



UNIVERSITY OF AMSTERDAM

*Chemistry  
research  
that matters*

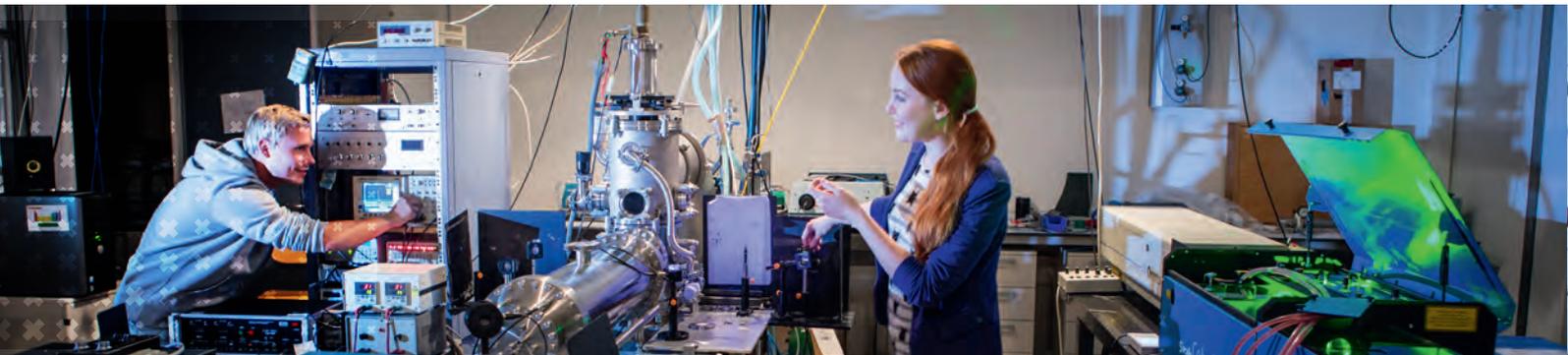


Van 't Hoff Institute  
for Molecular Sciences

# Molecular Photonics

*Focus:  
Solardam*

HIMS researchers participate in the Amsterdam Solardam initiative in which multiple partners aim at generating electricity and fuel through combinations of photovoltaics, photocatalysis and photosynthesis.



Synthesis, analysis, and computer simulations of molecular systems are key disciplines for advancing chemical sciences. However, the ultimate proof of the value in these molecular systems must come from 'seeing' them at work and 'steering' them to perform user-defined tasks. The interaction of Light and Matter is per se the basis of such endeavours. It not only allows the passive observation and characterization of molecular systems (molecular spectroscopy), but also enables us to obtain emerging properties from their synergy (molecular photonics). While the 20th century has been labelled as the century of the electron, it is now clear that the 21st century will be the century of the photon.

The Molecular Photonics group hosts a powerhouse of photochemical and photophysical expertise. It is in many aspects unique, as it covers the complete trajectory from design and construction of novel molecular systems to their application in areas of primary societal importance, such as energy, sustainability, and health.

This is reflected in the strong interactions within and outside HIMS, for instance in the Advanced Research Center for Nanolithography (ARCNL), the free electron laser facilities (FELIX, FELICE) at Radboud University Nijmegen and in medical research with the Academic Medical Center Amsterdam, FOM-Institute AMOLF and various companies.

Luminescent labels and probes

Solar energy conversion

Molecular machinery

Medical nanophotonics

Biomolecular dynamics

# Sustainable Chemistry

## *Focus: Science for Arts*

HIMS researchers participate in (inter)national Science for Arts projects that combine interdisciplinary research in art history, art conservation and molecular science.



Sustainable Chemistry research is focused on the development of new technologies that enable efficient and sustainable chemical transformations. Efficient production of chemicals is crucial for a sustainable society in which a growing world population faces problems associated with the scarcity of materials, energy and feedstock. Catalysis is the key enabling technique in ensuring atom and energy efficient synthesis and in storing and releasing chemical energy.

HIMS researchers aim to develop new, inexpensive and sustainable catalysts that improve the efficiency of chemical transformations and that enable the conversion of solar/electrical energy to fuels (electrocatalysis,

photocatalysis) and vice versa (fuel cells). The research team consists of a group of highly interdisciplinary and world-renowned top-scientists with expertise in the fields of catalyst design, synthesis, kinetics, (spectroscopic) characterization, modeling and testing under applied conditions. The team is strong in both fundamental research and applied catalysis, and Sustainable Chemistry was recently appointed as a university Research Priority Area.

On the fundamental side, the Sustainable Chemistry team collaborates with several top-scientists and renowned scientific institutes all over the world. Applied research is performed in close collaboration with various industrial partners and in spin-off companies.

- Transition (base) metal catalysis
- Kinetic DFT studies & spectroscopy
- Fuel cell technology & electrochemistry
- Homo-, hetero-, organo- and bio-catalysis
- Biomass conversion to fuels and chemicals
- Bio-inspired (supramolecular & metalloradical) catalysis
- Short-cuts and new methods in (enantio)selective synthesis

# Analytical Chemistry



Analytical Chemistry performs scientific discoveries at the molecular level. Our scientists establish which types of molecules are present, how many of them are present and, increasingly, what these molecules are doing – or have been doing. The Analytical Chemistry group at HIMS is involved with developments and applications in forensics, chemistry, materials, art, food, medicine and biotechnology.

In all these areas the group collaborates with leading companies and institutions nationally and internationally. Through cooperation with world-leading high-tech instrument companies the Analytical Chemistry group makes its scientific findings accessible to other scientists.

Locally the group collaborates with its counterparts from VU University in the Center for Analytical Sciences Amsterdam (CASA). This cooperation is recognized as a unique national Center of Expertise in the Netherlands. The research covers the development, improvement and optimisation of analytical (separation) methods and technologies.

In addition, advanced software (chemometrics) is developed to transform large amounts of data into useful information. Recently the group has strengthened its research in molecular analysis via mass spectrometry (MS). MS will further reinforce HIMS research in chemistry, biotechnology, health and forensic sciences, as well as 'Science for Arts'.

One- and two-dimensional separation techniques

Gas and liquid chromatography

Mass spectrometry

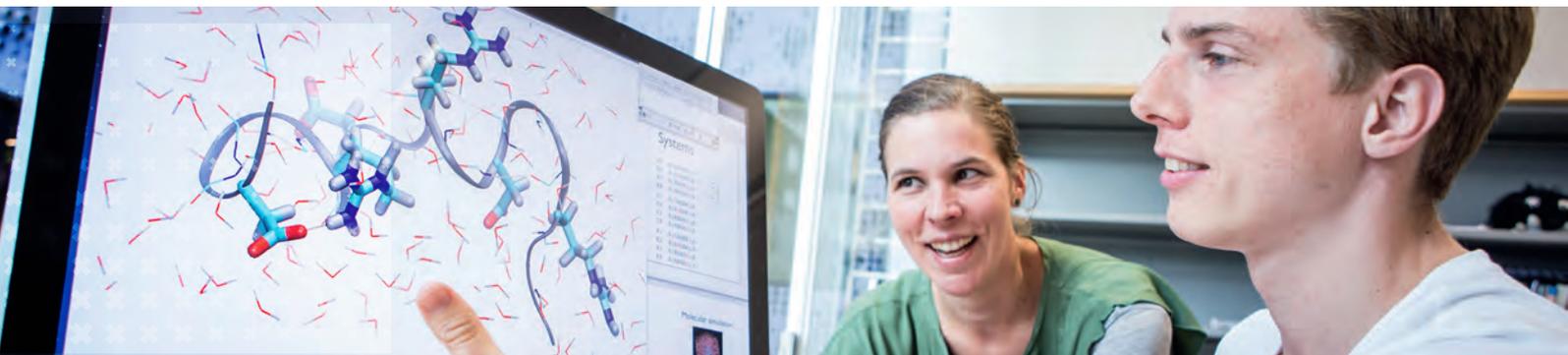
Electro-migration techniques

Field-flow fractionation

Data analysis and chemometrics

Biomolecular systems

# Computational Chemistry



Research in Computational Chemistry aims to develop computational tools to model and predict, from first principles, the behavior of complex chemical, biological, and physical processes.

The HIMS Computational Chemistry group is a worldwide leader in the fields of molecular simulations and multiscale modelling. Its expertise covers a wide variety of modelling techniques on multiple time and length scales. Examples include the unravelling mechanisms of homogeneous catalysis, the prediction of reaction coordinates in protein folding and conformational changes, the screening of optimal nano-porous materials for separation, and prediction of soft matter self-assembly.

**Molecular simulations**

**Biochemical and biophysical phenomena**

**Computational catalysis**

**Novel methodology development**

**Aqueous chemical processes**

**Nanostructured materials**

**Soft matter**

Over the past decade the group has developed a strong alliance with its counterpart at the VU science faculty, resulting in the Amsterdam Center for Multiscale Modeling (ACMM). Since 2007 the ACMM has developed a strong High Performance Computing infrastructure and an internationally recognized training program. It facilitates top research in all important modelling disciplines at one location, with direct access to essential infrastructure such as the Supercomputer Center (SURFSARA) and the eScience Center.

Research in Computational Chemistry is performed in collaboration with partners from industry, and knowledge valorization is further facilitated via scientific consultancy. In the High Performance Computing infrastructure of the ACMM a hands-on hosting environment enables the application of computational methods to systems of technological and industrial relevance.

# Van 't Hoff Institute for Molecular Sciences



The Van 't Hoff Institute for Molecular Sciences (HIMS) performs internationally recognized chemistry research, curiosity driven as well as application driven. This is done in close cooperation with the chemical, flavour & food, medical and high-tech industries.

Research is organised into four themes: Sustainable Chemistry, Analytical Chemistry, Computational Chemistry and Molecular Photonics. In all four themes HIMS has established a strong position in research areas of strategic importance to academia, society and industry. HIMS researchers actively participate in interdisciplinary initiatives, such as Solardam (energy research), Science for Arts (art conservation), Quantivision (medical imaging) and ARCNL (nanolithography).

The University of Amsterdam has established twenty Research Priority Areas over the entire spectrum of science. These RPA's are among the best the UvA has to offer and are internationally renowned. HIMS houses the UvA Research Priority Area Sustainable Chemistry.

As one of eight institutes of the University of Amsterdam Faculty of Science, HIMS is the only institute focusing solely on chemistry. HIMS has an academic staff of 30 researchers and a supporting staff of 20 employees. The number of postdoc researchers and PhD students - well trained for a future career in science or industry - totals 70.

HIMS has an extensive fleet of high quality analytical instrumentation, such as NMR, EPR, UV-Vis, HPLC and MS. HIMS offers companies, in particular small and medium enterprises (SME's), unique access to this infrastructure, scientific software and related know-how. HIMS scientists are always open to consider new collaborations and partnerships.

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