University of Amsterdam

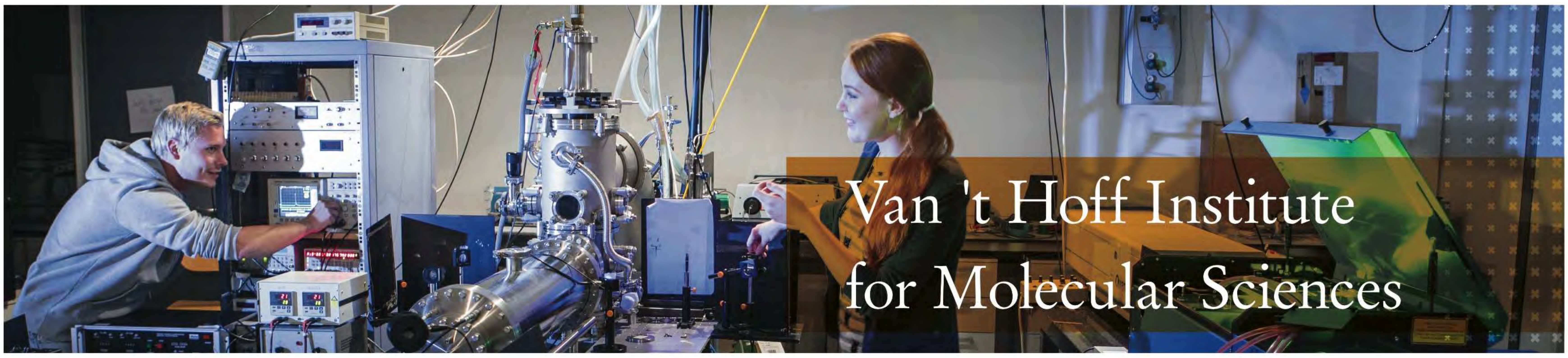
Valorisation at HIMS

Chemistry research that matters

Van 't Hoff Institute for Molecular Sciences

2015

Molecular Photonics



Synthesis, analysis, and computational understanding of molecular systems are key disciplines for advancing chemical sciences, but the ultimate proof of their value must come from ‘seeing’ them at work and ‘steering’ them to perform user-defined tasks. The interaction of Light and Matter is per se at the basis of such endeavours. Not only does it allow the passive observation and characterization of molecular systems (molecular spectroscopy) but also to obtain emerging properties from their synergy (molecular photonics).

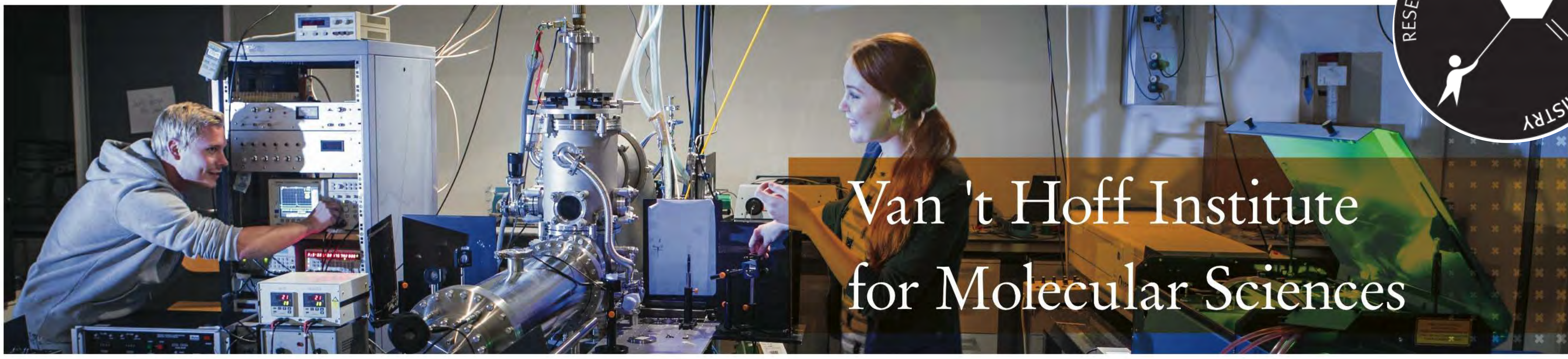
While the 20th century has been labelled as the century of the electron, it is now clear that the 21st century will be the century of the photon. The Molecular Photonics group harbours a power house of photochemical and photophysical expertise. It is in many aspects unique as it covers the complete trajectory from designing and constructing novel molecular systems to their application in areas of primary importance to society such as energy, sustainability, and health.

This is reflected in the strong interactions the groups has within and outside HIMS, such as the in 2014 started Advanced Research Center for Nano-Lithography, the free electron laser facilities (FELIX, FELICE) at Radboud University in Nijmegen, and medical research with the AMC and several companies.

Luminescent labels and probes
Solar energy conversion
Molecular machinery
Medical nanophotonics
Biomolecular dynamics

University of Amsterdam

Molecular Photonics



Research Priority Area Sustainable Chemistry

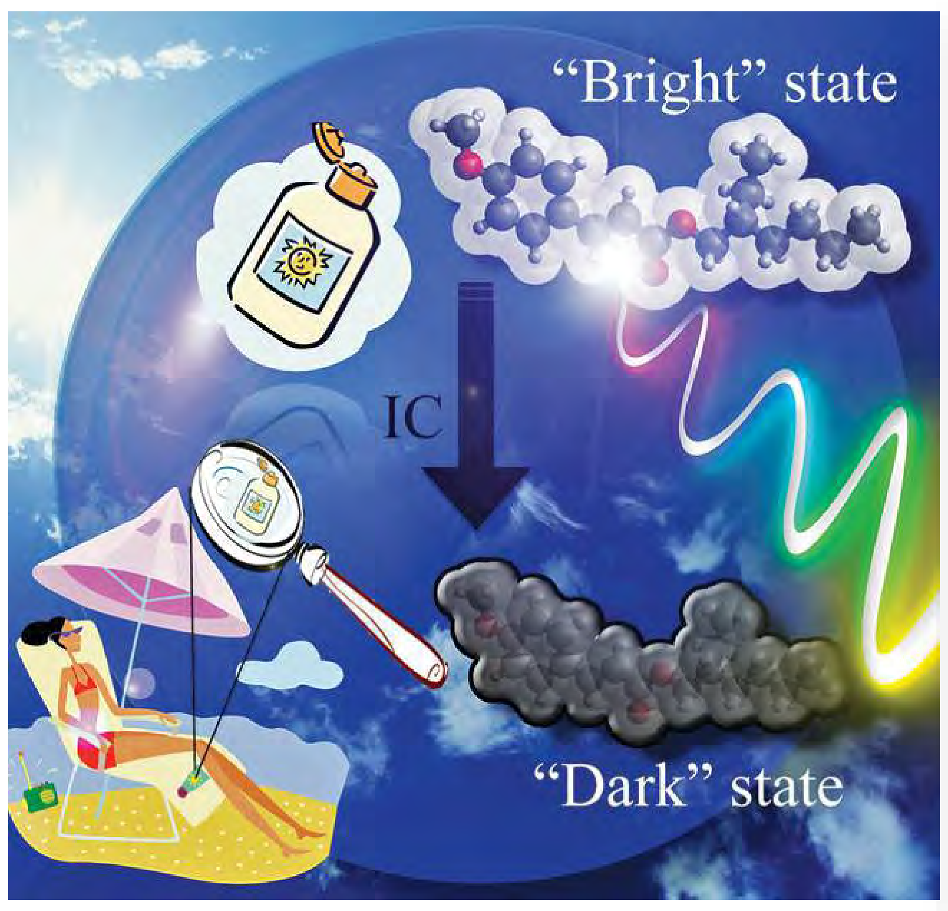
Molecules and Photons at Work

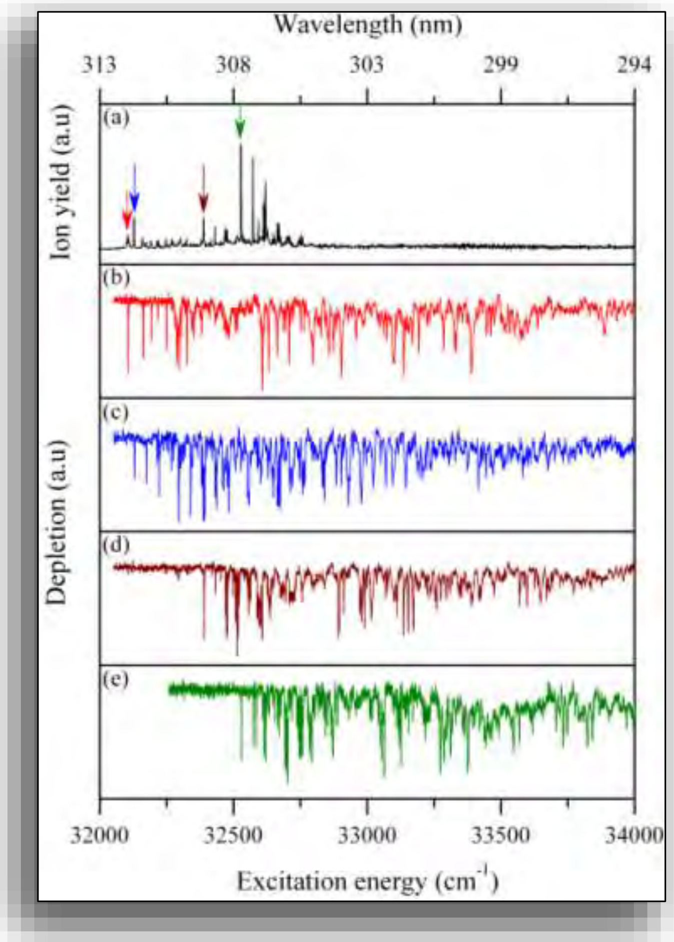
Photoactive Materials Sciences

The interaction between Light and Matter allows for the passive observation and characterization of molecular systems (molecular spectroscopy), but also to obtain emerging properties from their synergy (molecular photonics). Applications range from molecular machinery to medical imaging.

Example: advancing healthcare technologies

Understanding the intrinsic properties of molecular sunscreens is critical to developing more efficacious sunscreen products. Gas-phase spectroscopy and microsolvation studies provide innovative solutions.





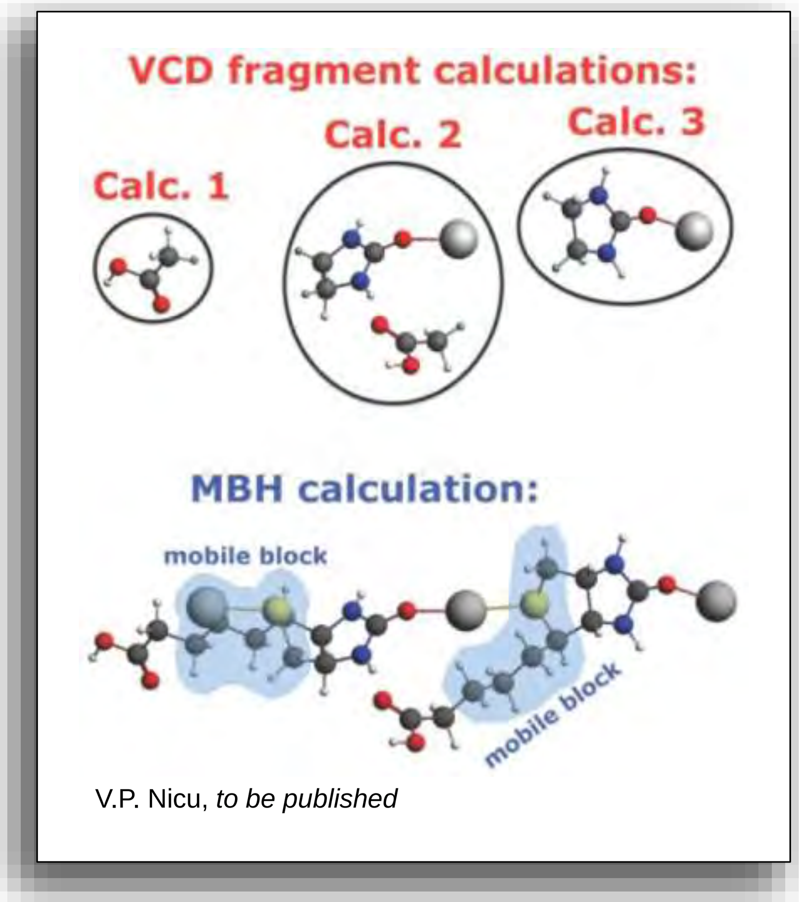
Chiral Structure Analysis

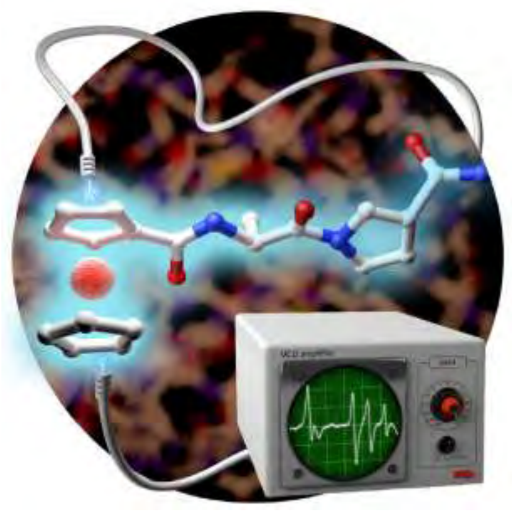
Chiroptical techniques are emerging as powerful means to determine the ***absolute configuration*** and ***conformational structure*** of chiral compounds.

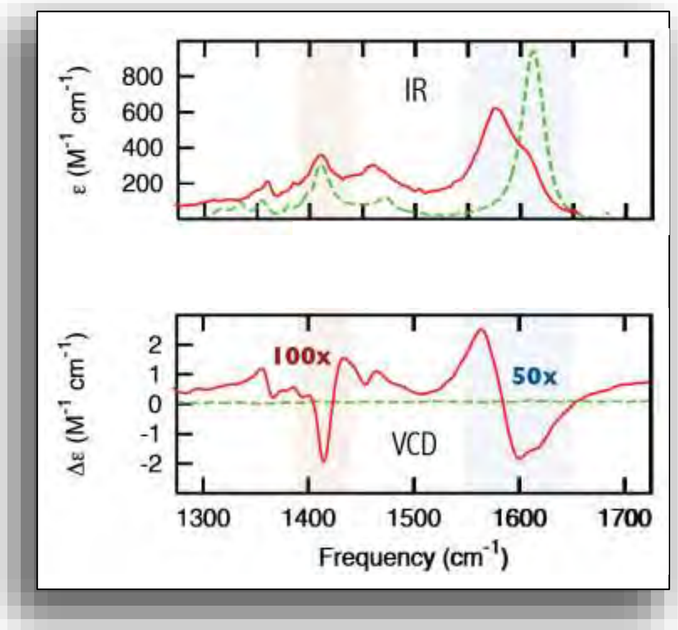
Example: development VOA analysis toolbox (together with Theoretical Chemistry (VU), SCM, and BioTools)

Example: novel methods to increase efficiency and utility Vibrational Circular Dichroism (together with Prof. S. Woutersen)

BioTools 'Tools for Discoveries of Life' — SCM Scientific Computing & Modelling



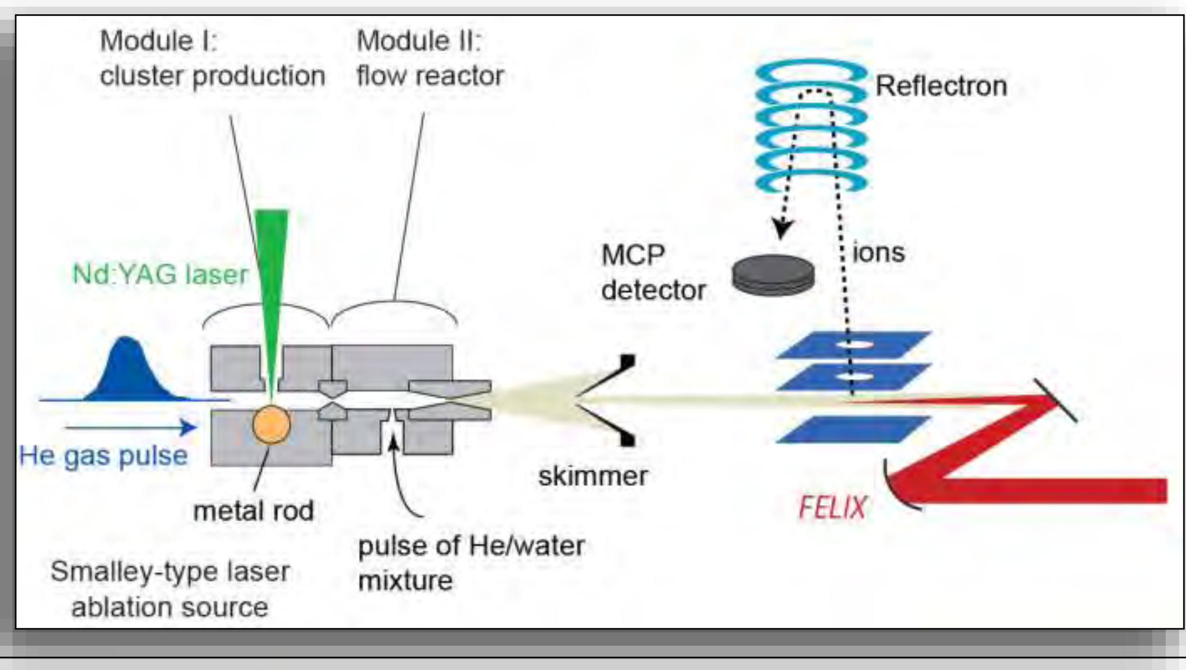


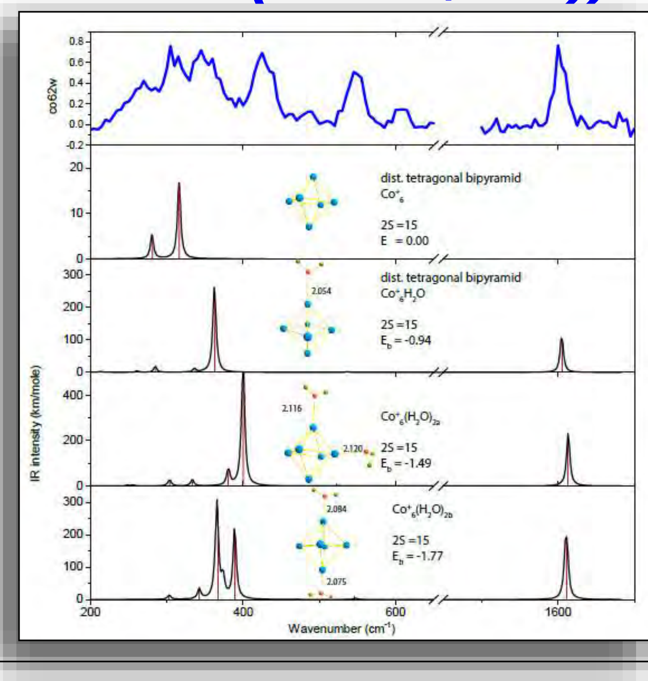


Tailoring Catalytic Activity on a Nanoscale

Nanoclusters are rapidly gaining commercial interest because of their unusual chemical reactivity. This reactivity finds its origin in the electronic properties of the clusters. Gas-phase studies of structure and substrate binding offer detailed insight and pave the way for optimizing these properties.

Example: structure and reactivity Co clusters (together with Dr. J. Bakker and Prof. J. Oomens (FELIX, RU))





Molecular Photonics

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References

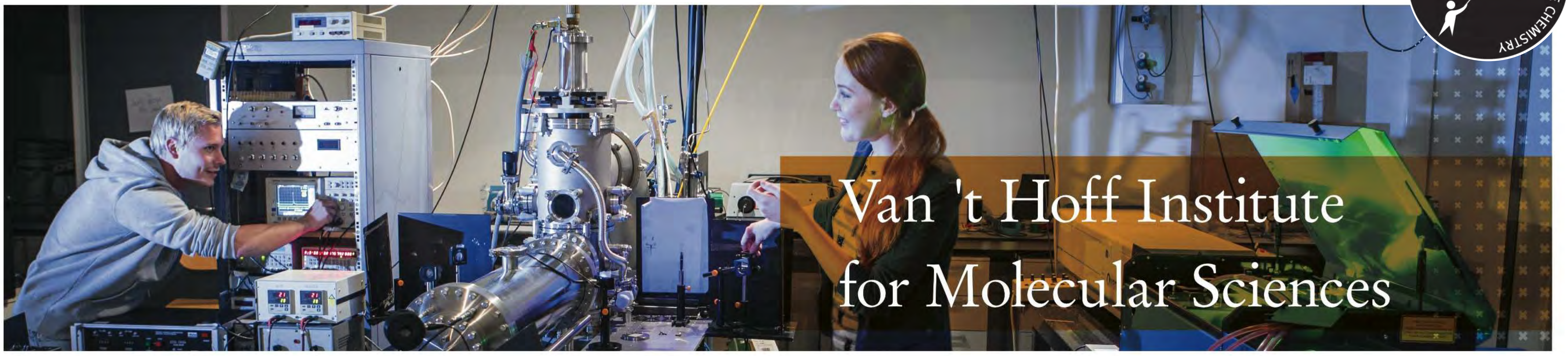
http://www.uva.nl/over-de-uva/organisatie/medewerkers/content/b/u/w.j.buma/w.j.buma.html

Valorization goals

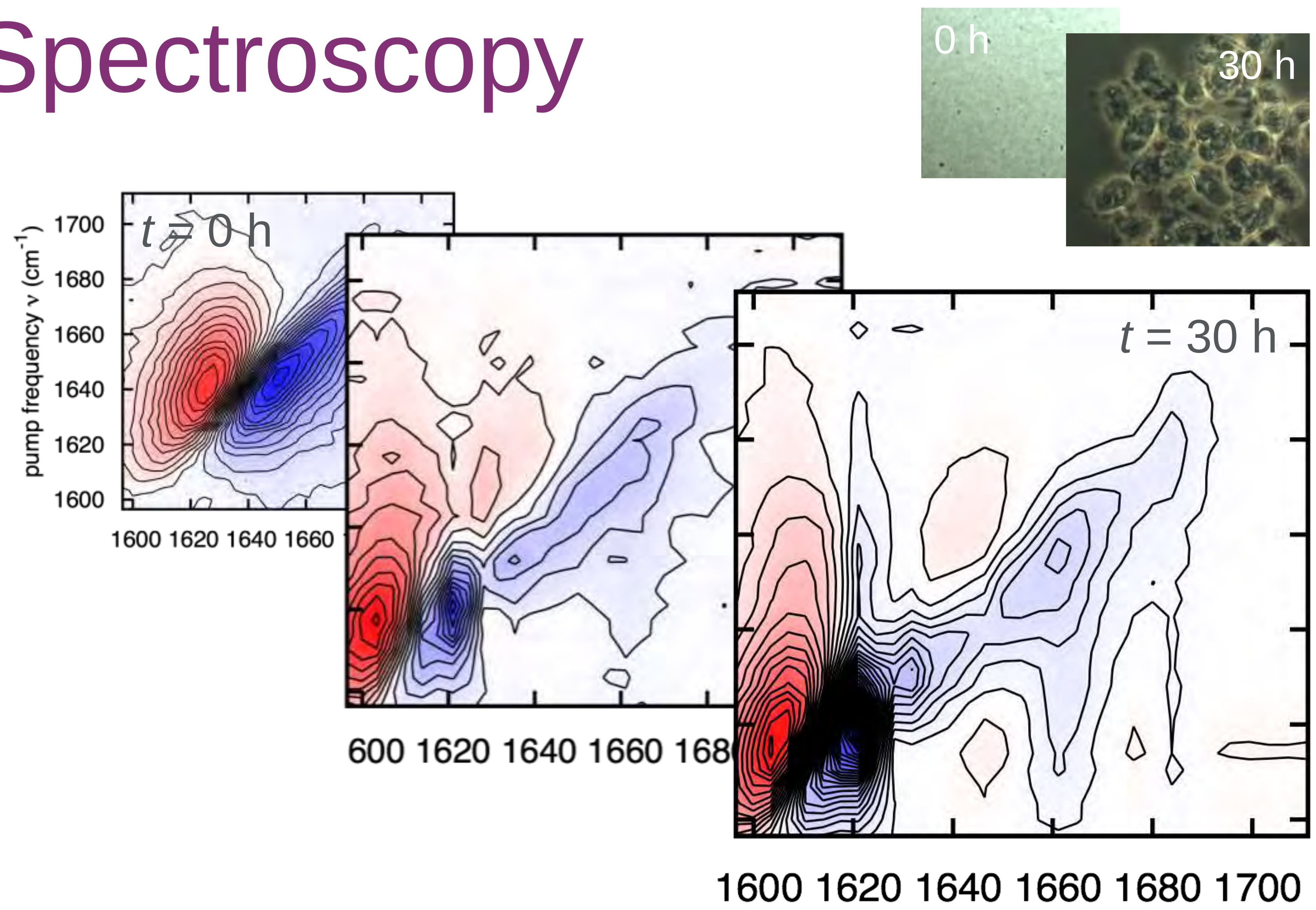
Develop photoactive materials with user-defined properties

Extend areas of commercial application of chiroptical techniques

Optimize catalytic activity nanoclusters

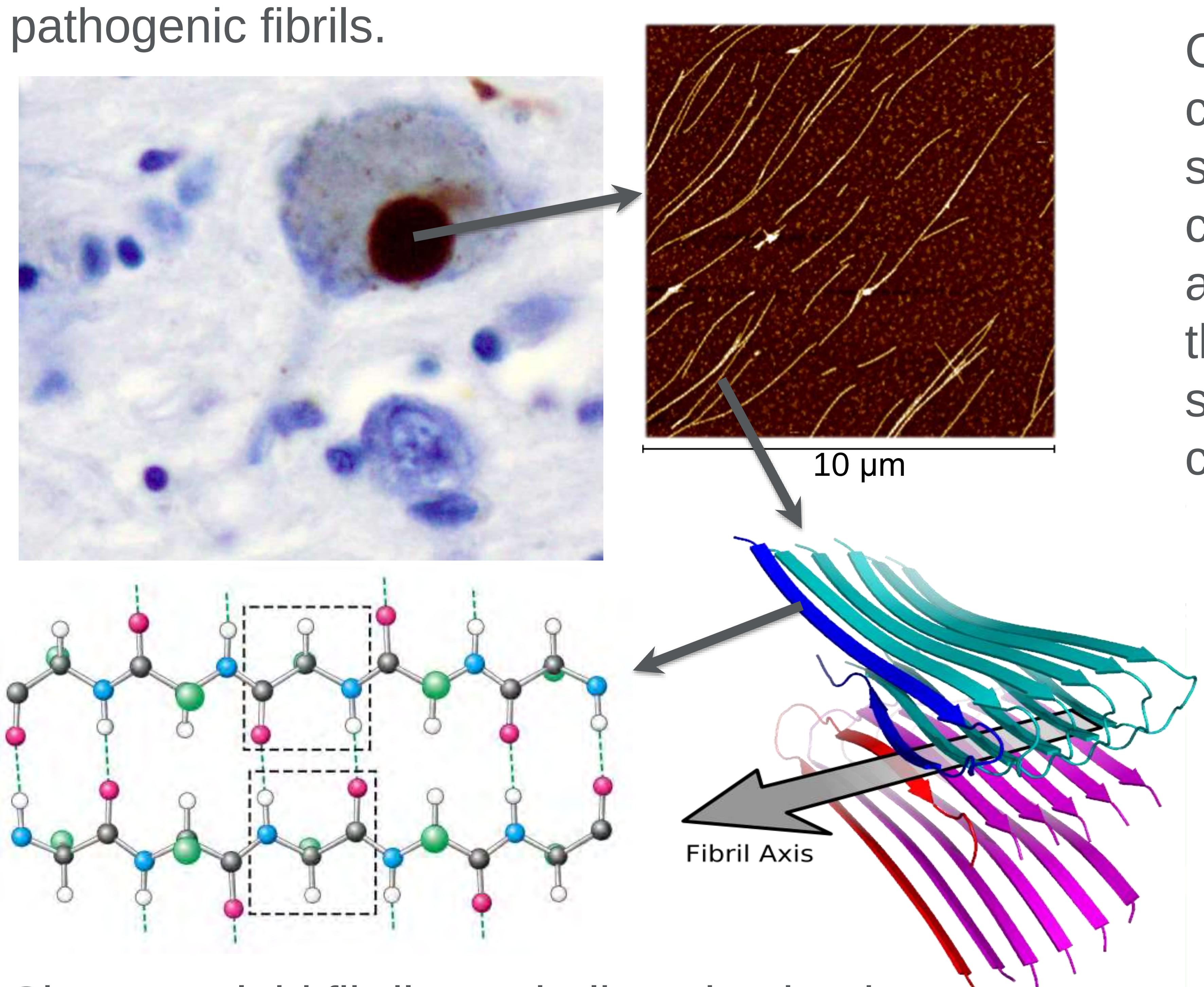


Multi-dimensional Infrared Spectroscopy



Unraveling the causes of Parkinson's

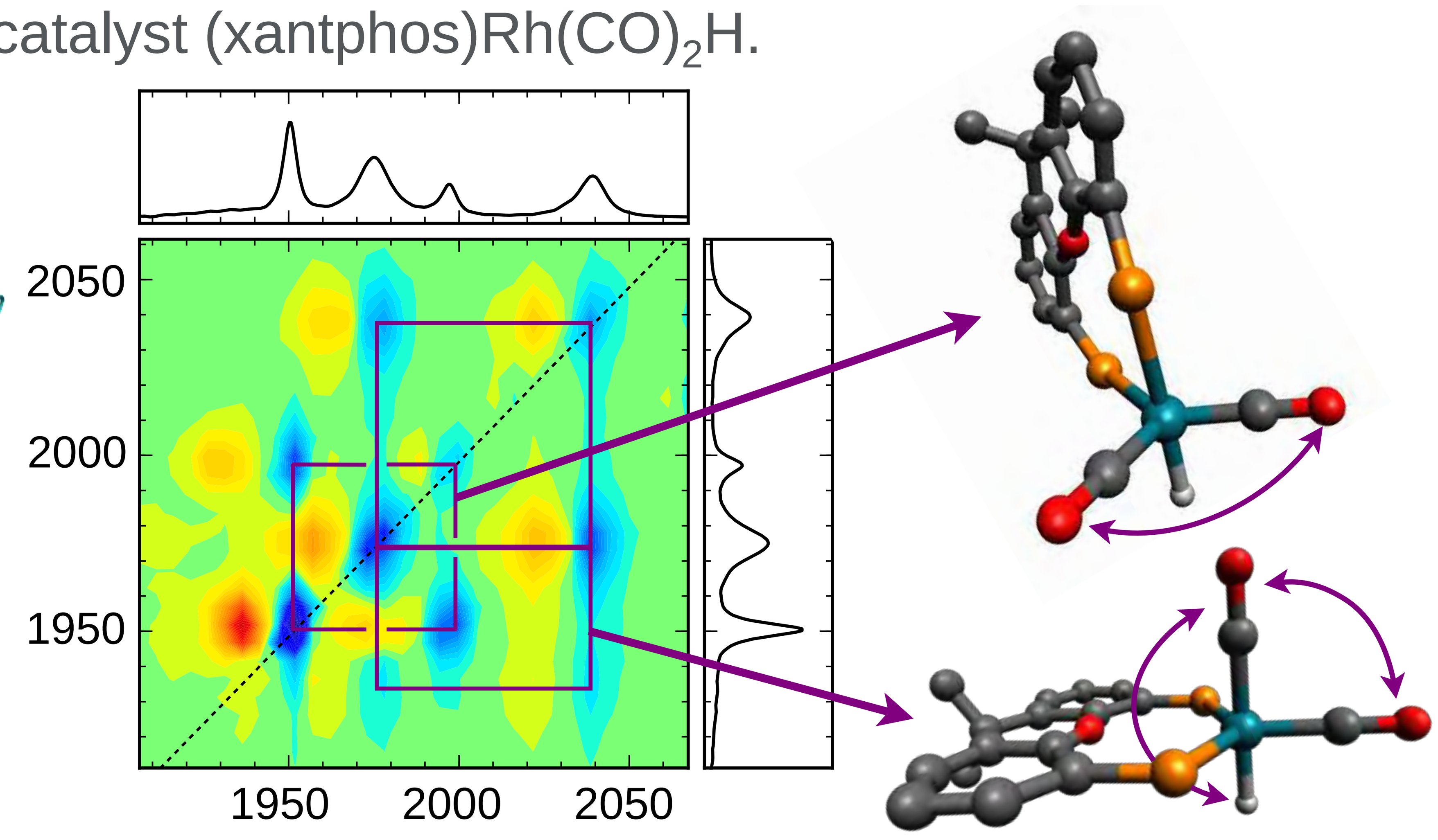
We study the aggregation into fibrils of the protein α-synuclein with infrared spectroscopy. This aggregation process is responsible for Parkinson's disease. The mechanism of amyloid formation is poorly understood, and the structure of the (pathogenic) intermediates and the final fibril are still largely unknown and difficult to determine with conventional techniques. The combination of 2D-IR spectroscopy and vibrational circular dichroism offers a unique insight into the kinetics and structure of the aggregation of α-synuclein into pathogenic fibrils.



Since amyloid fibrils are believed to be the thermodynamically most stable state of many proteins and peptides, the best hope for therapies lies in preventing fibril growth. The results of this research project, which is focused on the fibril nucleation and growth, should make a substantial contribution of our understanding of these processes, and thus help in developing therapies.

Catalyst structure and optimization

Catalytic complexes often occur in several conformations that exchange rapidly (<µs) in solution, so that their structures are difficult to characterize. Using 2D-IR spectroscopy on the CO and Rh-H stretching modes we have determined the structure of each of the two rapidly exchanging solution conformations of the hydroformylation catalyst (xantphos)Rh$(CO)_2$H.



This result demonstrates how 2DIR makes it possible to determine the structure of rapidly evolving, or exchanging, catalyst structures at the level of specific chemical bonds, and so to optimize their reactivity in a rationalistic manner.

Molecular Photonics

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References

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Inorg. Chem. **53**, 5373 (2014).

Valorization goals

Understanding amyloid formation to help developing therapies

Optimizing catalyst performance using mechanistic insights

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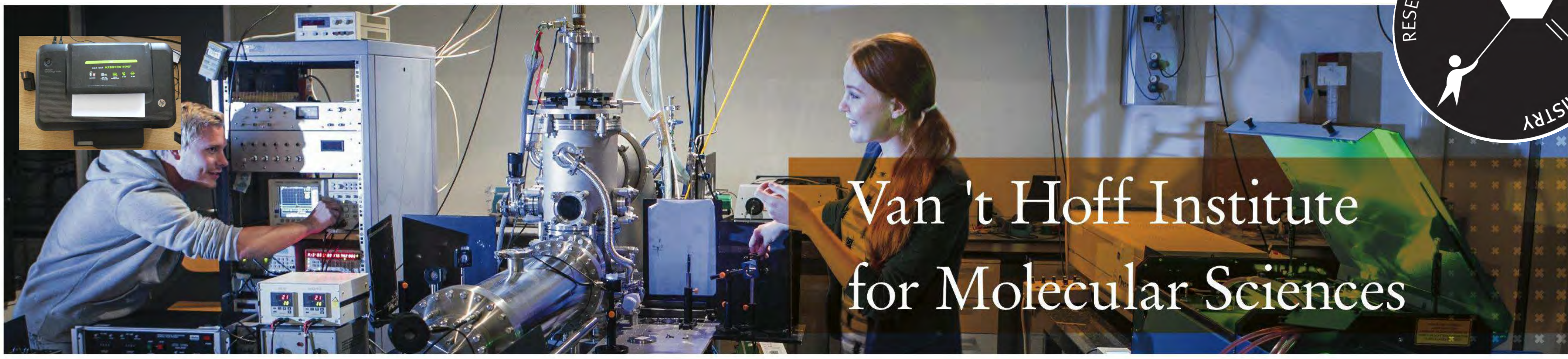
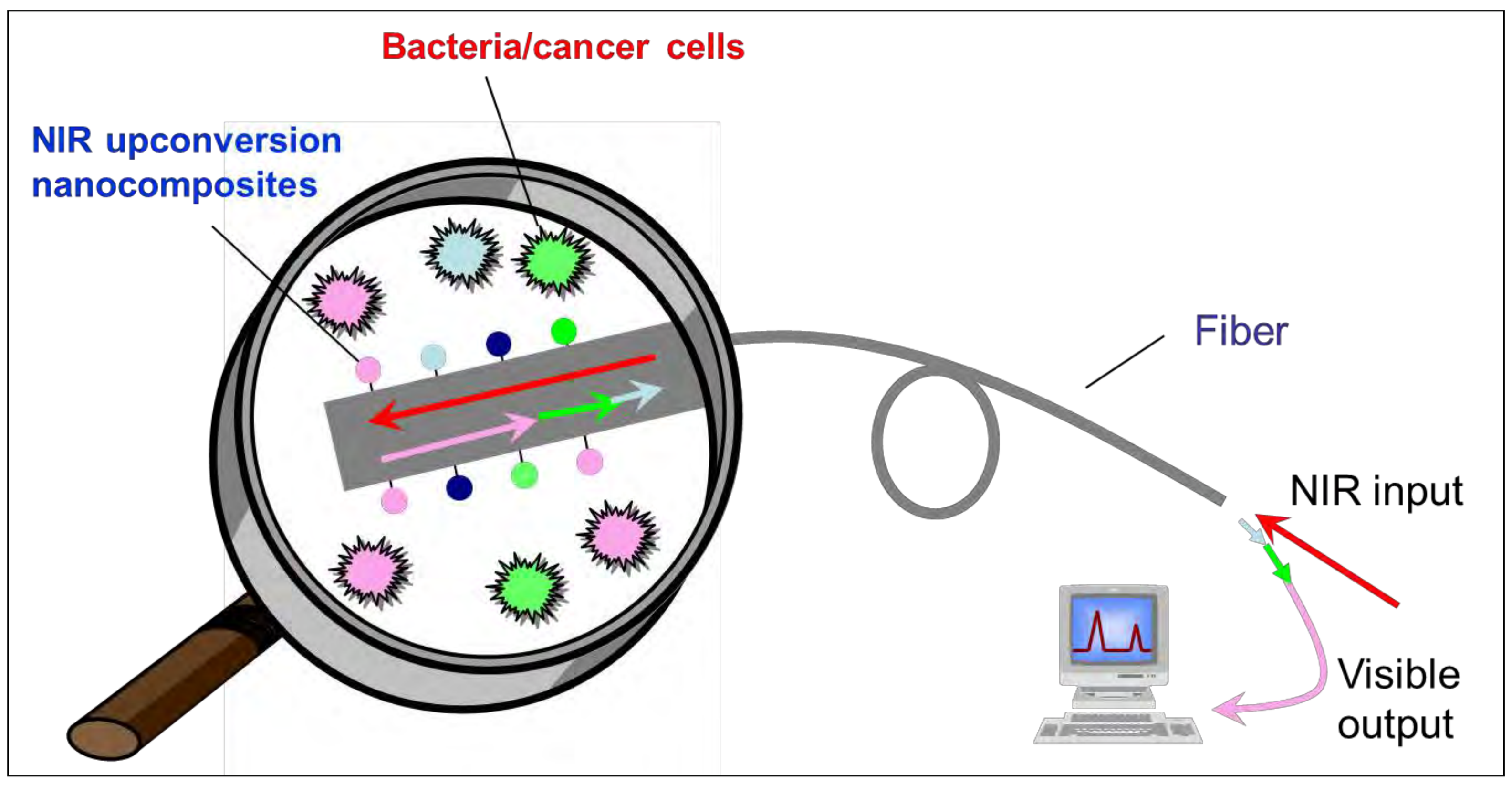


Functional Photonic Nanomaterials

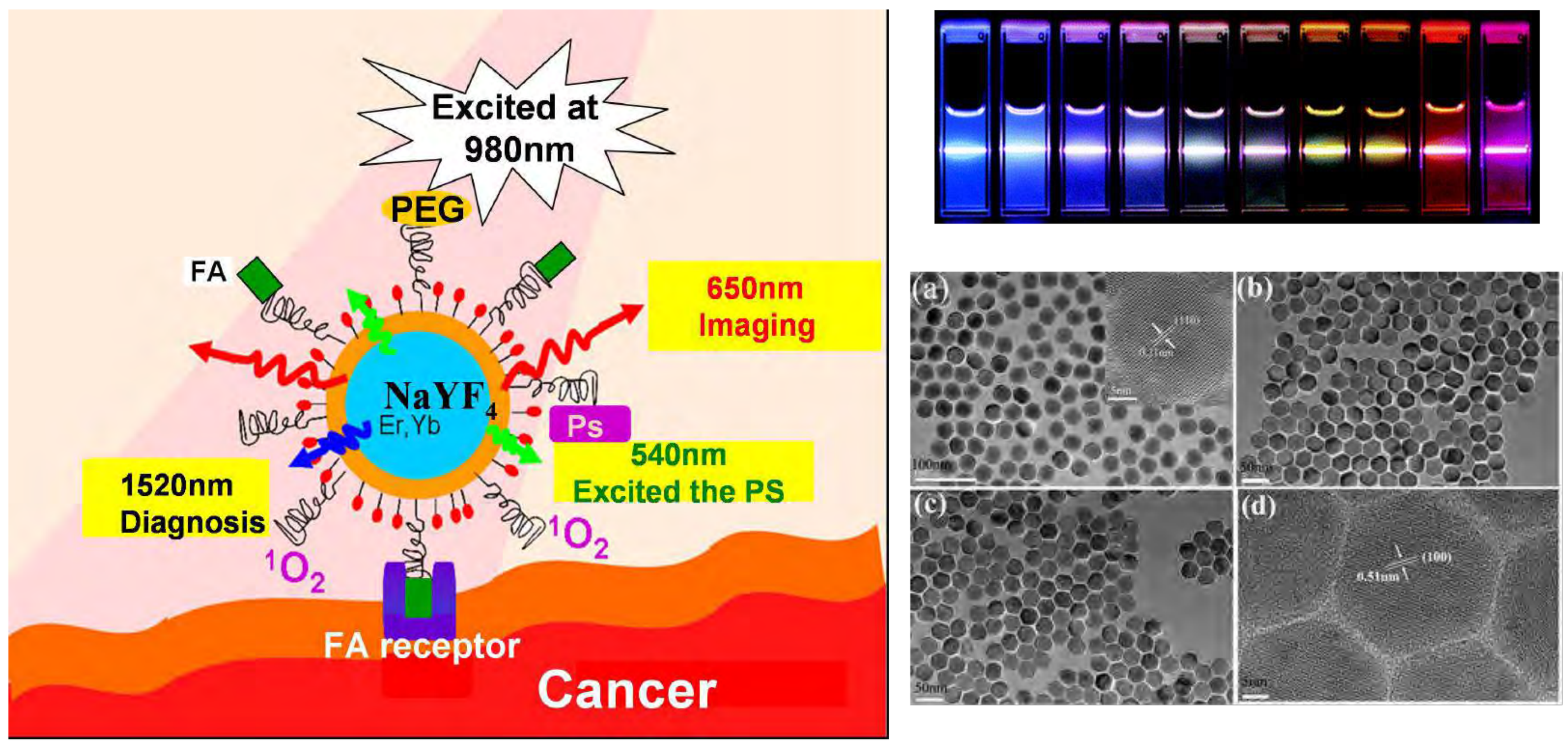
I. On-site Sensing in Biomedicine & Environment Without Background Emission Interference



Features:

- **Homogeneous detection**
  - > "Fishing" detection mechanism
- **Background emission free**
  - > employing NIR upconversion nanoparticles, only the nanoparticles are excited, and emission of surrounding biological entities will not be induced
- **Economic**
  - > fiber & cw NIR diode laser
- **Multiple targeting**

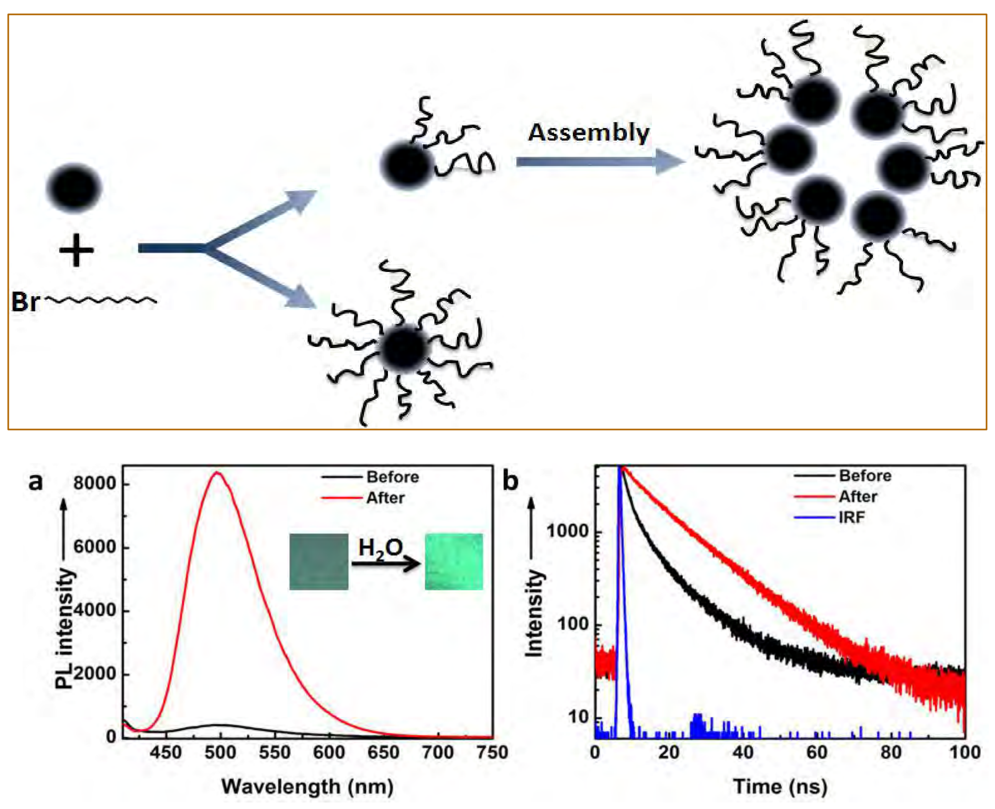
II. NIR Photonic Nanoplatform for Cancer Diagnosis & Therapy at Early Stage



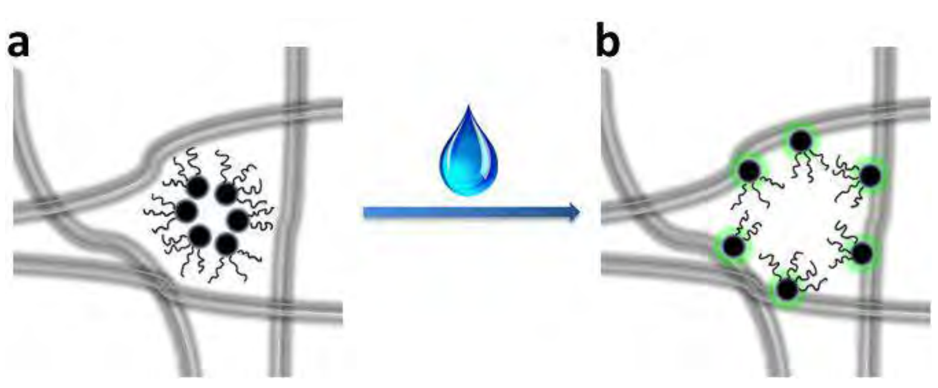
Features:

- **Image-guided photodynamic therapy**
  - > multi-color visible emission upon NIR excitation
- **Background emission free**
  - > NIR can only excite the nanoparticles, not biological background
- **Economic**
  - > cw NIR diode laser
- **Multiple targeting**
  - > Emission spectrum of the upconversion nanoparticles is characteristic of the dopants inside, thus nanoparticles of different dopants can be linked to different determinands based on one-to-one principle.

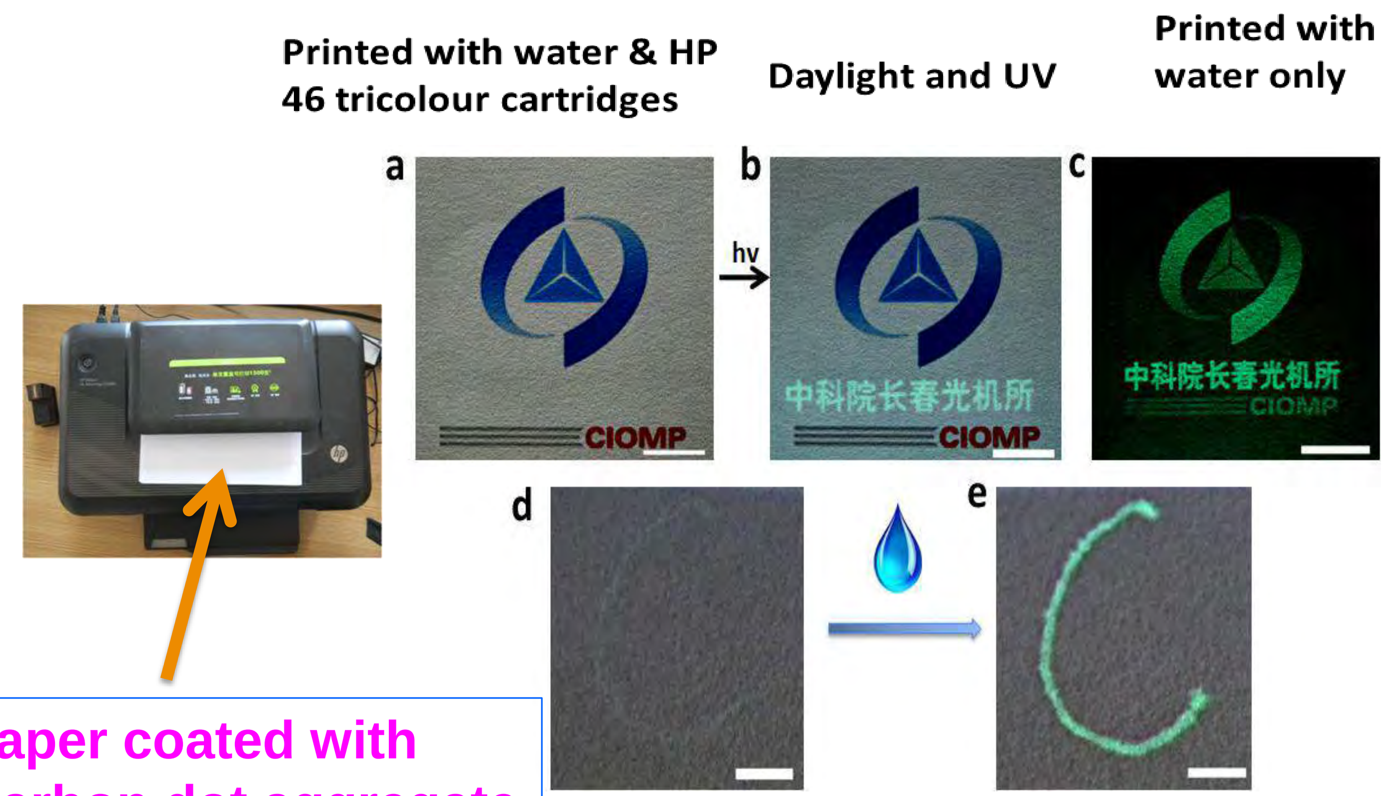
III. Water Printing & Patterning – Luminescent Carbon Nano-bombs



emission bomb formation



bombs merged in paper



paper coated with Carbon dot aggregate

Writing with water pen

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*Also at: CIOMP, Chinese Academy of Sciences and QuantiVision Institute-research center of IMDI.nl

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1. 2011 Amsterdam Science Park Innovation Prize
2. Chem. Soc. Rev., (tutorial review 2014), DOI:10.1039/c4cs00168k.
3. ACS Nano 6 (2012) 4054
4. Biomaterials 35 (2014) 4146

Valorization goals

1. Quick and sensitive on-site detection method
2. New generation of photosensitizers for cancer treatment
3. Environmental-friendly printing and writing technique

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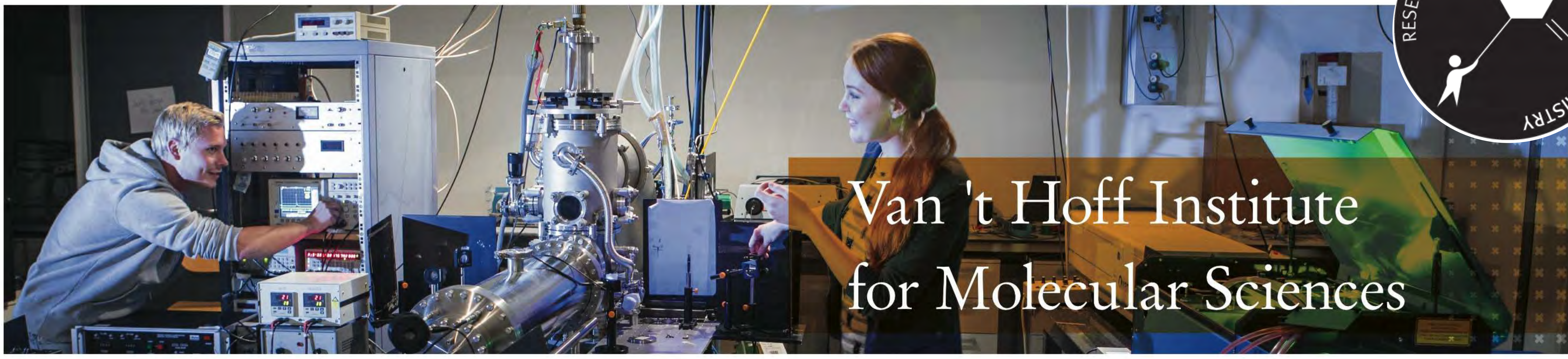
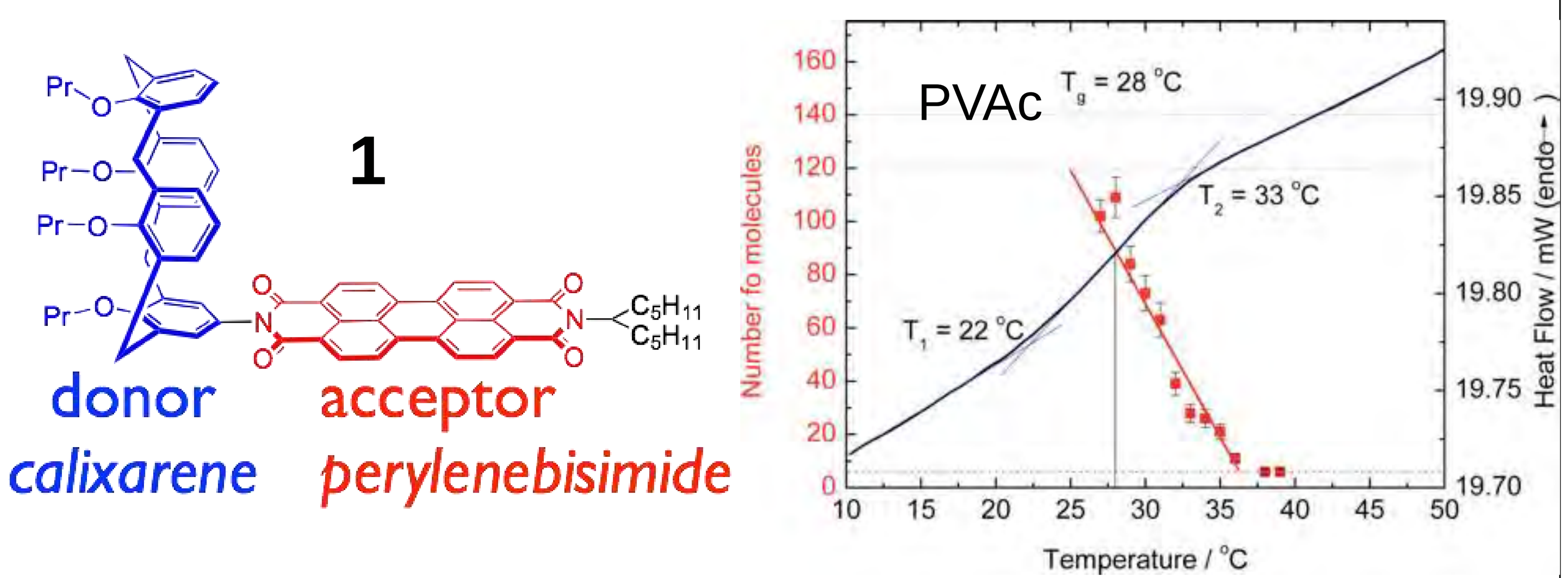


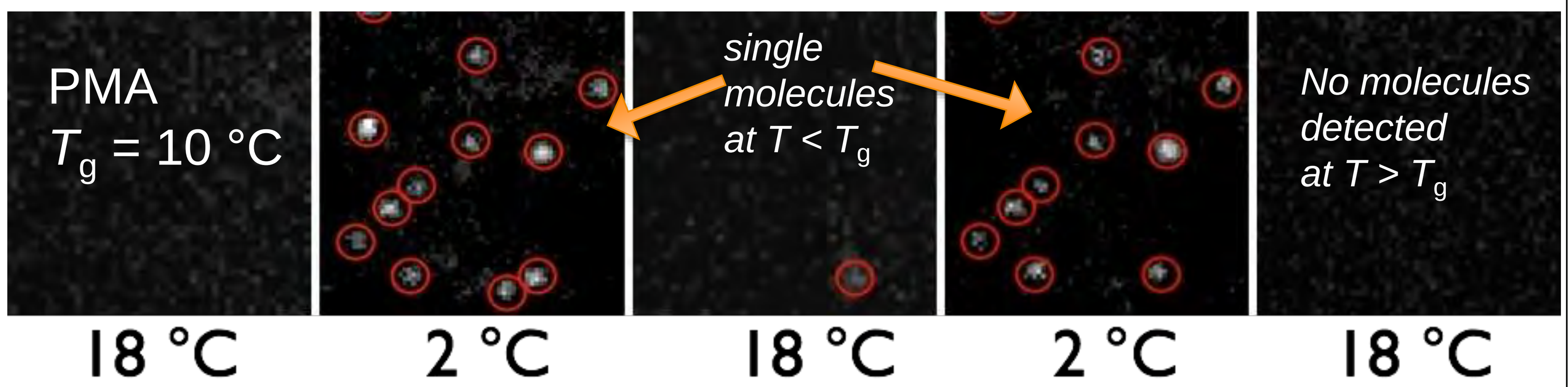
Fluorescence Microspectroscopy in Materials Science

Using a fluorescence microscope we image samples with spatial and temporal resolution and detect fluorescence parameters such as intensity, decay time, spectrum, etc. We apply this to the study of polymer dynamics, film formation in coatings and contact mechanics. Much of the potential of fluorescence microscopy for materials science is yet to be explored.

Single molecule free volume probe

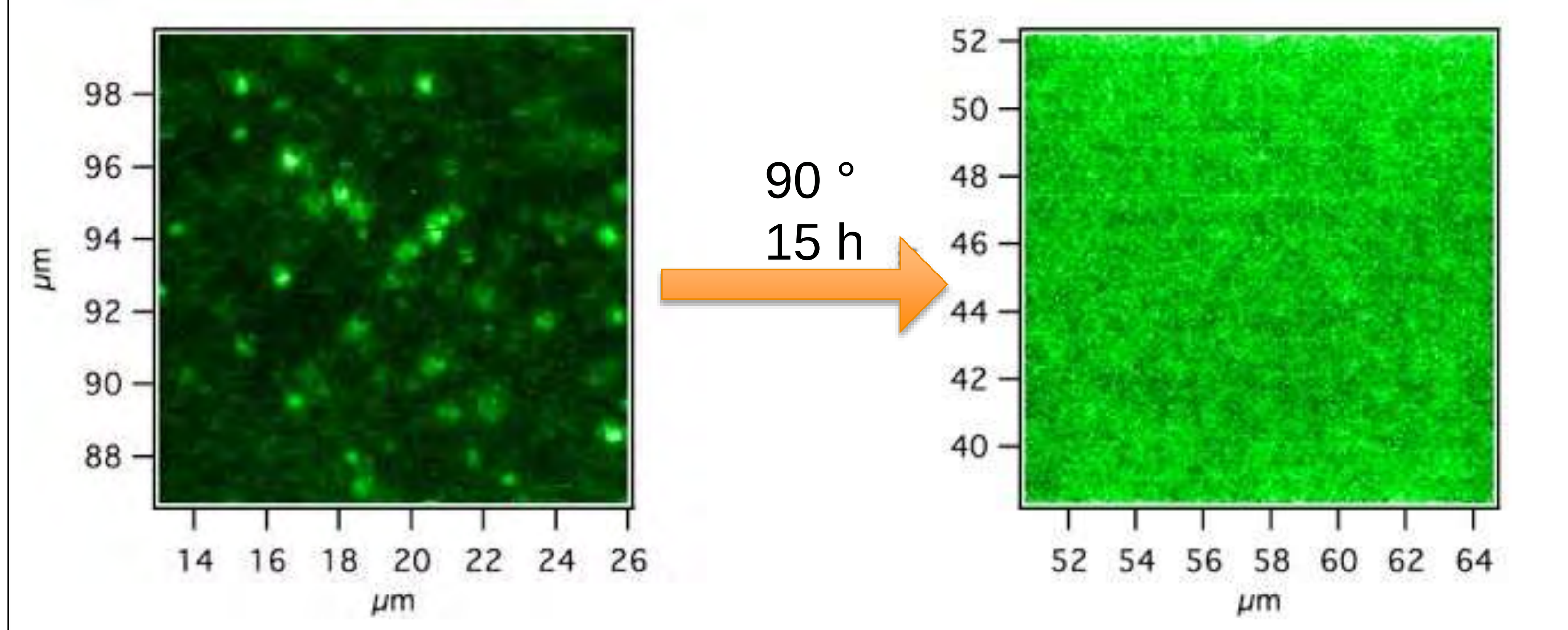
Compound **1** has the unexpected and unique property that it emits fluorescence when in a polymer at temperatures below the glass transition. Increasing the temperature above T_g leads to the disappearance of the fluorescence. This provides an optical method to observe the glass transition.



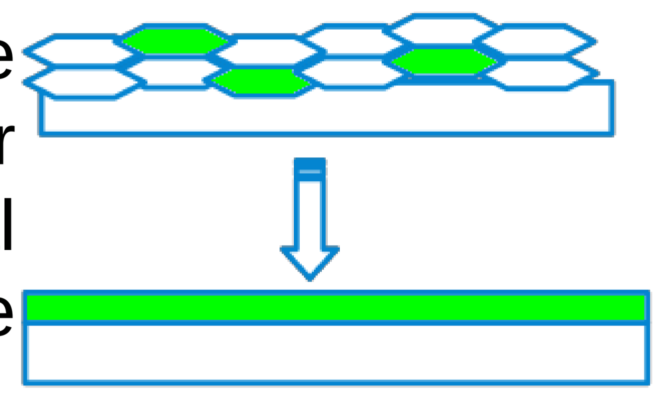


Single nanoparticles visualize latex film formation

Water borne coatings made from latex dispersions require coalescence of the particles in order for a robust film to be formed. We can observe this process directly by labeling the polymer in some particles with a fluorescent dye molecule.



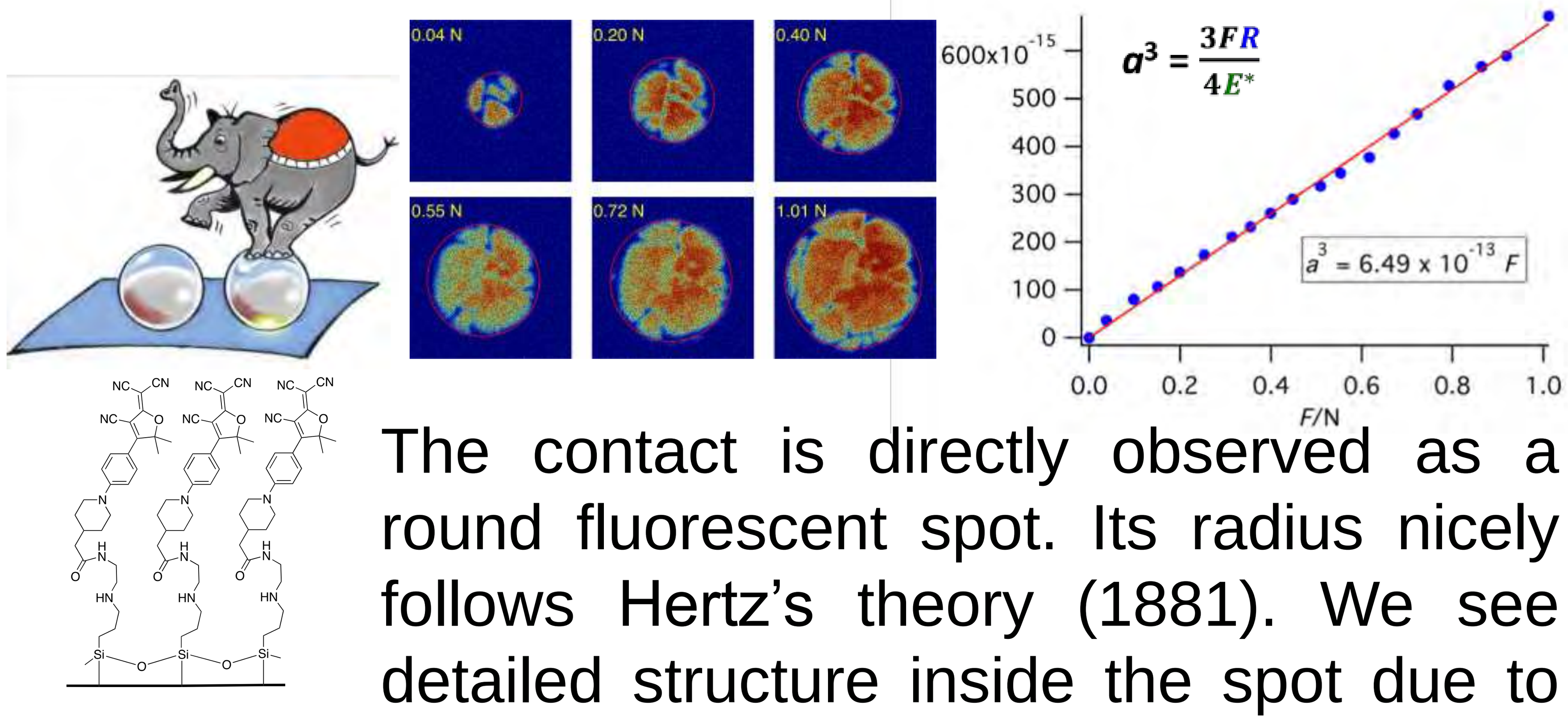
After heating overnight the original particles can no longer be recognized in the confocal image due to diffusion of the fluorescently labeled polymer.



Contact-sensitive fluorescent monolayer

Mechanical contacts between objects control many phenomena, from avalanches to friction. In collaboration with prof. Daniel Bonn (Institute of Physics) we develop methods to visualize contacts using fluorescence microscopy.

A viscosity sensitive molecule is in a monolayer on a glass surface, and a plastic bead is pressed down on it with controlled force. Due to the deformation of the bead, a contact area is formed.



The contact is directly observed as a round fluorescent spot. Its radius nicely follows Hertz's theory (1881). We see detailed structure inside the spot due to the roughness of the surface of the bead.

Molecular Photonics

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References

1. J. R. Siekierzycka, et al., *J. Am. Chem. Soc.*, **2010**, 132, 1240.
2. T. N. Raja, et al. *Colloid. Polym. Sci.*, **2012**, 290, 541–552.
3. T. Suhina et al.submitted, **2014**.

Valorization goals

In these projects we develop tools to enable better understanding of the physical properties of industrially relevant materials

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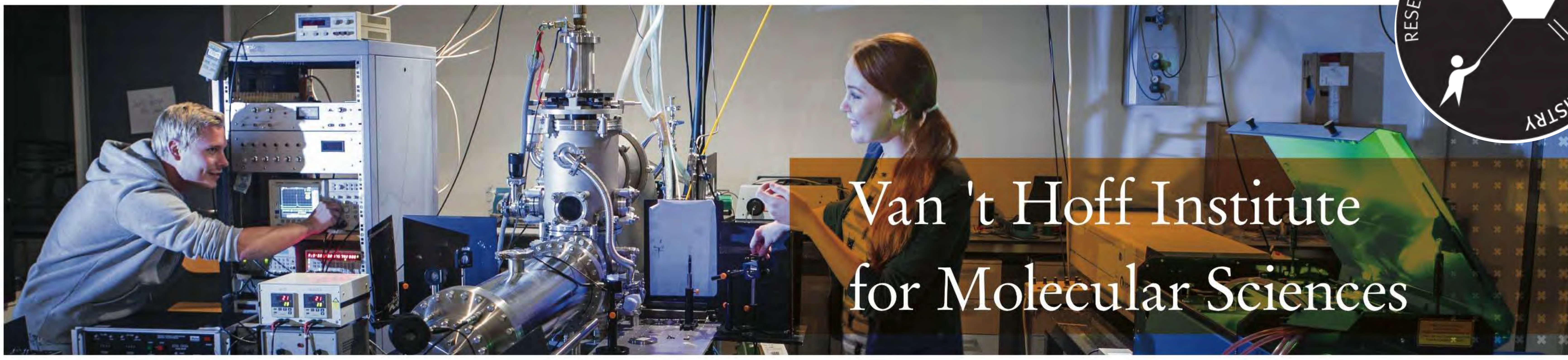
Molecular Photonics



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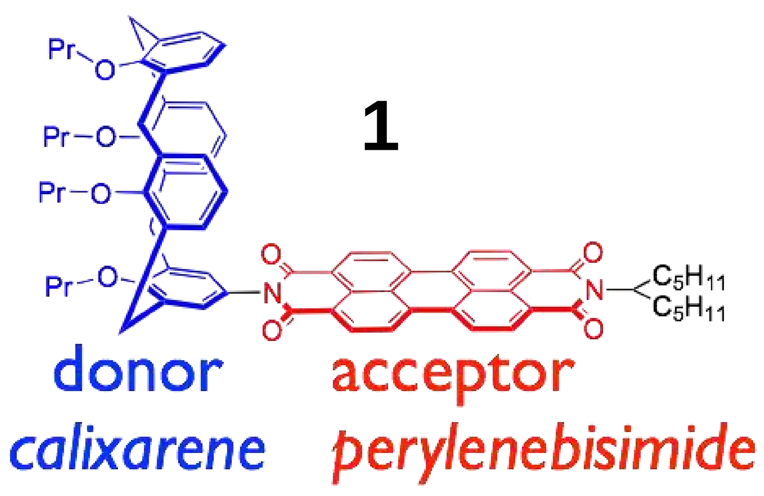

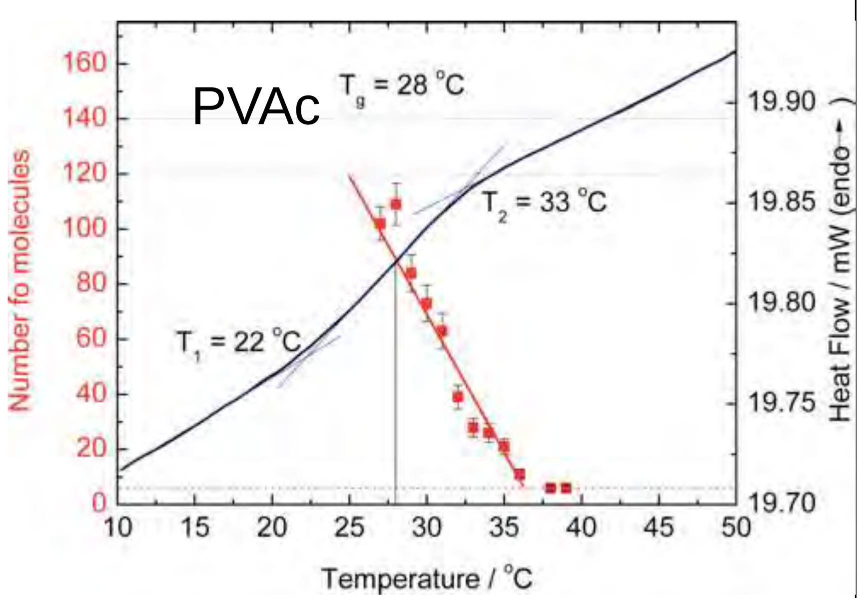

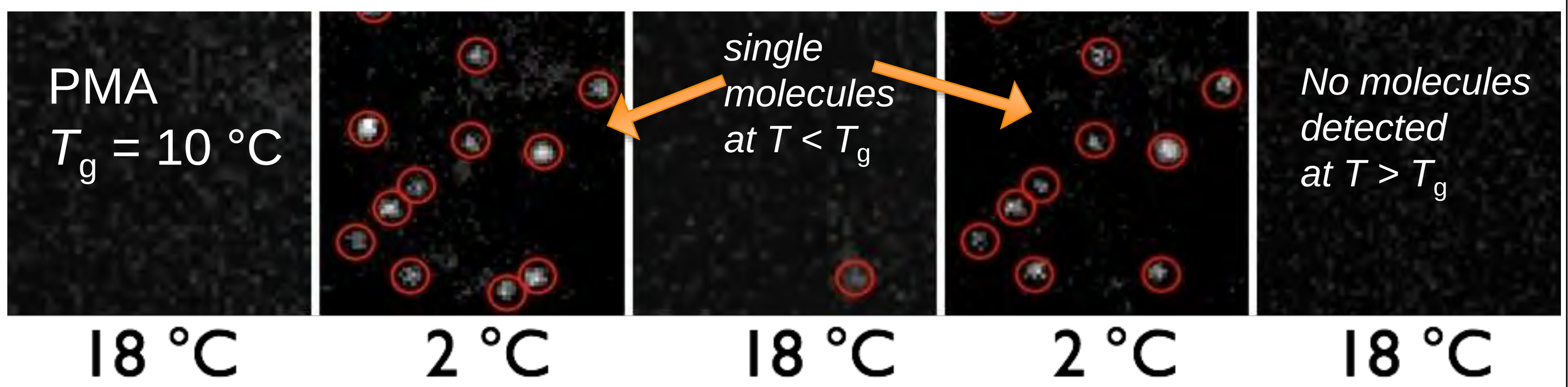

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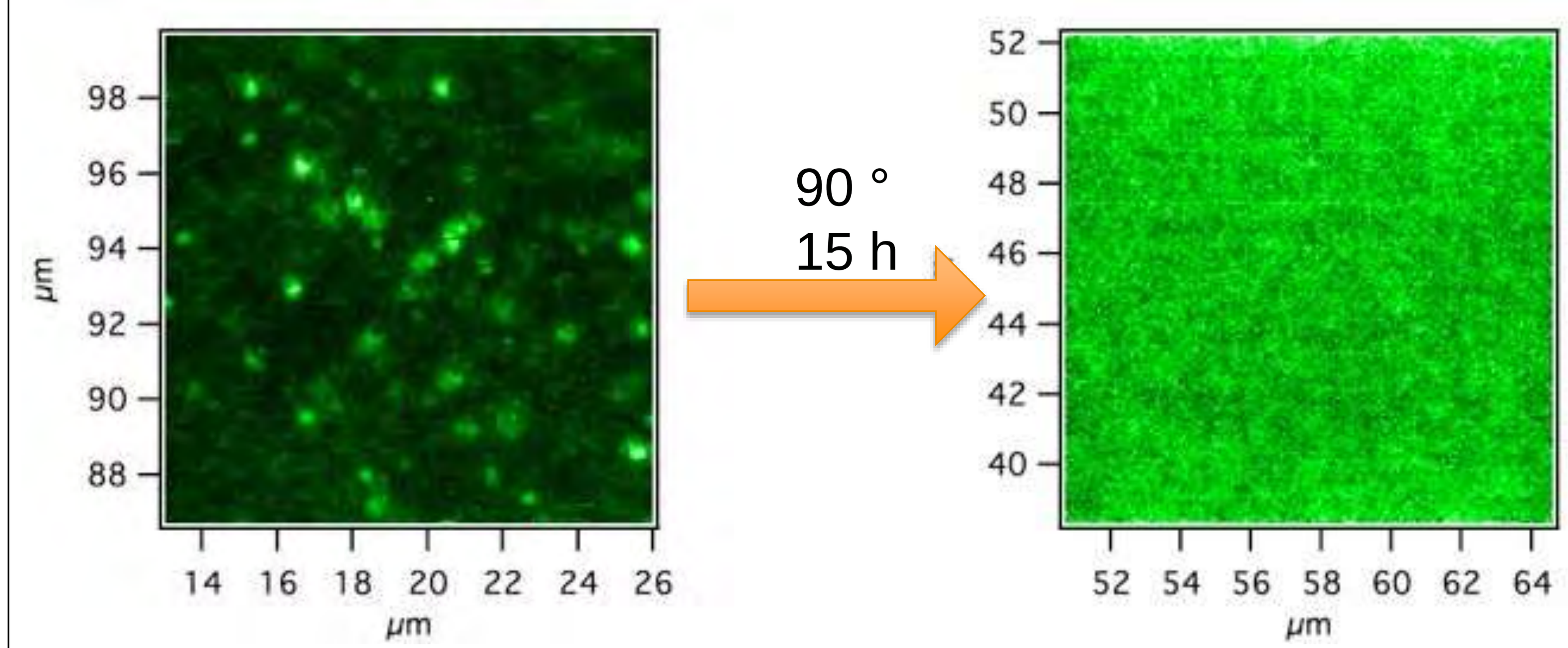

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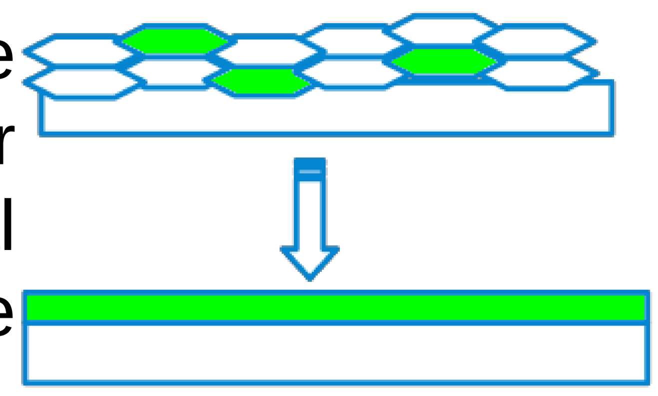

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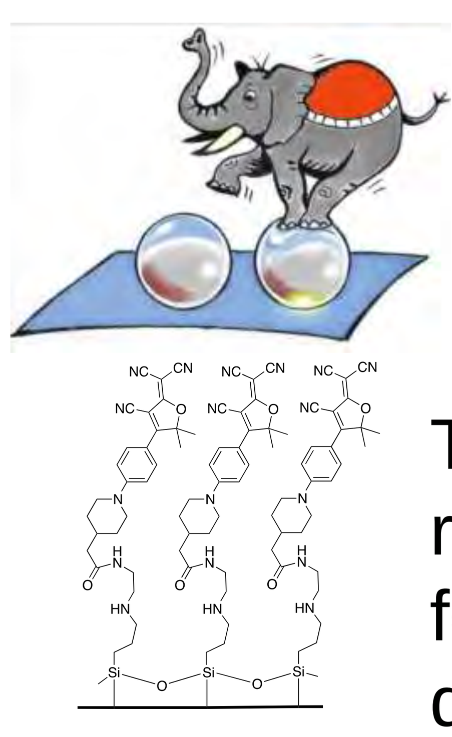

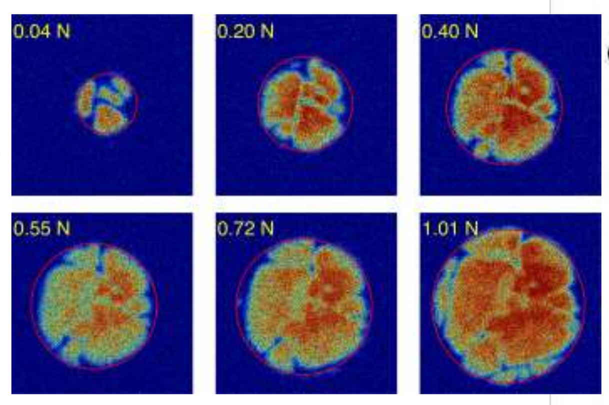

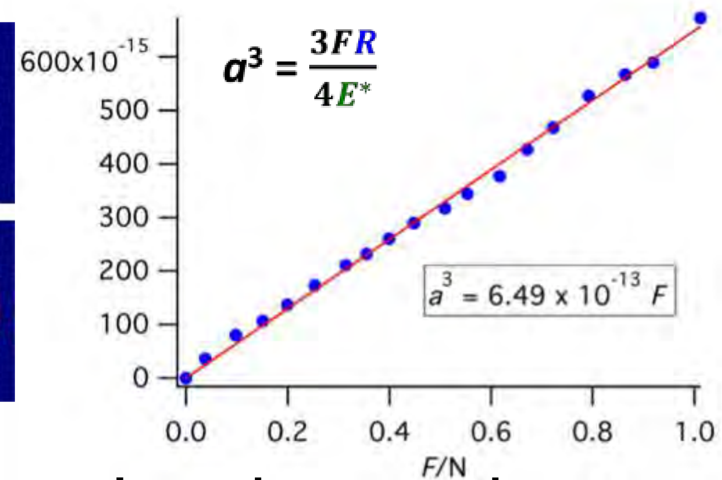

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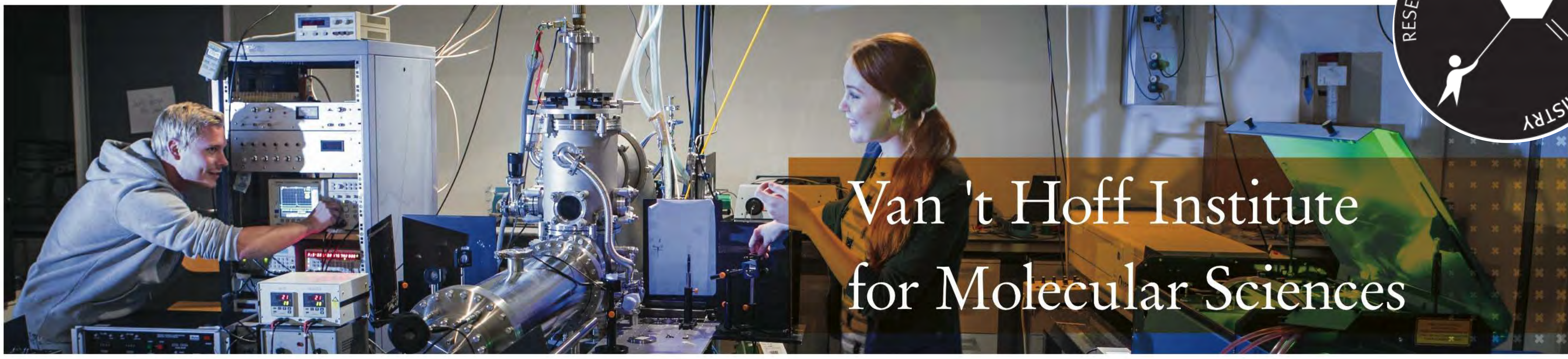
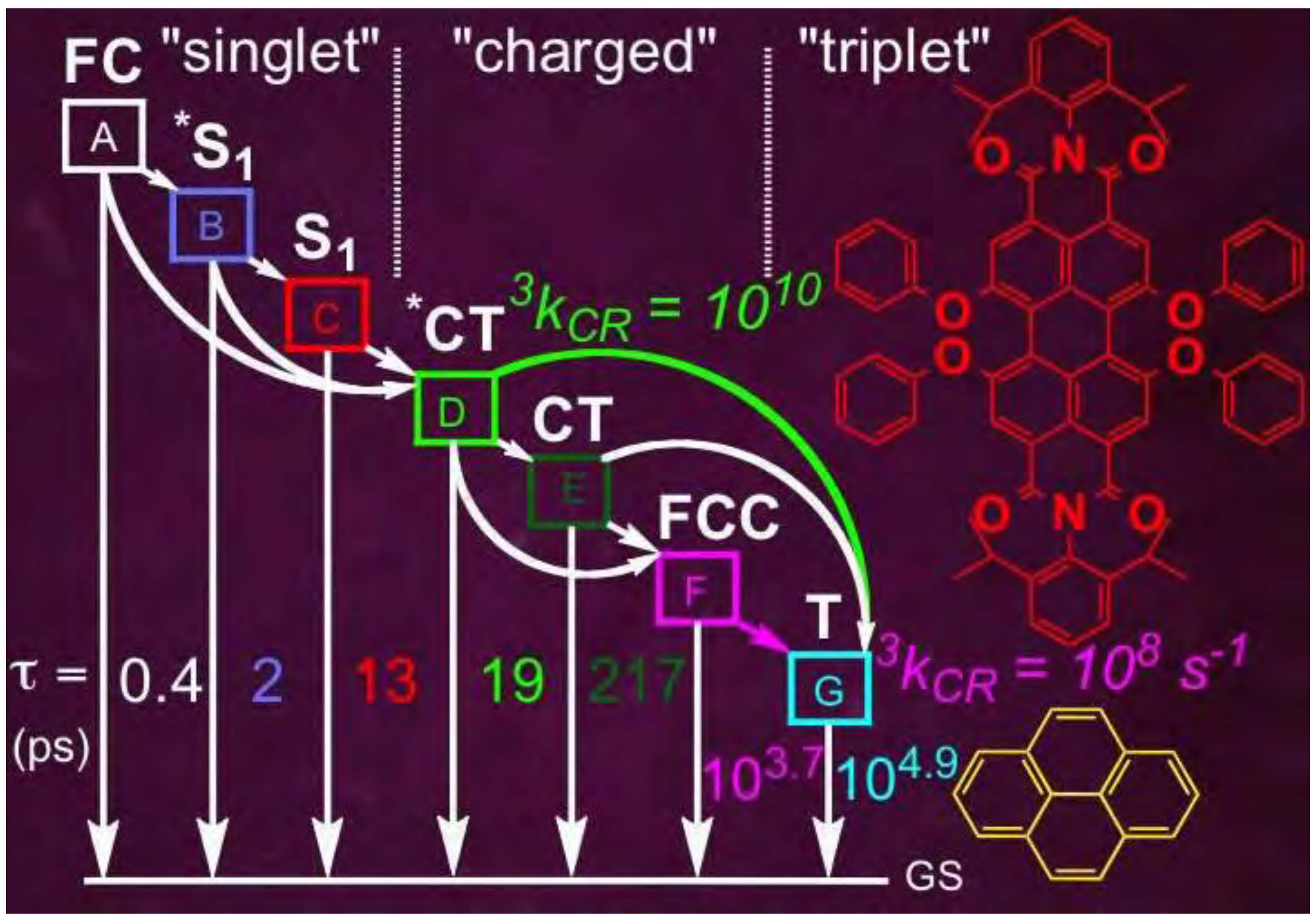


Photoinduced Electron and Energy Transfer in Molecular- Supramolecular- and Nano-systems: from Solar Cells to Solar Fuels

We use (time resolved) spectroscopy, supra-molecular organization and synthesis to get insight into and develop new materials for:

Primary in events in organic photovoltaics.

We focus on thin films containing perylene dyes or low band gap polymers and use fs pump-probe spectroscopy. We probe (non-)geminate charge recombination to the triplet state as charge loss.



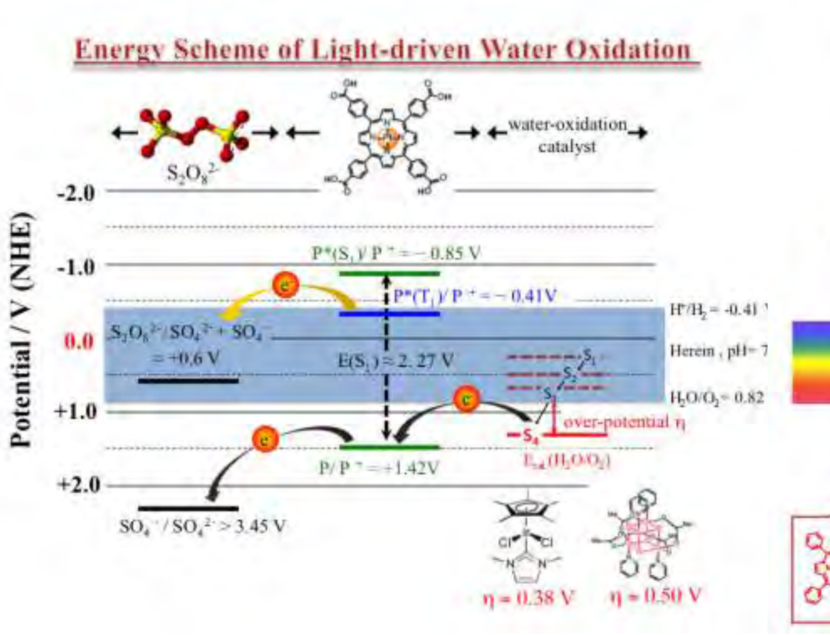
Primary in events in organic photovoltaics

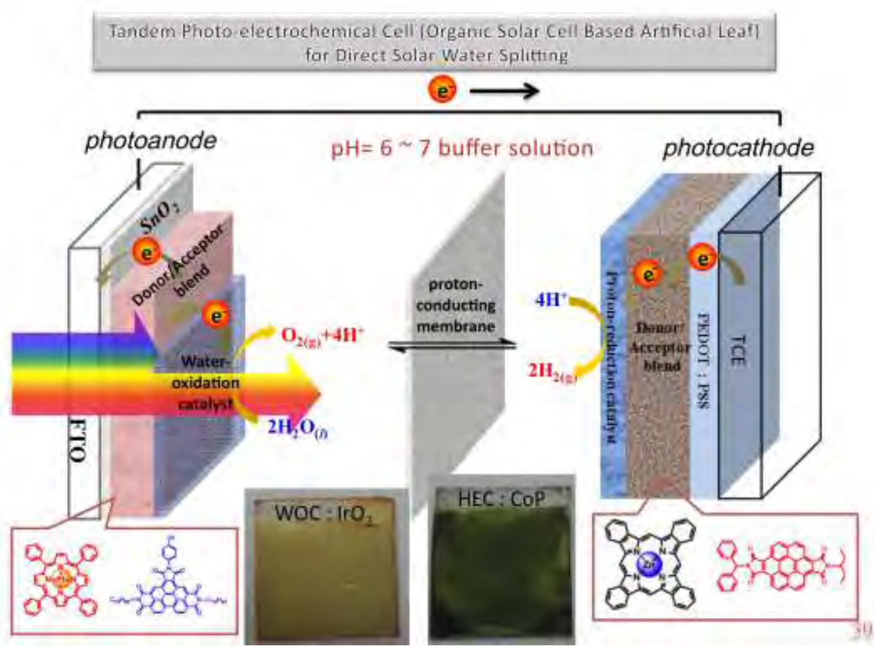
Photosensitizers for water oxidation and proton reduction in organized nano-materials.

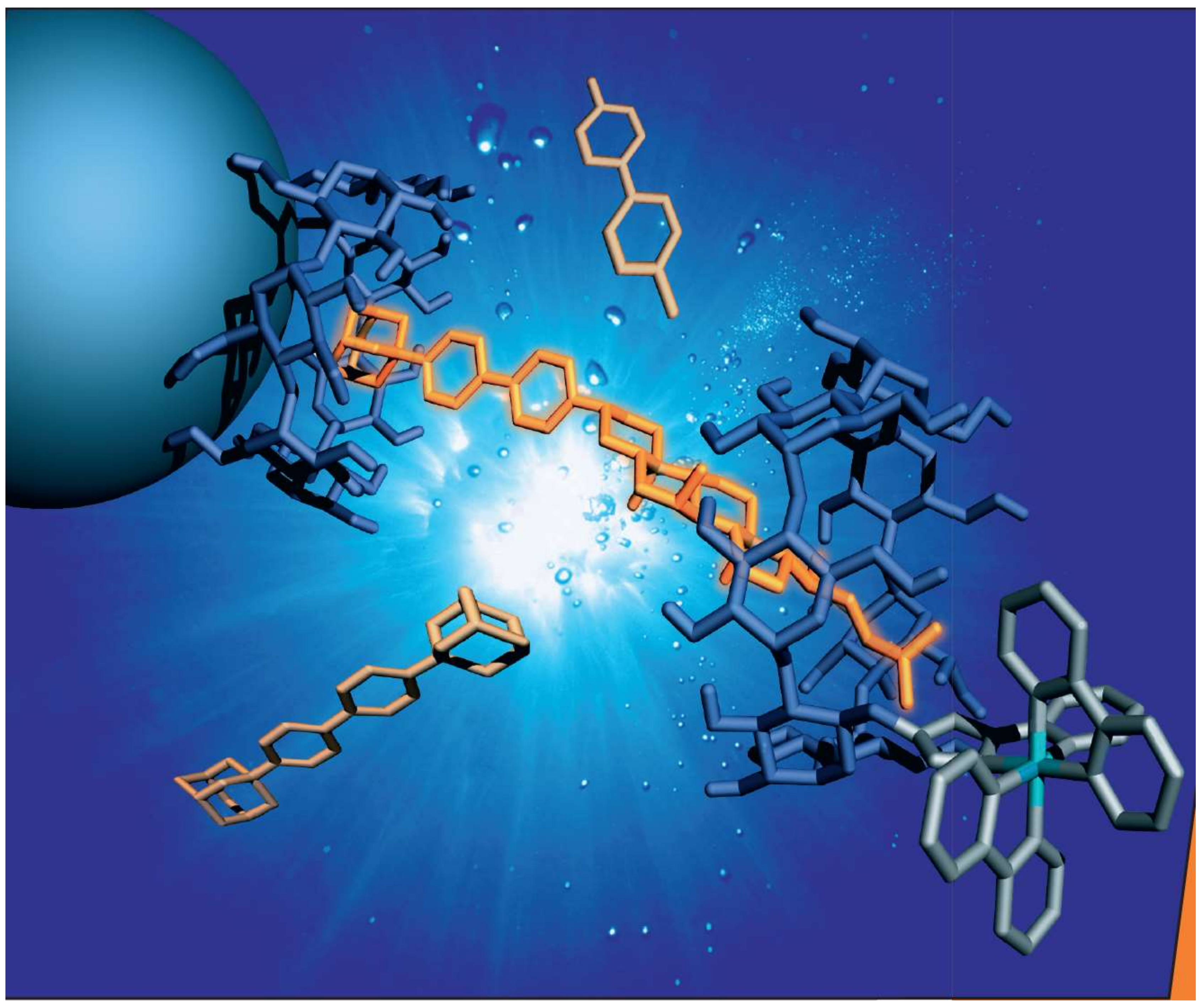
PS: Metal porphyrines, Ir and Ru complexes.

WOC: Ir and Co nanoparticles + complexes.

HEC: Pt and CoP nanoparticles.







Photoinduced proton reduction.

Metal organic frameworks containing perylene-bis(dicarboximides) for photocatalysis.

We use N-pyridyl as well as N-carboxyphenyl PDI compounds and focus on CO_2 fixation.

Photodynamic therapy. Using light to save lives. Anti-cancer, anti-bacterial, anti-inflammatory and immune-activating applications. NIR absorbing nanomaterials. *H2020 ITN project in development, looking for extra industrial partner.*

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References

DOI: 10.1021/jp402086p
DOI: 10.1002/ejoc.201200886
DOI: 10.1039/C0CP02867C

Valorization goals

Converting the energy of photons into usable energy, electricity and fuels.

Using light to save lives.