1 Amsterdam nanoCenter - soft-bio-nano-facility

PROF. DR L. KUIPERS

The Amsterdam *nano*Center is a modern facility for nanofabrication and nanocharacterization using a combination of techniques, operated by AMOLF. It includes a cleanroom, a thin-film deposition laboratory, and innovative tools for nanofabrication, manipulation and analysis. It serves as a user facility for users from inside and outside Amsterdam.

The *nano*Center cleanroom (total area 57 m^2) houses an electron beam pattern generator, mask aligner for optical lithography, resist processing equipment, a reactive ion-etching system, dual-beam focussed ion beam system, chemical benches for organic and inorganic processes, a profilometer and an inspection microscope. A rapid thermal annealing system and tube furnace are available for annealing. Evaporation tools include sputtering and electron-beam evaporation. A high-resolution scanning electron microscope is equipped with energy-dispersive X-ray spectroscopy, electron backscatter imaging, and cathodoluminescence spectroscopy. Rutherford backscattering spectrometry, spectroscopic ellipsometry, atomic force microscopy as well as optical tweezers for nanopatterning are also available.

7.2 Design Office

I. CERJAK

The Design Office supplies the scientific groups with mechanical designs of scientific equipment, advice on mechanical construction, and engineering solutions for analysis of mechanical problems. In some cases, commercially acquired equipment is modified or redesigned so that it suits the needs of the research programme.

Using specialized software packages, the physical properties of these designs, such as the mechanical and thermal response, can be tested before they are actually produced. The computer system employed by the design office allows some of the designs to be directly translated into a control code that can drive computerized machining tools available at the Mechanical Workshop.

7.3 Mechanical Workshop

W.H. BROUWER

The Mechanical Workshop group is responsible for building all of the state-of-the-art experimental equipment used at AMOLF. In close collaboration with the Design office, mechanical designs are realized using a variety of techniques such as diamond cutting, vacuum brazing and conventional and electron-beam welding. Computer-controlled equipment enables Computer Aided Design (CAD) drawings to be efficiently translated into machined components. These encompass standard milling machines and wire as well as microelectrical discharge machines that allow, e.g., holes with diameters of several micrometers to be made.

The Mechanical Workshop also serves as a training site for apprentices and graduates from mechanical engineering schools, helping them prepare for further careers in an environment where a steady stream of unique and challenging mechanical designs have to be produced to high specifications.

7.4 Electronics and Informatics

ING. C.B. OKHUIJSEN

The main task of the Electronics and Informatics (E&I) group is to design, build, maintain and support the electronic components, and increasingly, the software of the experimental set-ups in the lab. This requires a variety of skills ranging from computerized printboard design to software engineering in e.g. C++ or LabView. The group handles a mixture of high-urgency, short-term jobs and complex long-term projects.

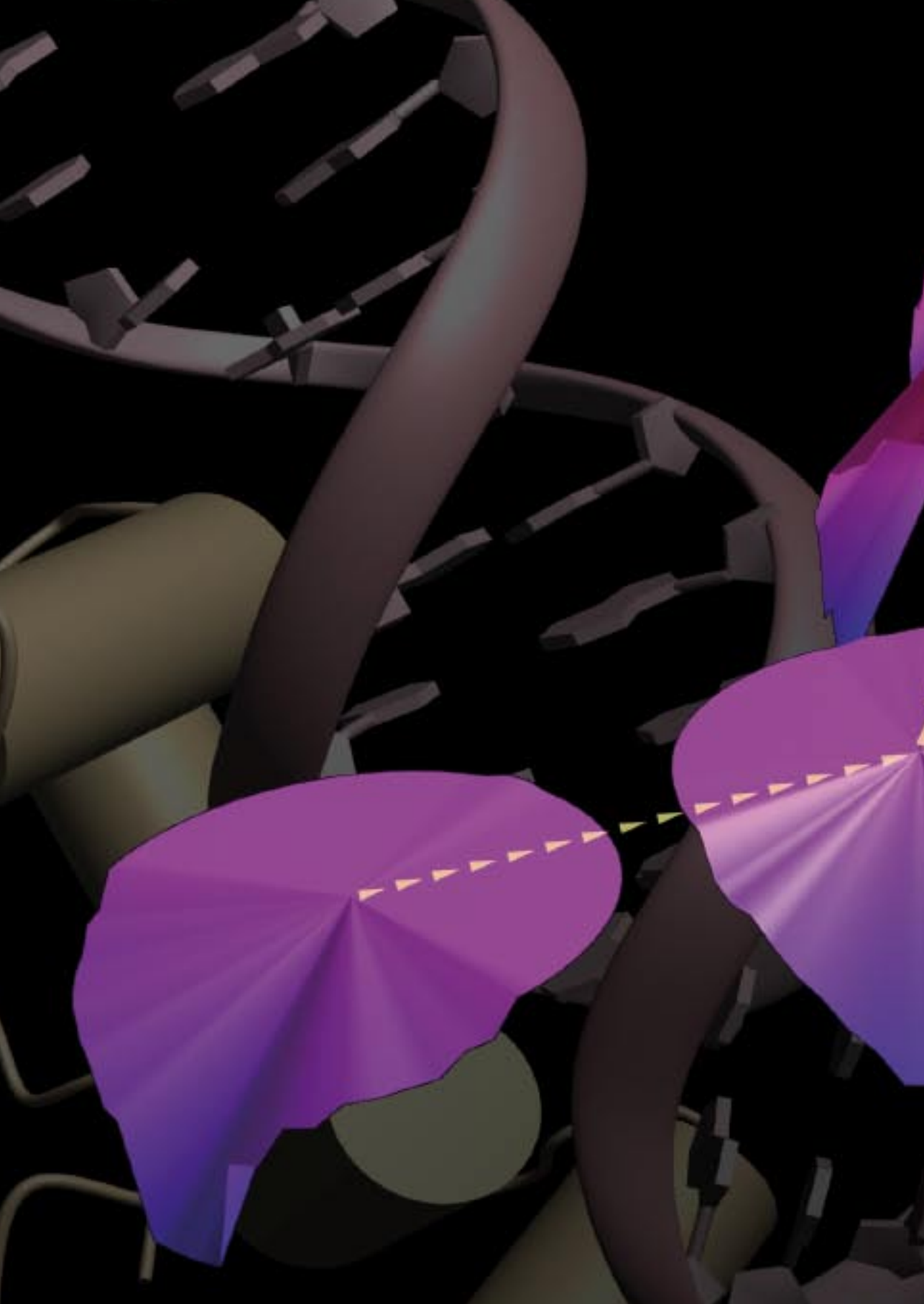
A webbased procedure is used to streamline the workflow, and providing the researchers with up-to-date insight into the progress of their projects.

E&I are also responsible for the computer infrastructure at AMOLF. This involves supporting a large number of PCs, workstations and specialized servers as well as the extensive network connecting them.

7.5 Facility Management

ING. H.H. KERSTEN

Four groups are involved with the care of the laboratory facilities:
The *Technical Services* group maintains the physical plant. An important task for this group is to prepare and install the necessary cables and wiring for new experiments and to provide security services for the physical plant.
The *Building Maintenance and Custodial Services* group is responsible for the cleaning and maintenance of the rooms and building and management of the cafeteria. A special task for the leader of the Custodial Services group is to allocate rooms to AMOLF employees.
The *Purchasing* group orders and receives goods and manages the stock. There are about 1,800 different items in stock, ranging from bolts and pencils to lecture bottles and connectors.
The *Occupational Health and Safety* group is responsible for safety at AMOLF and for taking all necessary measures to ensure healthy working conditions. AMOLF has an automatic fire alarm system as well as an emergency team of about 19 people trained in first aid, fire extinguishing, evacuation and accident prevention.



8 Support Groups
Administration

Visitors at the yearly organised open day

8.1 Financial administration

J. STIEL

The financial administration is responsible for arranging the financial aspects of ordering goods, checking invoices and charging the appropriate budgets. With the increasing number of externally funded projects, financial project adminstration has become an important task of this group as well. The financial administration provides regular reports to management and scientific group leaders.

8.2 Personnel management

W.C. HARMSEN

AMOLF is an institute with PhD students and postdocs coming from all over the world. Therefore, in addition to "conventional" human resource management, much time is involved in arranging the necessary paperwork for the foreign newcomers and, where necessary, in assisting them through the required legal procedures. Every year, some 50-80 new employees join AMOLF, and a similar number leave AMOLF.

8.3 Travel and housing

R. VAN WIJK

Assisting our constantly changing group of foreign guests in finding accommodation in Amsterdam requires much time and ingenuity. The travel & housing officer at AMOLF arranges housing for most of our foreign employees and guests at approximately 90 addresses, ranging from rooms/studios to family apartments. Most of the apartments are close to AMOLF, making it easy to commute by bicycle or public transport. Short-term visitors often stay at AMOLF's guest residence adjacent to the institute.

8.4 Secretariat, reception

DRS E. LAMMERS

The secretariat is responsible for providing management support to the AMOLF director and department heads, as well as for personnel management and public relations. In addition, it handles all regular electronic mail, manages agendas and helps organise national and international workshops.
The receptionists are responsible for telephone calls, incoming mail, faxes and attendance records.

8.5 Information Services

G. JOSEPH

The Library and Information Services group is responsible for library services, maintenance of the AMOLF website and developing databases. The librarians are specialized in providing the scientists with appropriate information in the form of books, journals and international databases, and through contacts with other libraries.

Job opportunities at AMOLF

Every year AMOLF welcomes some 50-80 new employees in all of the research and support groups. Details of the application procedure can be found on the homepage www.amolf.nl.
All vacancies are advertised on the “vacancies” section of AMOLF’s website.

PROJECT LEADERS (1-2 PER YEAR)
Every year, AMOLF hires one or two young scientist to start a new, independent, research group. These project leaders are hired for a 5-year period with the possibility of tenure afterwards.

POSTDOCS (~10 PER YEAR)
Postdoctoral fellows typically make a transition from running an individual research project (as PhD students) towards running (part of) a group. At AMOLF, postdocs carry out a well-defined project, with many opportunities for aquiring a more independent research attitude.

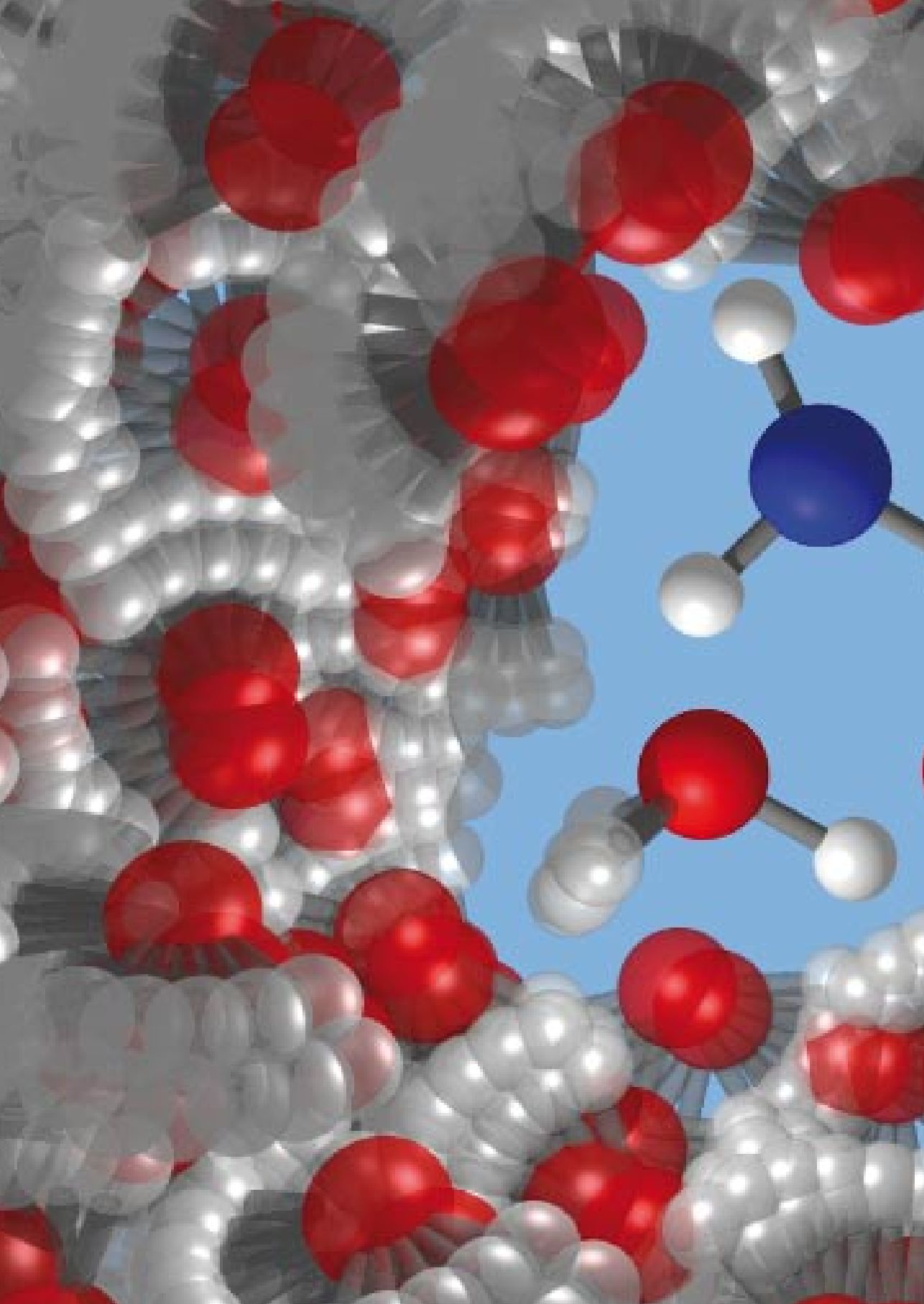
PHD STUDENTS (~10 PER YEAR)
AMOLF welcomes Dutch and international students to enroll in a PhD programme that takes about 4 years. The graduation examination takes place at one of the Dutch universities. Each student has a well-defined research programme that is part of the research programme of the group. Interactions with other members of the department are an essential part of all research projects, and are further stimulated during combined work discussions. The PhD training programme includes specialized courses on presentation skills, project planning, English writing and project management. Visits to (inter-)national conferences and collaborations or exchange visits with international partners are a regular ingredient of a PhD programme at AMOLF.

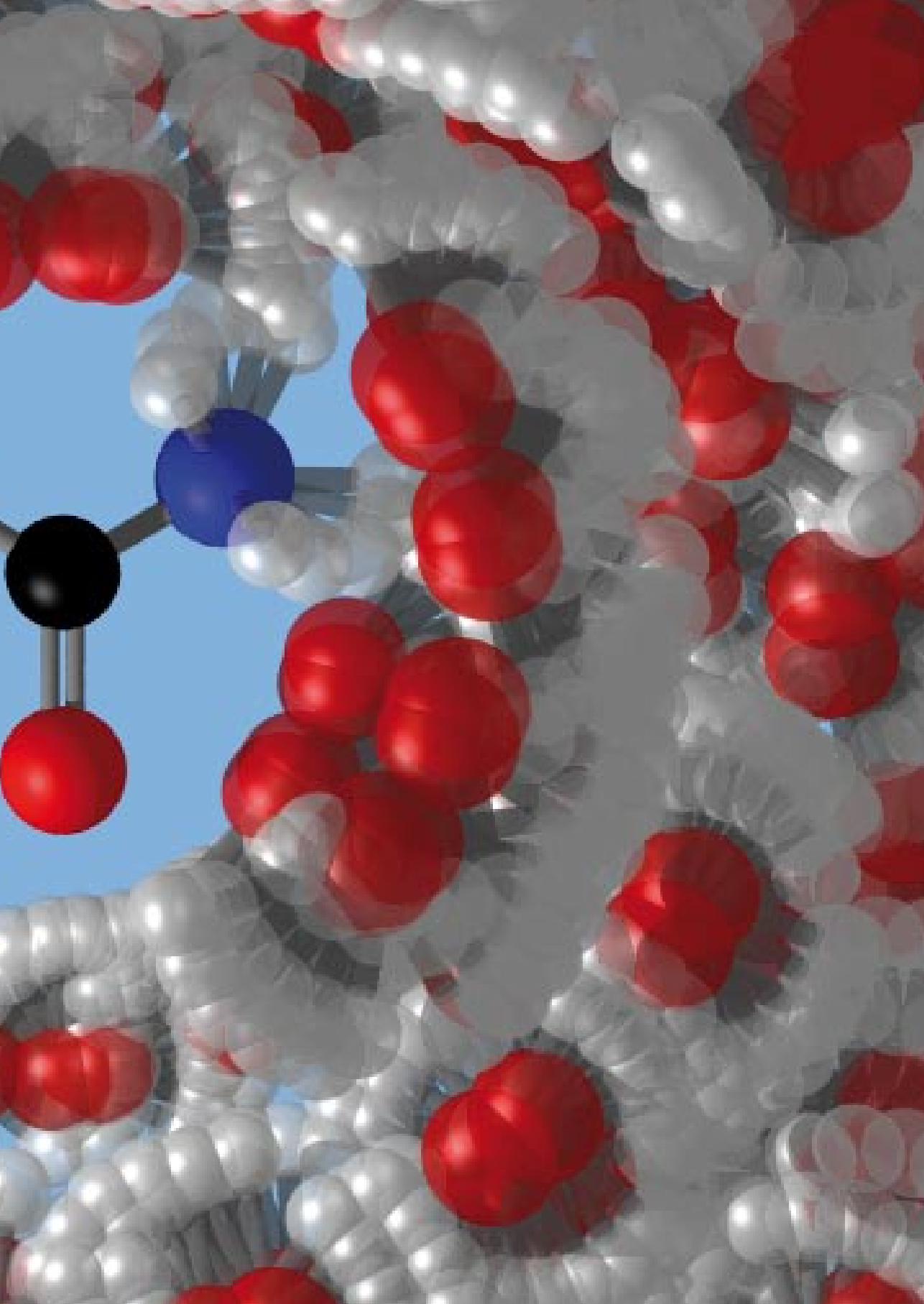
MASTER STUDENTS (~5 PER YEAR)
Master students can do a (part-time) internship (*afstudeerstage*) in one of the research groups at AMOLF. Students have their own research project, the results of which are presented in a publication or internal report. A PhD student or a postdoc gives daily supervision. An internship contract arranges remuneration and working hours.

SCIENTIFIC GUESTS (~20 PER YEAR)
AMOLF welcomes a large number of guests from all over the world, visiting AMOLF for periods ranging from a few weeks to a year.

TECHNICAL SPECIALISTS (~5 PER YEAR)
Students from technical eduction institutions can find a traineeship in AMOLF's technical support groups. Technical specialists that have graduated are regularly hired on a project basis.

Upon completing their training at AMOLF, junior researchers and technical specialists find jobs in a wide range of organisations. PhD students most often pursue a career in either industry (55%) or academia (40%); postdocs too go into academa (60%) or industry (30%). Technical staff that finish training at AMOLF nearly all move into industry. AMOLF has a network of alumni that assists AMOLF researchers in taking the next step in their careers.





How to get to AMOLF

FROM SCHIPHOL AIRPORT

1. Take a train to Amsterdam Central station (approximate costs: € 4,-), and then follow **public transport** instructions below.
2. Take a train to Amsterdam Central station, and then take a **taxi**. Approximate costs: € 20,-
3. Take a taxi from the airport. Approximate costs: € 45,-

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1098 SJ Amsterdam
Tel: +31 (0)20-6081234
Fax: +31 (0)20-6684106
e-mail: secr@amolf.nl
www.amolf.nl

Below: current building, new building ready in 2008 (see page 2)

PUBLIC TRANSPORT

1. From Amsterdam-Central railway station: Take the train to either Amsterdam-Amstel or Muiderpoort station, from there see 2 or 3 respectively. To Amsterdam-Amstel station you can take the 'metro' (subway) too.
Alternative: take tram 9 to the corner of Middenweg and Kruislaan and take bus 40 at this crossing or walk about 1 km along Kruislaan (initially in direction 'Jaap Edenbaan'). After passing through the railway tunnel, AMOLF is on the left hand side.
2. From Amsterdam-Amstel railway station: Take bus 40 to Muiderpoort station. This bus departs from the bus platform in front of the station. On Kruislaan, get off at the second stop after going through the railroad tunnel.
3. From Amsterdam-Muiderpoort railway station: Take bus 40 to Amsterdam-Amstel station. This bus departs from the Muiderpoort bus station. On Kruislaan, get off at the second stop.

BY CAR

All motorways to Amsterdam lead to the **A10 ring road**. Take exit **S113/ Watergraafsmeer**, and head for "**Science Park**". After 2 km, **turn right** onto the **Kruislaan**, following the sign '**Science Park**'. After passing through the railway tunnel AMOLF is on your left hand side.