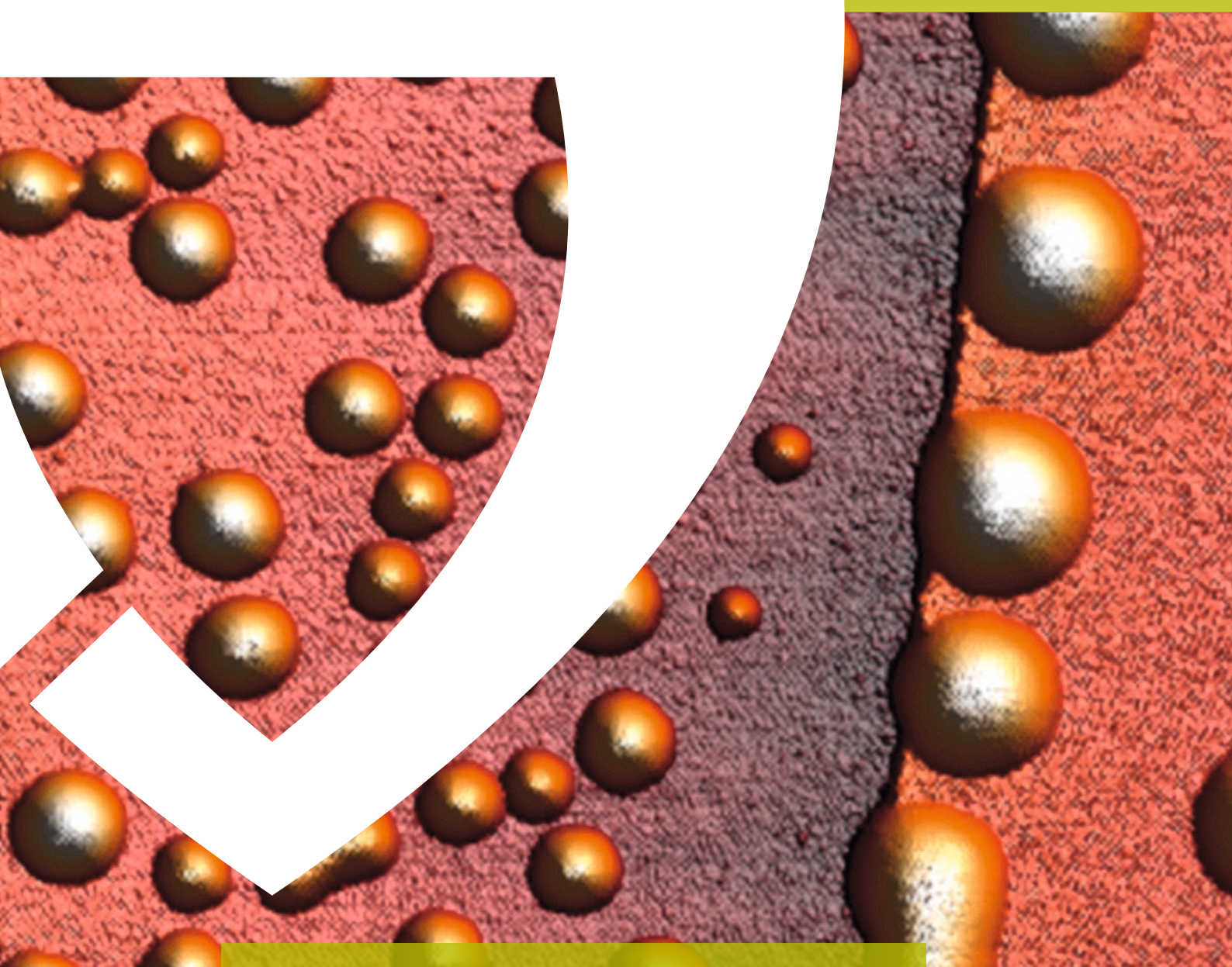




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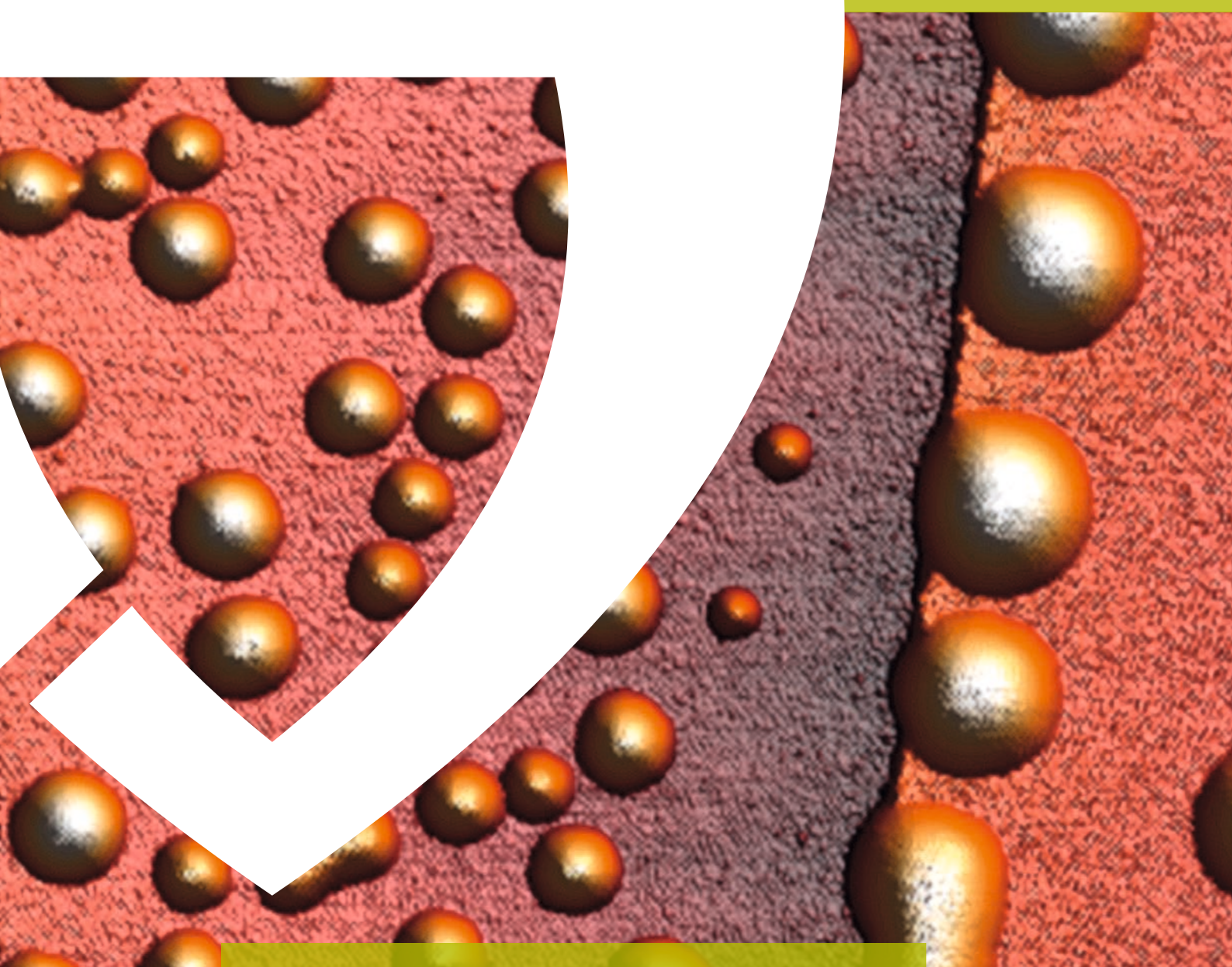
School of Engineering and Science

# Nanomolecular Science

Graduate Program



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# 1 Nanomolecular Science at Jacobs University

## 1.1 Concept

### 1.1.1 What is Nanomolecular Science

The physical sciences have reached a state that enables us, at least in principle, to build objects at the ultimate level of finesse, one atom or molecule at a time, with ultimate precision. At the nanometer length scale, the traditional sciences of physics, chemistry and biology lose their distinctiveness and merge into a new transdisciplinary science, commonly known as "Nanoscience" and its concomitant technology. In this new scientific endeavour, each of the traditional sciences has an invaluable contribution to make. Given the scope of Nanoscience and Nanotechnology, it is not surprising that they hold answers to our most pressing material and technological needs. For example, advanced organic solar cells based on new functional materials, fuel cells incorporating nano-catalysts and novel hydrogen storage systems based on molecularly engineered materials could help solve our energy problems in a sustainable way. Wires, transistors, and storage media of the size of single molecules will introduce a paradigm shift in information technology. The construction of molecular shuttles, rotors and wheels realizes mechanical tools at the nanoscopic level, while the design of molecular barrels, cups, chains and knots transfers macroscopic objects to the nanoscale. Molecular medicine is looking for ultrasmall and less invasive detection techniques in diagnostics and delivering systems employing nanocontainers to advance progress and treatment of diseases. These are just a few examples of how (molecular) nanotechnology can transform our future.

### 1.1.2 Nanomolecular Science at Jacobs University: A Broad-based Education in a Technology of the Future

Nanomolecular Science is highly transdisciplinary. Physics has developed novel observation and manipulation tools for single atoms and molecules and provides quantum physics as the fundamental science of the small. *Chemistry* as the science of molecules reveals the functional, conformational and structural relationship within and between molecules; it can nowadays design molecules and supramolecular assemblies with unprecedented complexity. Research in *biology* is currently revealing the toolbox of real-life molecular machinery and teaches us how nanosized objects can be self-assembled into complex systems in which dynamic nanomolecular functions like signalling, catalysis, transport, and locomotion can be realized in a controlled way. Finally, *materials science* converts the nanoscale properties of components into macroscopic materials with entirely novel properties and functionalities.

The Graduate Program in Nanomolecular Science at Jacobs University reflects the need for transdisciplinary training. Faculty from the physical, chemical and biological sciences provide lectures and lab classes in the nano-related aspects of their fields. The education covers different classes of nanomaterials, different synthesis and characterization methods, various theoretical and computational approaches as well as application areas of nanomaterials. The course work provides interdisciplinary breadth to the degree granted. The M.Sc. or Ph.D. thesis allows for the in-depth study of a particular topical research area in the lab of the participating faculty. Thus participants emerge from the program with a versatile background in Nanomolecular Science, as well as with the ability to perform independent research in a results-oriented approach.

### 1.1.3 Prospects for Graduates/Career Options

Nanomolecular Science is inherently cross-disciplinary, probably more so than many other areas of research. It has an impact on a very broad range of industries and technologies, including the chemical, pharmaceutical, semiconductor and computer industries and biotechnology as well as environmental, energy, information, materials and medical technologies.

In most of these fields, the introduction and application of nanoscale science requires novel, specialized technology and instrumentation, often developed by small innovative companies. As a consequence, a host of new employers is emerging, in addition to those well-established companies already engaged in the field. A well-recognized major bottleneck is the lack of talented, motivated and well-trained nano scientists.

The prospects of graduates from the fields of molecular-scale physics, chemistry and biology are both extremely good and exceptionally varied. The reason is simple: the students are not merely degree holders in one of the traditional core sciences, e.g. physics, chemistry, biology or engineering, but are also scientists with a thorough training in key areas of *each* of the above disciplines. They will certainly have an edge over graduates from classical disciplinary programs, because an education in Nanomolecular Science offers them a broader view of science and technology. This enables them to communicate and collaborate effectively with scientists and engineers across the disciplines, while still being able to understand their language and problems, and most importantly providing these teams with problem solving strategies. This translates into a competitive advantage even in traditional research institutions and industry, not to speak of the increasing number of institutions focusing on Nanoscience and Nanotechnology. Jacobs University's graduate program is firmly embedded in interdisciplinary research co-operations within Jacobs University and with various external partners, academic or commercial. These opportunities provide our graduates with the high caliber training sought after by potential employers.

While Jacobs University's graduate program in Nanomolecular Science will certainly equip students for careers at the frontiers of research and development in universities, research institutes and company laboratories, almost all of these employers also need trained graduates for positions in administration, technical support, service, and sales, to name but a few examples. Finally, the fact that graduates of the program have learned to communicate with specialists from different fields is a highly relevant qualification in many consulting, policy-making, administration, and governmental jobs. In an increasingly technology-driven world, individuals in decision-making positions need to have sound knowledge on diverse topics such as computers and microelectronics, biotechnology, energy resources and sustainability, all of which are touched upon by an education in Nanotechnology such as Jacobs University's graduate program in Nanomolecular Science.

## 2 Structure of the Program

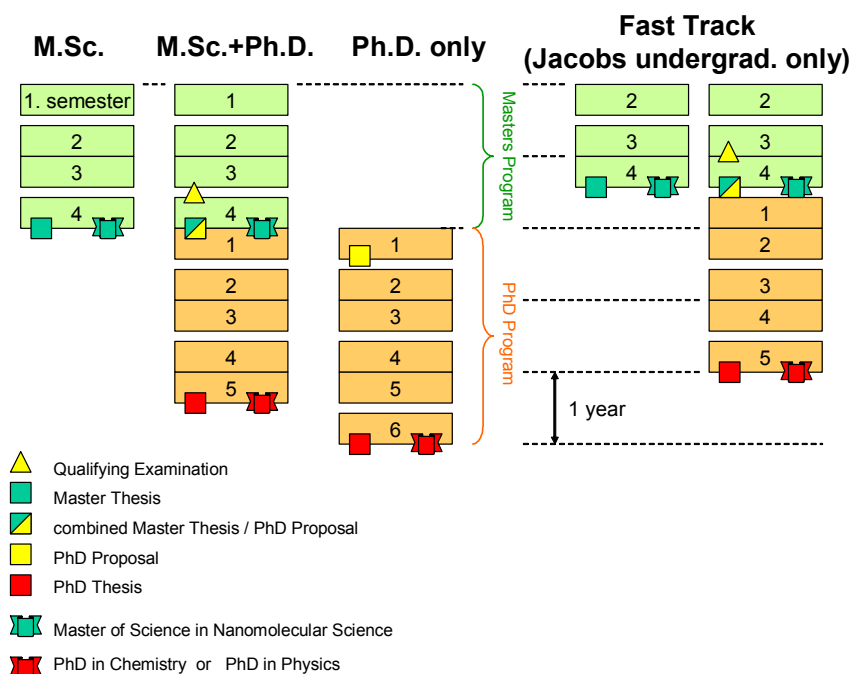
### 2.1 General Information

The graduate program consists of two phases.

**Phase 1** is the course work (3 semesters, 9 courses, and further seminars and research) and a Master Thesis in the 4<sup>th</sup> semester. Courses are designed to provide a broad education in the physics, chemistry, biology and technology of nanoscale systems and their applications. The 2-year program leads to a M.Sc. in Nanomolecular Science and contains a mandatory research component.

**Phase 2** is a Ph.D. thesis under the supervision of one of the faculty members of the Nanomolecular Science graduate program, which provides independent in-depth research experience and trains individuals in problem-solving skills. The program character is constituted mainly by research activities but also academic events such as seminars and colloquia, which all Graduate Students have to participate/attend on a regular basis. The 3-year program awards a Ph.D. in Chemistry or a Ph.D. in Physics.

**Advanced Admission:** The Nanomolecular Science Graduate Program facilitates the progress of students from the Master's Program to the Ph.D. Program by offering a Qualifying Exam before the 4th semester of the Master's Program. Passing the Qualifying Exam will the student allow to combine the preparation of the Master Thesis with initial Ph.D. research. Furthermore, a Fast Track option exists for Jacobs University's undergraduate students, which allows to bring forward one semester of coursework.



Note: A successfully passed Qualifying Examination and combined Master's Thesis / Ph.D. Proposal does not automatically imply Jacobs University funding during the 3-year Ph.D. Program following the 2-year Master's Program.

## 2.2 Degrees and Requirements

**M.Sc. Program (Phase 1):** Students with a B.Sc. or equivalent degree (for example a German Vordiplom plus at least one more year of study) in a relevant field (for example physics, chemistry, materials science etc.) can enter the course program (semesters 1-3) and accumulate the required number of credit points. There is the option for Jacobs University's undergraduate students to start with semester 1 topics already during the undergraduate studies (see Fast Track option). The degree program culminates with the M.Sc. Thesis (semester 4). Participants receive a M.Sc. in Nanomolecular Science. Depending on their results in a Qualifying Examination before semester 4 students are allowed to submit a combined Master Thesis / Ph.D. Proposal to facilitate the progress towards the Ph.D. Program.

**Ph.D. Program (Phase 2):** Students with an Jacobs University recognized M.Sc. or equivalent degree (for example a German Diplom) in a relevant field can directly enter the Ph.D. program (semesters 5-10). They conduct independent research in the group of one of the participating faculty. They are required to develop a Ph.D. Proposal, which is presented in public no later than eight months after the entrance into the Ph.D. Program. The proposals outcome decides if they can continue. Upon completion of the research, a Ph.D. thesis is written. The students receive the Ph.D. in the field of their supervisor (physics, chemistry, etc.).

For further information see also Jacob University's general graduation requirements

## 2.3 Overview of Phase I

*Semesters 1 - 4 leading to the M.Sc.*

Students accumulate a minimum total of 120 ECTS credit points (CP), with the following requirements:

1. 45 CP from mandatory courses and electives (9 courses)
2. 10 CP from the Nanomolecular Science Graduate Seminars (2 semesters)
3. 15 CP from laboratory rotations (3 units of app. 5 weeks each) in the laboratories of Nanomolecular Science faculty
4. 20 CP from research in the laboratories of Nanomolecular Science faculty (2 semesters)
5. 30 CP from the M.Sc. Thesis in the laboratory of a Nanomolecular Science faculty member

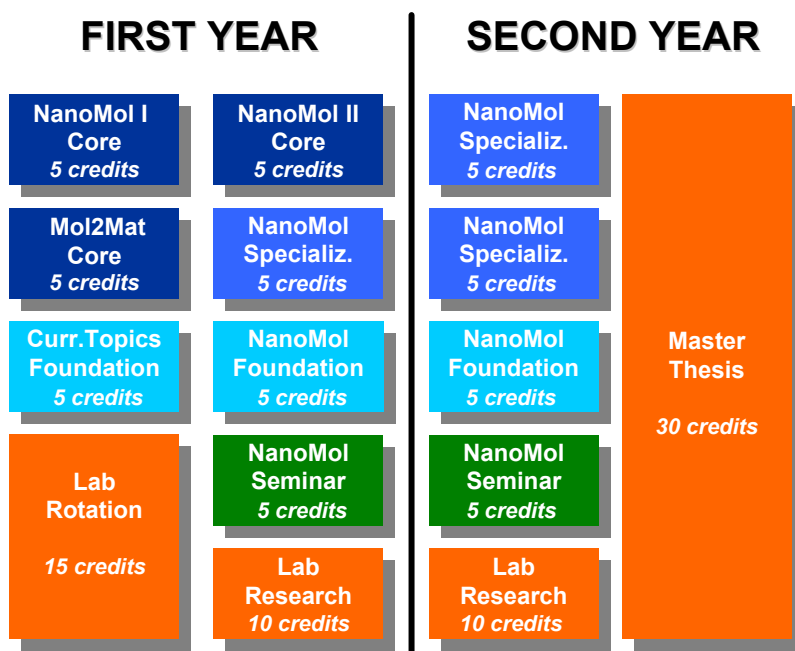
Of the credits in (1), 15 CP are from mandatory (core) courses (Nanomolecular Science I and II, From Molecules to Matter), 15 CP are from Nanomolecular Science specialization subjects, and 15 CP are from Nanomolecular Science foundation topics. Up to 20 CP of the electives can be substituted by suitable graduate courses from other graduate programs at Jacobs University or certain 3<sup>rd</sup> year undergraduate specialization courses. Substitutions are subject to approval by the Graduate Advisor. 3<sup>rd</sup> year courses may only be credited if they have not been credited towards their undergraduate degree. Students can take additional courses (lectures, labs, seminars; within or outside the Nanomolecular Science graduate program; graduate or undergraduate level) in order to broaden or deepen their field of study.

## 2.4 M.Sc. Course Plan - Phase I

Notes:

- The Lab-rotation in the first semester consists of 3 units of about 5 weeks each.
- The graduate seminar includes training in presentation skills and scientific discussions.





Semester	Courses	Graduate Seminar	Research	M.Sc. Thesis	Credits per Semester
1	3 (15 CP)	-	1 (15 CP)	-	30
2	3 (15 CP)	1 (5 CP)	1 (10 CP)	-	30
3	3 (15 CP)	1 (5 CP)	1 (10 CP)	-	30
4	-	-	-	1 (30 CP)	30
<b>Credits per Theme:</b>	<b>45</b>	<b>10</b>	<b>35</b>	<b>30</b>	<b>120 Total ECTS Credits</b>

CP =ECTS credits

## 2.5 M.Sc. Courses - Phase I

Graduate Courses in the Nanomolecular Science Master's Program are categorized (besides labs and seminars) as core courses, specialization courses and foundation courses :

- core courses [CC] are mandatory lectures.
- specialization courses [SC] are lectures focusing on a single subject or area of nanoscience providing in depth knowledge.
- foundation courses [FC] are lectures on basic phenomena/tools or reviewing a broad field of nanoscience and thus providing a broader overview and understanding of the field.

Depending on the student's focus (Chemistry or Physics), non-core courses are labeled as either specialization or foundation courses [SC&FC].

For detailed course descriptions, see Section 3 (Courses).

**Mandatory (Core) Courses [CC]:**

Are given on a regular basis

1. Nanomolecular Science I (n.n)
2. Nanomolecular Science II (Kuhnert, Fritz)
3. From Molecules to Matter (Nau, Kleinekathöfer)
4. Nanomolecular Science Graduate Seminar (alternating faculty)
5. Nanomolecular Science Lab Rotations (Wagner)
6. Nanomolecular Science Lab Research (advisor specific)
7. Nanomolecular Science Master Thesis (advisor specific)

**Nanomolecular Science Electives:**

Not every course is taught in every year

1. Nanomolecular Science Master Research Seminar (advisor) [SC&FC]
2. Current Topics in Nanomolecular Science (all faculty) [FC]
3. Structural Methods in Nanoscale Science (Kortz) [FC]
4. Optical Spectroscopies & Appl. to Nanostructures (Materny) [SC]
5. Advanced Organic Synthesis (Nau/Nugent) [FC]
6. Structure and Mechanism (Nugent) [SC&FC]
7. Structuring by Lithography and Electronic Applications (Wagner) [SC]
8. Transport Physics and Electronic Devices (Wagner) [SC&FC]
9. Quantum Theory in Condensed Matter Physics (Kleinekathöfer) [SC&FC]
10. Techniques for Analysis and Structure Determination of Biomolecules II (Zacharias, Fritz) [SC]
11. Nanomechanics (Fritz) [SC]
12. Biomimetic Materials: The Cell as a Factory (Winterhalter) [SC]

These Electives are taught on an irregular basis:

1. Coordination Chemistry in Nanoscale Science (Kortz) [SC]
2. Organic and Molecular Electronics (Wagner) [SC]
3. Silicon Biology (Fritz) [SC]
4. Biopolymers (Nau) [SC]
5. Nanomolecular Materials in Biotechnology (Fernandez-Lahore) [SC]

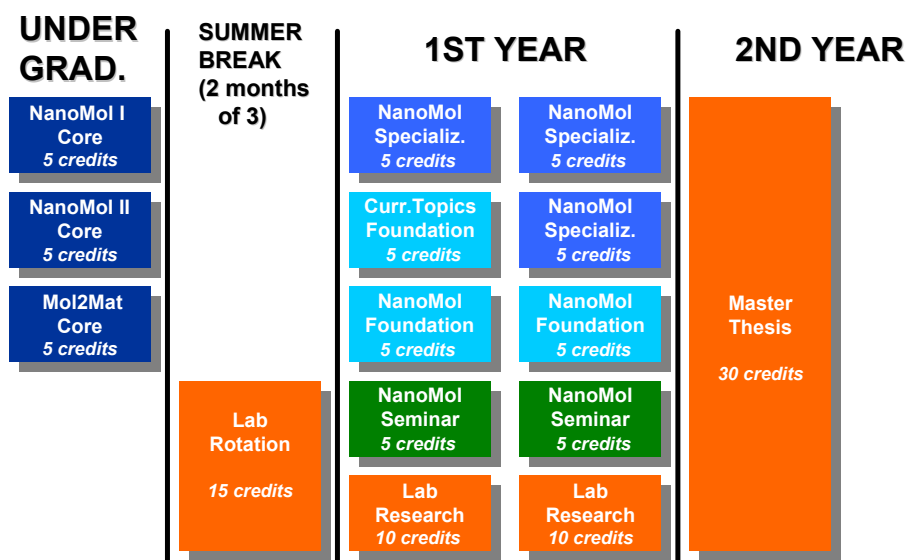
**Suitable 3rd year undergraduate specialization courses**

- 200352 Principles and Applications of Optical Spectroscopy [FC]
- 200362 Surfaces of Condensed Matter [SC&FC]
- 201321 Biophysics [FC]
- 400301 Computational Chemistry and Biochemistry [FC]
- 400302 Structure and Mechanism [SC&FC]
- 400312 Advanced Synthesis [FC]
- 300331 Electronic Devices [SC]
- 201302 Applications of Statistical Physics I [FC]
- 201311 From Classical to Quantum Networks in Physics and Biology [SC]
- 201362 Computational Materials Science [SC&FC]
- 500351 Introduction to Biophysical Chemistry I [FC]
- 560311 High-throughput Screening Technology I [SC]

**Note:** Additional eligible courses and further updates might be announced by the Steering Committee of the Nanomolecular Science Graduate Program.

## 2.6 Fast Track Option (Jacobs University Undergraduates only) - Phase I

The Fast Track option is available for Jacobs undergraduate students, which have already successfully attended a minimum of two Nanomolecular Science courses which have been not counted towards their undergraduate degree. Fast Track students are allowed to do the course Nanomolecular Science Laboratory Rotation starting with the 1<sup>st</sup> of July during the summer break before the start of the 1st semester and can afterwards directly enter the 2nd semester of the Nanomolecular Science Master's Program. Jacobs University students have to indicate in their application or after admission to the program if they want to apply for the fast track option of the Nanomolecular Science Program. The Nanomolecular Science Program Admission committee will finally decide on valid Fast Track applications. A potential course plan for the Fast Track option is shown below.



## 2.7 Overview Phase II

*Semesters 5 - 10, leading to the Ph.D.*

Students conduct research in the group of a member of the Nanomolecular Science faculty. Doctoral students, who *completed Phase I at Jacobs University*, can be admitted to Phase II subject to their Ph.D. research proposal and available funding. Student in Phase I can facilitate their advance to Phase II by successfully passing a Qualifying Examination before semester 4, which allows them to submit a combined Master Thesis / Ph.D. Proposal (not later than 8 months after the Qualifying Examination). Also in this case admittance to Phase II is subjected to available funding.

Doctoral students, who are *directly* admitted to Phase II, are required to present a Ph.D. research proposal not later than 8 months after entering the program.

There are no required courses for doctoral students. Students can, however, take courses subject to approval by their Graduate Advisor.

## **2.8 Possible Research Areas**

Research (Intersession, M.Sc. Thesis, Ph.D. Thesis) can be carried out with all faculty of the Graduate Program in Nanomolecular Science. For a quick overview of the faculty members's research areas, see Section 4.

## **2.9 Graduate Advisors**

Each Graduate Student in Nanomolecular Science is assigned to a personal Graduate Advisor upon entering the Graduate Program. Graduate Advisors are members of the Nanomolecular Science faculty. The student is responsible by him/herself for his/her course selection and curriculum planning. The role of the advisor is to guide the student through the curriculum, to suggest and to approve course selections, creditations, etc. Upon entering Jacobs University, the student is initially assigned to a temporary Advisor. Later, the Advisor is normally the thesis supervisor.

## **2.10 Graduate Requirements**

(See Jacobs University's general graduation requirements)

## 3 Courses: Nanomolecular Science

### 3.1 Mandatory (Core) Courses

#### 420431 – Nanomolecular Science I

*Short Name:* Nanomol I  
*Instructors:* Nanomolecular Science Faculty  
*Credit Points:* 5 ECTS, mandatory  
*Semester:* Fall

**Course content** This course is the first in a series of two mandatory courses on Nanomolecular Science which provide a survey of the field, both from a chemical and physical point of view. They consist of two modules each, one closer to chemistry, the other closer to physics. After a general introduction to the field, the first module of Nanomolecular Science I will focus on the (chemical) synthesis of various nanoparticles, including fullerenes and carbon nanotubes as well as metallic, semiconducting and ceramic nanoparticles. Aspects of their structure, properties and selected applications (catalysis) will also be covered. Finally, nanoporous materials (zeolites) and nanocrystalline materials will be treated. The second module will start off with an introduction to imaging, characterisation and manipulation techniques of nanoobjects and single molecules. This includes scanning probe microscopies (e.g. STM, AFM, SNOM) and other single molecule detections and analysis techniques (patch clamp, optical tweezers, fluorescence spectroscopy and microscopy). Also, fundamental properties of nanoscale materials (confinement, size dependent properties) will be discussed. The module is rounded off by a short account of methods to create nanostructures at surfaces.

#### Textbooks

- **Module 1:** (Synthesis and Properties of Nanomaterials)
  - Nanoscale Materials in Chemistry, Ed. Kenneth Klabunde
  - Chemistry of Advanced Materials, Ed. Leonard Interrante and Mark Hampden-Smith
- **Module 2:** (Nanodiagnostics and Nanomanipulation, Nanostructures at Surfaces)
  - Scanning Probe Microscopy: Analytical Techniques, Ed. R. Wiesendanger
  - Nanoelectronics and Information Technology, Ed. R. Waser

#### 420432 – Nanomolecular Science II

*Short Name:* Nanomol II  
*Instructors:* Nikolai Kuhnert, Jürgen Fritz  
*Credit Points:* 5 ECTS, mandatory  
*Semester:* Spring

**Course content** This course is the second in a series of two mandatory courses on Nanomolecular Science which provide a survey of the field, both from a chemical and physical point of view. The course will introduce the principal design of nanomolecular systems, their characteristic properties, principal functions and applications. The focus will lie on organic and biological functional systems and on applications in the physical sciences, thus complementing

the inorganic, materials-related and methodological aspects covered in Nanomolecular Science I. Nanomolecular Science II is divided into two parts, one taught by a physicist and one by a chemist. The physics part will mainly cover nanoelectronics and nanooptics, including molecular wires, single electron transistors, nanomagnetism, optical nearfield, and single molecule fluorescence. The chemistry and biology part will deal with supramolecular chemistry, the construction of nanomolecular functional systems including shuttles, photonic devices, molecular rotors and machines, and molecular containers, including biological examples and applications, e.g., drug delivery and high-throughput screening. Synthetic aspects of supramolecular assemblies, both of discrete monodisperse nature (calixarenes, functionalized fullerenes, cyclodextrins, cucurbiturils, as well as less well defined polydisperse systems like dendrimers will be discussed.

## 420441 – From Molecules to Matter

*Short Name:* MoltoMat  
*Instructors:* Werner Nau, Ulrich Kleinekathöfer  
*Credit Points:* 5 ECTS, mandatory  
*Semester:* Fall

**Course content** From Molecules to Matter is a mandatory course for all students enrolled in the Nanomolecular Science program. The course provides foundations as basis knowledge necessary for understanding and describing nano-scale systems, and it is divided into two parts devoted to essential chemical and fundamental physical aspects. The first part deals with the description of molecules and matter from a chemical point of view, with emphasis on basic concepts of chemical bonding, including simple covalent bonds, delocalization, intermolecular interactions to create assemblies, and the mechanical bonding relevant in supramolecular and nanomolecular systems. An introduction into photonic processes will be given in terms of photochemical reactions and photoinduced electron transfer. Properties of matter are viewed in terms of thermodynamic aspects, highlighting enthalpic and entropic effects as the driving force of chemical reactions, solvent effects, isotope effects, properties of phase mixtures, etc. In the first part of the lecture, the student is expected to get both an intuitive understanding of molecular properties and reactions as well as the tools for an appropriate quantitative description of isolated molecules, small molecular assemblies, and bulk material. The second part covers the statistical approach to thermodynamics of multi-particle system. Quantum statistics of electrons, vibrations and photons are introduced to calculate various thermodynamic properties. Furthermore electromagnetic fields and their modification in matter and in cavities is addressed. Throughout the second part special emphasis is given to the scaling behaviour from infinite systems to systems of finite size.

### Textbooks

- Principles of Physical Chemistry, H. Kuhn, H.-D. Försterling (Wiley, 1999);
- Structure and Mechanism, F. A. Carroll (Brooks/Cole, 1998);
- Stimulating Concepts in Chemistry, F. Vögtle, J. F. Stoddart, M. Shibasaki (Wiley-VCH, 2000);
- Fundamentals of statistical and thermal physics, F. Reif (McGrawHill, 1965);
- Solid State Physics, N.W. Ashcroft, N.D. Mermin (Rinehart&Winston, 1976);

- Classical Electrodynamics , John David Jackson (Wiley, 1998).

## 420511 – Nanomolecular Science Graduate Seminar

*Short Name:* NanoGradSem  
*Instructors:* alternating  
*Credit Points:* 5 ECTS, mandatory  
*Semester:* All semesters

**Course content** The graduate seminar exposes the students of the graduate program in Nanomolecular Science to actual developments in the field. The scientific content is provided via three routes: (i) The participants write essays on subjects designated by the instructor, which are based on own literature research. They also present their findings to the class in seminar talks. (ii) Faculty of the Nanomolecular Science program give short presentations. (iii) The instructor of record can also designate talks at Jacobs University by external speakers as mandatory for this seminar (e.g. chemistry and physics seminars, Wednesday colloquium) if they thematically fit into its scope. In addition to the scientific content, the seminar pursues other important objectives. Through their own essays and presentations (i) students train to conduct literature research, to write scientific papers and to prepare and present scientific talks. The presentation of faculty research (ii) gives them an overview of research possibilities at Jacobs University and helps them select their lab rotations, and their M.Sc.. or Ph.D.. theses. Attendance of talks by external speakers (iii) exposes them to the current research carried out worldwide. Last but not least, the regular meetings of Nanomolecular Science graduate students and faculty helps to give the program an identity.

Grading is based on attendance, the essay and the presentation. In the latter two, not only the scientific content but also the quality of presentation is graded.

## 420421 – Nanomolecular Science Laboratory Rotation

*Short Name:* NanomolLabRot  
*Instructors:* Instructor of Record, Coordinator Veit Wagner  
*Credit Points:* 15 ECTS, mandatory, 18 h per week  
*Semester:* All Semesters

**Course content** Lab-rotation is mandatory for students enrolled in the Nanomolecular Science graduate program. This course exposes the student to different research areas of nanotechnology and should be taken in the first semester at Jacobs University. The student is required to participate in the research activities of at least three Jacobs University faculty members that participate in the Nanomolecular Science graduate program. The research will be conducted in three consecutive modules in the groups of three different faculty members. Depending on his/her interest, availability and previous knowledge the student chooses from a list of offered modules. The research could involve experimental and/or theoretical topics. Each module ends with the preparation of a short report. Grading for this course is based on lab performance and the quality of the research reports. Furthermore, the lab-rotation should support the student in the process of selecting a M.S. advisor or an advisor for a Ph.D.. thesis.

## 420462/420461 – Nanomolecular Science Research I/II

*Short Name:* NanomolSciRes I/II  
*Instructors:* M.Sc. Advisor  
*Credit Points:* 10 ECTS, mandatory, 12h per week  
*Semester:* Spring/Fall

**Course content** The Nanomolecular Science Research courses is mandatory for students enrolled in the Nanomolecular Science graduate program. During two consecutive courses the students are exposed to a specific research area of nanoscience/nanotechnology in-depth. For this the student is required to participate in the research activities of a Jacobs University faculty member that participate in the Nanomolecular Science graduate program. Typically a continuous project defined by the supervising faculty member is conducted during the consecutive Nanomolecular Science Research courses. The research can involve experimental and/or theoretical topics. Grading for this course is based on lab performance and the quality of research reports. Furthermore, the Nanomolecular Science Research should enable the student for preparing a M.Sc.. thesis in the 4th semester or entering the Ph.D.. phase.

## 420522 – Nanomolecular Science Master Thesis

*Short Name:* NanoMasterThesis  
*Instructors:* M.Sc. Advisor  
*Credit Points:* 30 ECTS, mandatory, full week  
*Semester:* Spring/Fall

**Course content** The Nanomolecular Science Master Thesis courses is mandatory for students enrolled in the Nanomolecular Science graduate program. The student is required to participate in the research activities of a faculty member of the Nanomolecular Science graduate program. The research can involve experimental and/or theoretical topics. The research work of the student has to be summarized in written document, the Master's Thesis. Furthermore the work is presented in a scientific seminar. Grading for this course is based on lab performance and the quality of the Master's Thesis research reports.

## 420532 – Nanomolecular Science Master Research Seminar

*Short Name:* NanoMolMResSem  
*Instructors:* M.Sc. Advisor  
*Credit Points:* 2 ECTS  
*Semester:*

**Course content** The Nanomolecular Science Master Research Seminar exposes the students to research topics relevant for their Master Thesis. This includes attendance of selected research seminars/colloquia as well as presentations and discussions with the research group of the Master Thesis's advisor. The course is graded as passed or failed without further explicit grade. The Master Thesis advisor selects suitable topics on an individual basis (typically one event per week). An attendance of at least 70% is required to pass the course.



## 3.2 Nanomolecular Science Electives

### 420472 – Current Topics in Nanomolecular Science

*Short Name:* Topics in Nano Sci  
*Instructors:* Nanomolecular Science faculty  
*Credit Points:* 5 ECTS, elective  
*Semester:*

**Course content** The course introduces current topics of nanoscience and nanotechnology. Lectures will be taught by various faculty members according to their expertise. For each field an overview of the scientific background, the motivation and major challenges is provided. This is complemented by an in depth discussion of a specific research topic in each discipline. Each student will select two different fields of nanoscience and nanotechnology, for which (s)he writes a term paper following the scheme of a PhD proposal under the supervision of the corresponding faculty member. Grading is based on the quality of the term papers and attendance.

### 420452 – Structural Methods in Nanoscale Science

*Short Name:* StrucMethNanoScaleSci  
*Instructors:* Ulrich Kortz  
*Credit Points:* 5 ECTS, elective  
*Semester:*

**Course content** This course deals with modern analytical instrumentation used for the structural characterization of inorganic compounds, e.g. nuclear magnetic resonance spectroscopy, electron spin resonance spectroscopy, NQR, mass spectrometry, Mössbauer spectroscopy, and diffraction techniques. The course is designed to teach students interpret experimental data, understand the material published in modern research journals, and make decisions about what techniques will be the most useful in solving particular structural problems. The course makes a strong connection between theoretical topics and the real world of practicing chemists.

#### Textbooks

- Structural Methods in Inorganic Chemistry, Eds. Ebsworth, Rankin, Craddock (CRC Press)

### 200352 – Principles and Applications of Optical Spectroscopy

*Short Name:* Spectroscopy  
*Instructors:* Arnulf Materny  
*Credit Points:* 5 ECTS, elective  
*Semester:*

**Course content** Optical spectroscopy is a powerful technique for investigating electronic and vibrational properties of a variety of systems. In nanostructured systems, the techniques of absorption, reflection, luminescence, and light-scattering spectroscopies are capable of providing

invaluable information about diverse aspects. This course gives an introduction to the different spectroscopic techniques which are used in the field of laser spectroscopy. The prerequisites will be the lectures on quantum mechanics of atoms, molecules, and solids. In the beginning, the instrumentation of laser spectroscopy will be introduced. Especially the different types of lasers will be explained. Then techniques making use of the spectral information will be discussed, starting with absorption and luminescence spectroscopy. Other examples are Raman spectroscopy and finally also nonlinear spectroscopic methods. The course will after this introduce the methodology of femtosecond time-resolved spectroscopy, which gives access to the dynamics of both internal molecular processes and chemical reactions. At the end of the course, possible applications of the spectroscopic techniques (e.g. in combination with SNOM) for the investigation of nanostructures will be discussed.

#### Textbooks

- Wolfgang Demtröder, Laser Spectroscopy (Springer, NY, 2002), 3rd ed.

### 400342 – Advanced Organic Synthesis

*Short Name:* AdvOrgSynthesis

*Instructors:* Thomas Nugent

*Credit Points:* 5 ECTS, elective

*Semester:*

**Course content** Building on your basic knowledge of functional group transformations and stereochemistry, strategies for the synthesis of complex organic molecules (natural products and pharmaceutical drugs) will be discussed. In this context, you will learn the importance of the order and type of transformation (retrosynthetic analysis) required for brevity in synthesis. To do so, we will cover functional group compatibility, the use of modern reagents, and the control of stereochemistry (chirality) through the use of chiral auxiliaries vs. enantioselective catalysis. Finally, all of these aspects will be assessed, learned and applied through the use of reaction mechanisms (arrow pushing).

#### Textbooks

- Organic Chemistry, Oxford University Press 2001, Clayden, Greeves, Warren, and Wothers, ISBN: 0 19 850346 6
- Supplementary material: Current Literature

### 400341 – Structure and Mechanism

*Short Name:* StrucMech

*Instructors:* T. Nugent, W. Nau

*Credit Points:* 5 ECTS, elective

*Semester:*

**Course content** The course will deal with the area of physical-organic chemistry and requires the fundamental knowledge from undergraduate organic and physical chemistry courses, such

as Advanced Chemistry AI and BI. The course will cover the following areas: Conformational analysis and molecular mechanics, applications of molecular orbital theory and valence bond, reactive intermediates, spectroscopic methods of studying chemical reactions and reaction mechanisms, and applications to various reaction types. Two special chapters will be dedicated to mechanistic photochemistry and supramolecular chemistry.

### Textbooks

- Structure and Mechanism, F. A. Carroll (Brooks/Cole, 1998)

## 420xxx – Nanomechanics

*Short Name:*

*Instructors:* Jürgen Fritz

*Credit Points:* 2.5 ECTS, elective

*Semester:*

**Course content** This interdisciplinary course introduces to the mechanics of nano- and micrometer sized objects at the interface between physics, molecular biology, and chemistry. The first section introduces the necessary theory and experimental methods to measure molecular forces. We show how microfabricated nanomechanical sensors can be used as biosensors, spin detectors, and as the next generation of data storage devices. We then turn our attention to mechanical properties of single biomolecules. Here we discuss the stretching and unzipping of DNA, forces and kinetics when receptor-ligand systems are pulled apart, and mechanical unfolding of proteins. The concepts of entropic elasticity, entropic traps and molecular ratchets are introduced. We investigate the nanomechanics and chemomechanical coupling of nature's molecular machines focusing on muscle motor proteins, biomolecular rotors and polymerases.

### Textbooks

- Current Literature

### Prerequisites

- Nanomolecular Science I or II
- Biochemistry
- Permission of Instructor

## 420xxx – Biomimetic Materials: The Cell as a Factory

*Short Name:*

*Instructors:* Mathias Winterhalter

*Credit Points:* 5 ECTS, elective

*Semester:*

**Course content** Nature has optimized the synthesis and the function of macromolecular assemblies. It is tempting to combine recently developed techniques in nanoscience and biochemistry to create new types of intelligent materials and devices based on natural cellular functions. This course first introduces the underlying molecular interactions relevant for the assembly of

mesoscopic structures and has a closer look on thermodynamics in confined systems. Then we show a few applications where reconstituted natural assemblies can already be used as a tool to build an artificial cell. Artificial surfaces can be rendered biocompatible. Reconstituted receptor proteins allow recognition of specific molecules. Insertion of channel forming proteins in polymer matrices allows to filter and harvest specific molecules. Encapsulation of enzymes preserves their optimal function in a hostile environment.

#### Textbooks

- Recent Publications

### 3.3 Infrequently offered Specialization Courses

#### 420xxx – Coordination Chemistry in Nanoscale Science

*Short Name:*

*Instructors:* Ulrich Kortz

*Credit Points:* 5 ECTS, elective

*Semester:*

**Course content** This course deals with the state of coordination compounds in modern chemistry. In addition to methods of synthesis, studies of structure and reactivity, particular attention is paid to the application of coordination chemistry in fields as varied as biochemistry and medicine, organometallic chemistry, solid state chemistry, catalysis, and molecular receptors and devices.

#### Textbooks

- Perspectives in Coordination Chemistry, Eds. Williams, Floriani, Merbach (VCH Publishing)

#### 420xxx – Organic and Molecular Electronics

*Short Name:*

*Instructors:* Veit Wagner

*Credit Points:* 5 ECTS, elective

*Semester:*

**Course content** Organic and molecular electronics seeks to build electrical devices to implement computation (logic and memory) using collections of molecules or even individual molecules. Due to the huge potential of reduction in device size and/or fabrication costs relative to conventional CMOS these devices are expected to be superior in a multitude of applications. The course will introduce to basic circuit ideas by MOS-FET designs using organic semiconductor as active materials. Principal device characteristics and their dependence on the various electrode geometries (down to nm-scale), channel lengths, metal-organic junction properties, organic semiconductor bulk properties, etc. will be introduced in the first part. Thereafter concepts of realization of switches and diodes formed by individual molecules or by single mono layers will be given and how contacts to them can be realized. Finally, the assembly to logic

gates (XOR, NAND, 1-bit adder) is addressed, which is strongly influenced by the specific organic device technology used. Further topics such as defect and fault tolerance are treated in this context.

## 420xxx – Silicon Biology

*Short Name:*

*Instructors:* Jürgen Fritz

*Credit Points:* 5 ECTS, elective

*Semester:*

**Course content** This course teaches the fundamental effects and laws which govern the interface between silicon technology and molecular biology. It provides a background in silicon microfabrication, bioelectronics, microfluidics, and the solid liquid interface. We discuss electronic field-effect sensors and nanowires to detect charges on biomolecules and to transmit action potentials via silicon - neuron - silicon interfaces. DNA chips and microarrays for proteomics are then introduced as recent examples of massively parallel solid state biosensors. We investigate how cells assemble inorganic materials and how molecular biology can be used to self-assemble semiconducting materials. We conclude with selected topics of current research on electronic remote control of DNA hybridization and on running feedback loops in cells.

## 420xxx – Biopolymers

*Short Name:*

*Instructors:* Werner Nau

*Credit Points:* 5 ECTS, elective

*Semester:*

**Course content** The polymerization of amino acids and nucleotides gives rise to the most fascinating classes of biomolecular functional nanostructures: enzymes, DNA and RNA. In this course we will study their properties and functions. Understanding how proteins fold and assemble to their final three-dimensional structures and how domain motions in proteins lead to enzymatic activity greatly assists the development of nanomolecular biomimetic materials. The molecular structure and flexibility of proteins, in particular, is a crucial factor in determining their biological activity, including binding affinity, antigenicity, and enzymatic activity. The identification of regions in proteins with highest conformational flexibility and rigidity is essential for predicting the mechanism of protein folding, for understanding domain motions in proteins, and for predicting the rate of non-local interactions as well as intramolecular reactions, including electron and proton transfer. Consequently, there is a considerable interest to predict the flexibility or, conversely, the rigidity of peptides from their amino acid sequence. Another frontier is the *ab initio* prediction of protein structure from the primary sequence, which has direct implications for the *de novo* design of peptides and for the theoretical understanding of peptide dynamics. The course will also cover concepts of solution and solid-phase synthesis of biopolymers.

## **420xxx – Nanomolecular Materials in Biotechnology**

*Short Name:*

*Instructors:* Marcelo Fernandez-Lahore

*Credit Points:* 5 ECTS, elective

*Semester:*

**Course content** The course is intended to give an overview on nanomolecular materials and systems used in various fields of biotechnology such as product recovery and polishing. Theoretical as well as experimental aspects will be presented in detail including methods for tailoring materials and proteins. Applications and scale-up problems will be explained on selected examples of chemical and pharmaceutical companies. In addition we intend to use a software tool, recently developed at the university Bremen, for modelling, predicting and designing product recovery procedures.

## 4 Nanomolecular Science Faculty and their Research

**Marcelo Fernandez-Lahore** (Biochemistry):

- Bioprocess intensification and Process proteomics
- Downstream processing of natural compounds
- Meta-Integration in downstream processing
- Continuous processing unit operations for biotechnology
- Process modeling, simulation, design and scale-up

**Jürgen Fritz** (Biophysics):

- Single molecule biophysics
- atomic force microscopy & force spectroscopy
- nanomechanical sensors

**Thomas Heine** (Computational Physics)

- Hydrogen Storage in Nanoporous Materials
- Electromechanics in Nanostructures
- Development of Scalable Methods Based on Density-Functional Theory

**Ulrich Kleinekathöfer** (Computational Physics):

- Computational physics
- dynamics of excited electronic states
- transport in molecular wires
- DNA and membrane proteins

**Dietmar Knipp** (Electrical Engineering):

- Electronic devices
- photonics
- organic materials and electronics
- nanooptics
- optical sensors
- thin film technologies
- nano fabrication

**Ulrich Kortz** (Chemistry):

- Synthesis and structural characterization of nanoscale polyoxometalates with applications in catalysis and medicine

**Nikolai Kuhnert** (Chemistry):

- Analytical Chemistry
- Supramolecular chemistry
- Natural Product Chemistry

**Arnulf Materny** (Chemical Physics):

- Laser spectroscopy on nano-structured systems in the frequency and time domain

**Hildegard Meyer-Ortmanns** (Physics)

- Synchronization in excitable media
- Mass transport on arbitrary graphs
- Interaction-driven condensation phenomena
- Algorithms for simulating evolutionary processes
- Optimization problems in networks

**Werner Nau** (Chemistry):

- Supramolecular functional materials
- biopolymer dynamics and function
- fluorescent sensors and probes

**Thomas Nugent** (Chemistry):

- Total synthesis (pharmaceutical and natural product drugs)
- enantioselective catalytic methods development
- organometallic chemistry
- process research

**Veit Wagner** (Physics):

- Nanoelectronics
- single molecule transistors
- functionalized organic materials and plastic electronics

**Mathias Winterhalter** (Biophysics):

- Substrate recognition and translocation on a single molecular level
- functionalisation of surfaces and nanocapsules with biomaterials

**Danilo Roccatano** (Chemistry):

- Solvent models for MD simulations
- Peptide secondary structures in solution
- Protein dynamics and folding
- Development of bioinformatics tools for bioengineering



