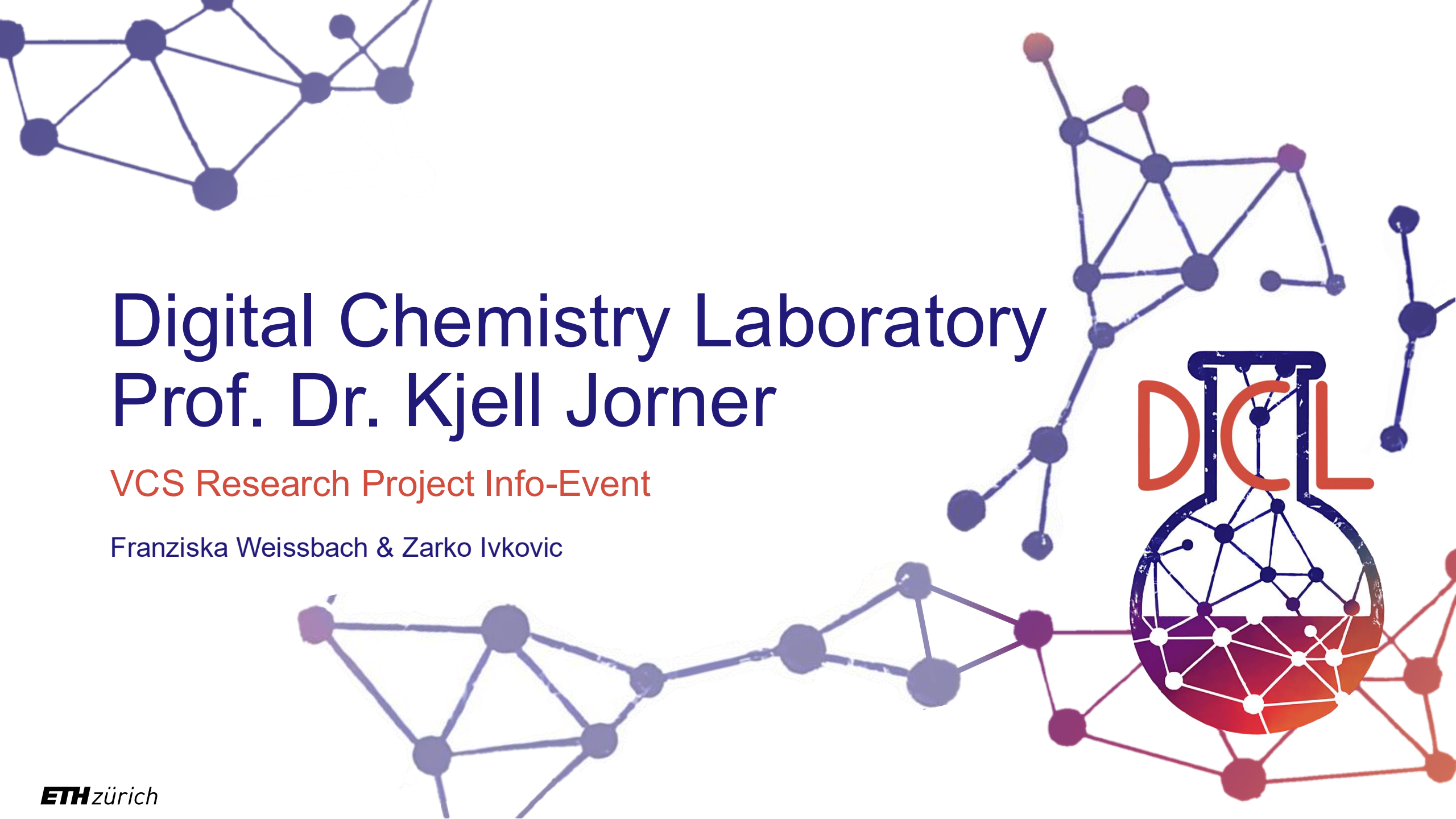


The background of the slide features a complex, abstract molecular network. It consists of numerous dark blue and purple nodes connected by thin lines, forming a web-like structure that spans the entire frame. In the lower right quadrant, there is a prominent graphic of a round-bottom flask. The flask is filled with a red-to-orange gradient liquid. Inside the flask, a white molecular structure is visible. Above the flask, the letters 'DCL' are written in a large, bold, orange font. The overall aesthetic is scientific and digital.

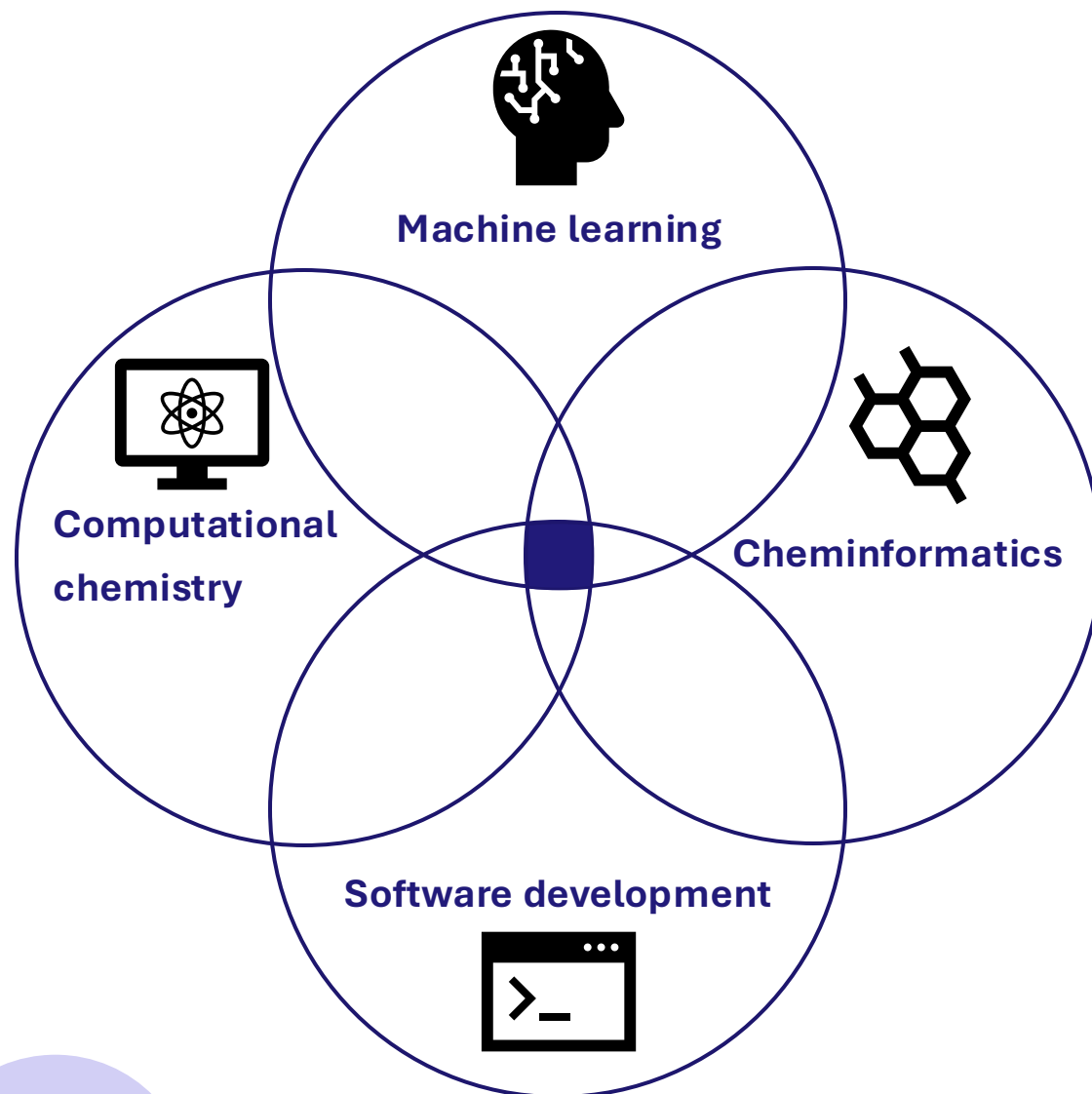
Digital Chemistry Laboratory

Prof. Dr. Kjell Jorner

VCS Research Project Info-Event

Franziska Weissbach & Zarko Ivkovic

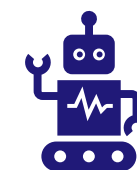
Digital Chemistry



Lab chemists



High-throughput
experimentation



Self-driving labs

Mission: Accelerate chemical discovery with digital tools



Strategic core research



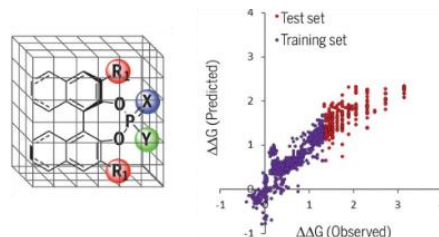
Opportunity-driven

Reactivity and catalysis

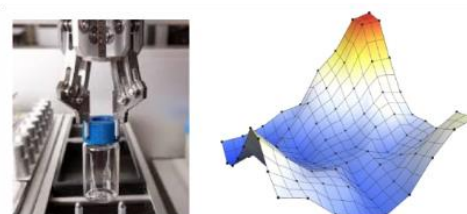
Computer-aided molecular design

Organic electronic materials

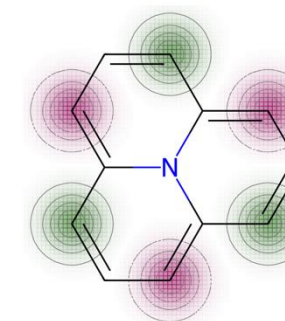
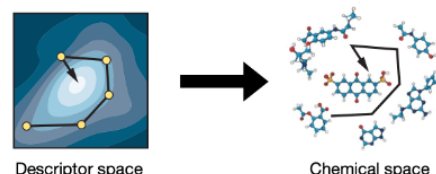
Reaction outcome prediction



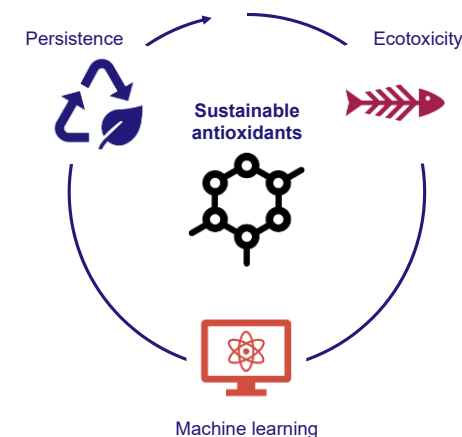
Reaction optimization



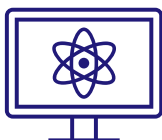
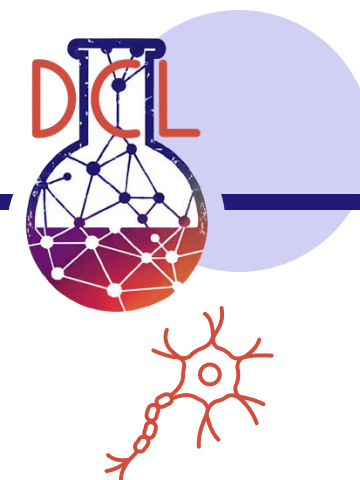
Catalyst & reaction design



Safe and sustainable by design

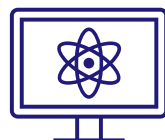


Our niche: Models in the low-data regime

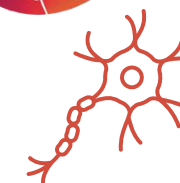
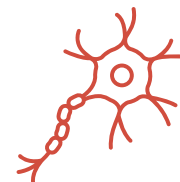


Simulations

No data



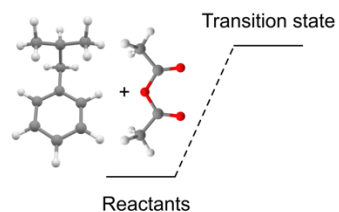
Chemistry-informed
machine learning



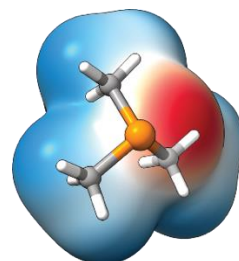
Machine learning

Lots of data

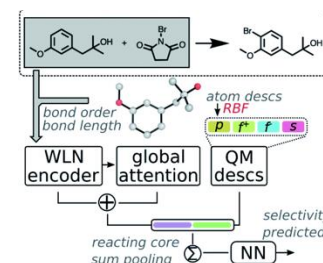
Mechanistic DFT



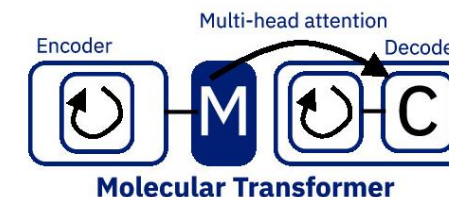
Chemical descriptors



Chemistry-augmented deep learning



Deep learning



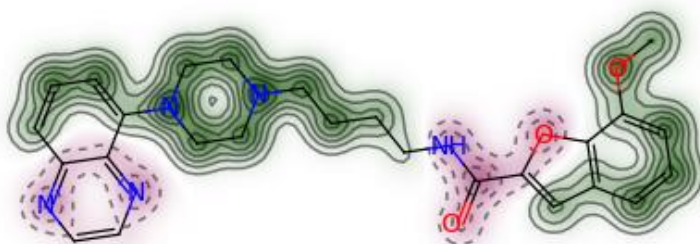
Examples of recent student projects



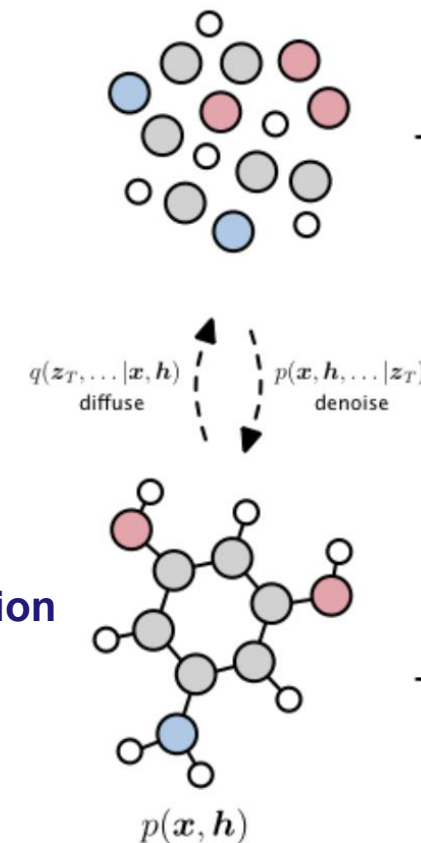
Developing ML models for antioxidant activity prediction

Fine-Tuning of Diffusion Models for Molecule Generation

Integrating numerical descriptors into language models for property prediction



Delta learning for the prediction of reaction barriers in combinatorial libraries



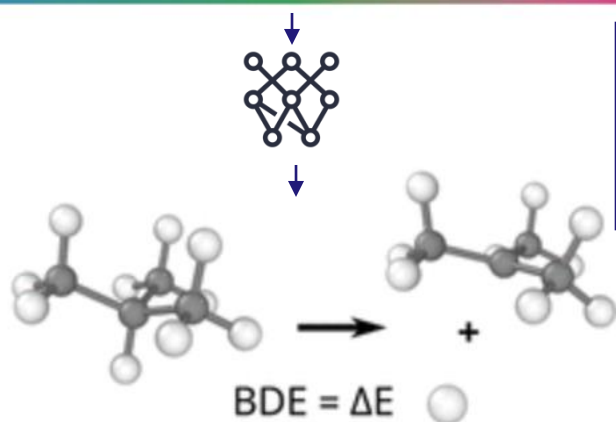
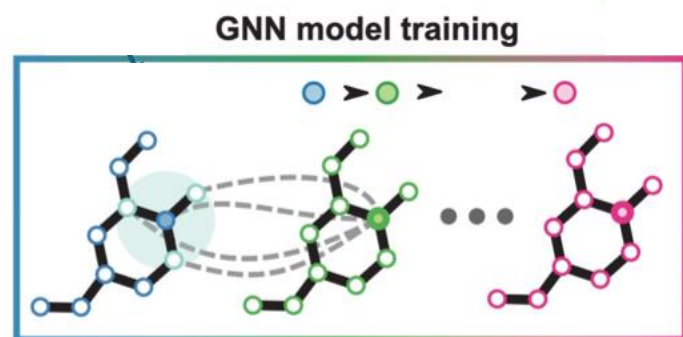
Upcoming projects



Big picture: De-novo computational design of safe and sustainable antioxidants

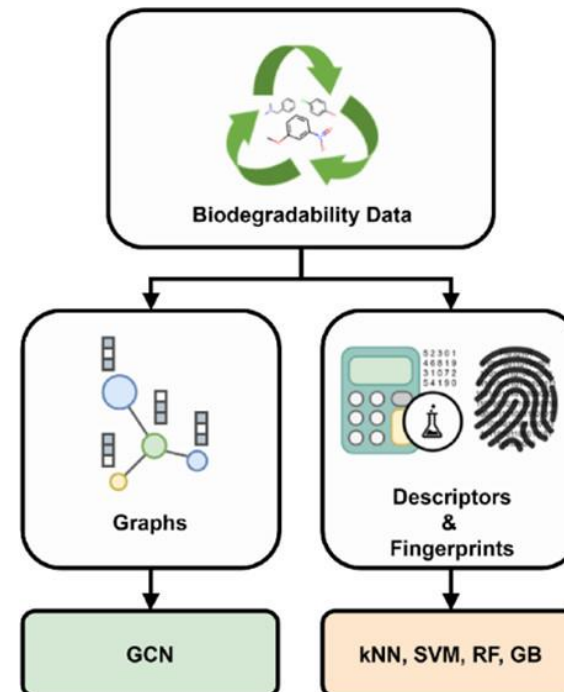
Finetuning a GNN for BDE prediction

ML models for biodegradation



Project requires:

- Running DFT calculations
- Pretraining and finetuning a neural network



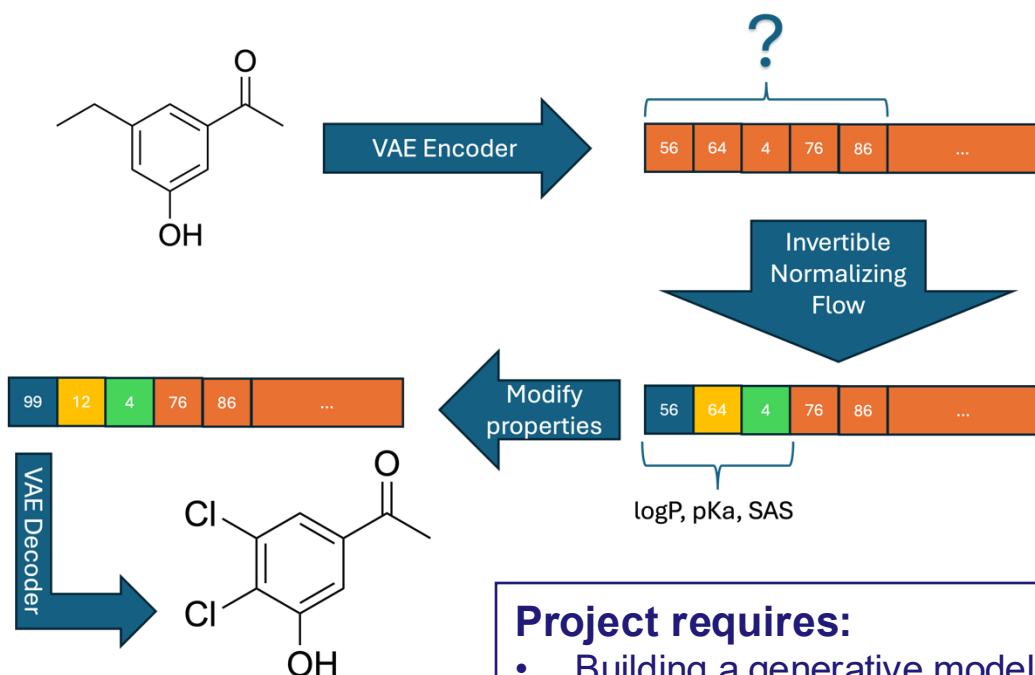
Project requires:

- Data curation
- Training simple ML models

Upcoming projects



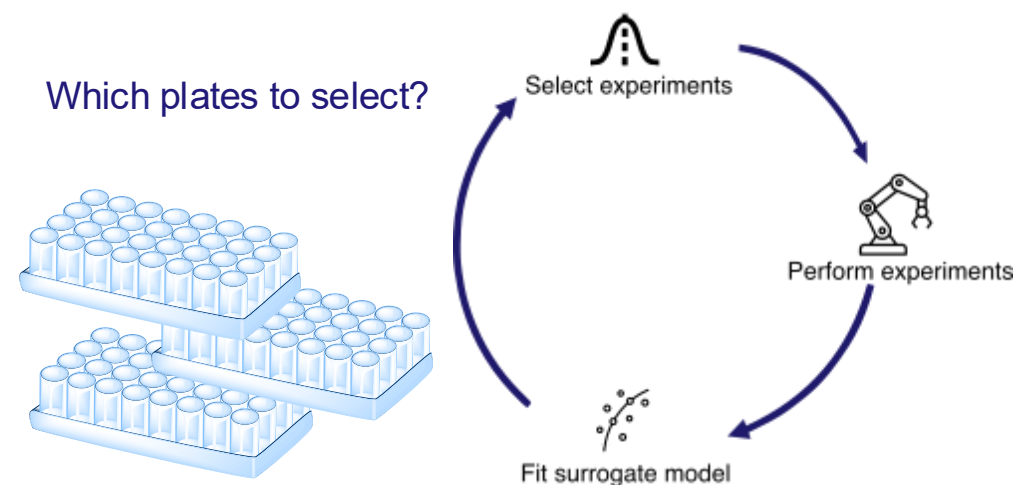
Optimising molecular properties in reorganized latent space



Project requires:

- Building a generative model
- Chemical analysis of results

Bayesian Optimization over wellplates



Project requires:

- Mathematical thinking
- Use of ML workflows

The Digital Chemistry Laboratory

Department of Chemistry and Applied Biosciences (D-CHAB)
Institute of Chemical and Bioengineering (ICB)



Principal investigator

Prof. Dr. Kjell Jorner

PhD students

Lauriane Jacot-Descombes

Giustino Sulpizio

Stefan Schmid

Luca Schaufelberger

Franziska Weißbach

Zarko Ivkovic

Ghali Sekkat

Aline Hartgers



Post-doc

Dr. Hanwen Zhang

Contact us!

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zivkovic@ethz.ch

HCI E133-135



@dcl-ethz.bsky.social



Doing a Semester Project in the Reiher Research Group

21.05.2025

Overarching Goal

- Develop a theoretical framework for chemistry which is
 - fully predictive
 - applicable to any chemical system
 - straightforward to use
- This endeavour requires advances in many areas
- Hence, research in the Reiher group is very diverse

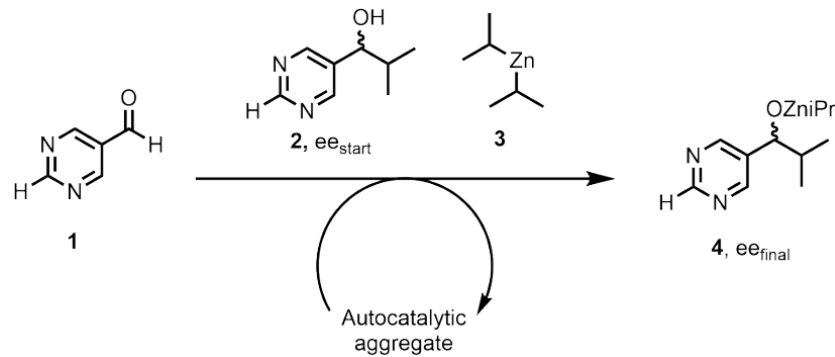
Research Areas

- Exploration of Chemical Reactions and Reaction Networks
- Theoretical Spectroscopy
- Development of Highly Accurate Methods
 - Density Matrix Renormalization Group
 - Pre-Born-Oppenheimer Theory
 - Relativistic Quantum Chemistry
- Embedding Approaches for Complex Systems
- Uncertainty Quantification
- Machine Learning
- Haptic and Interactive Quantum Chemistry
- Quantum Computing

Organizational Aspects

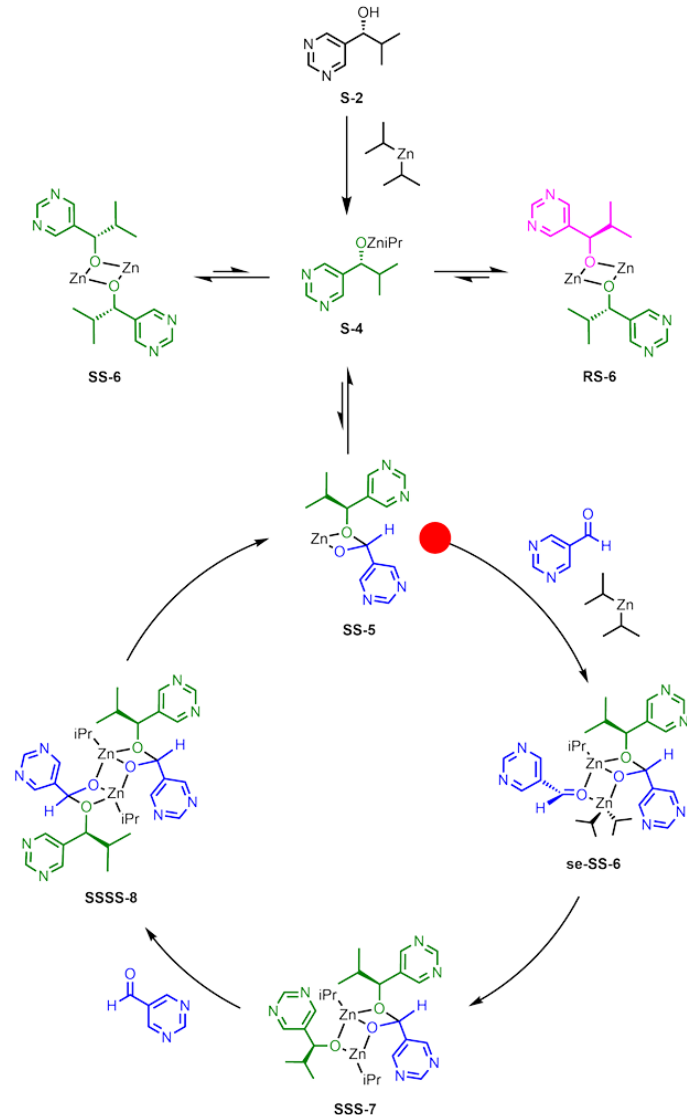
- Every project is tied to and important for our research
- Hence, the list of possible topics is very dynamic
- An experienced PhD student or PostDoc will oversee your project and help you
- Timewise, the organization of the project is very flexible (e.g., 14 weeks half-day, 7 weeks full-time)
- You are required to write a report and present your project at the end of the semester in the group's seminar

Example Project 1: Exploring the Soai Reaction



- The Soai reaction is an alkylation of the carbaldehyde **1** with diisopropylzinc **3**
- The reaction is autocatalytic
- Starting with a low enantiomeric excess of **2**, one obtains a product with very high enantiomeric excess
- Important model system for studying the origin of homochirality
- Discovered 1995, still not fully understood

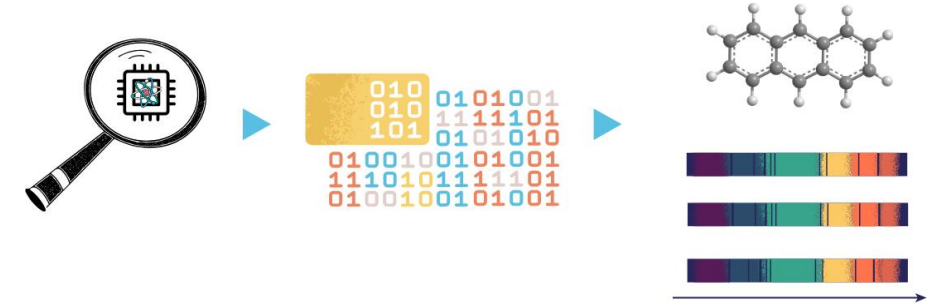
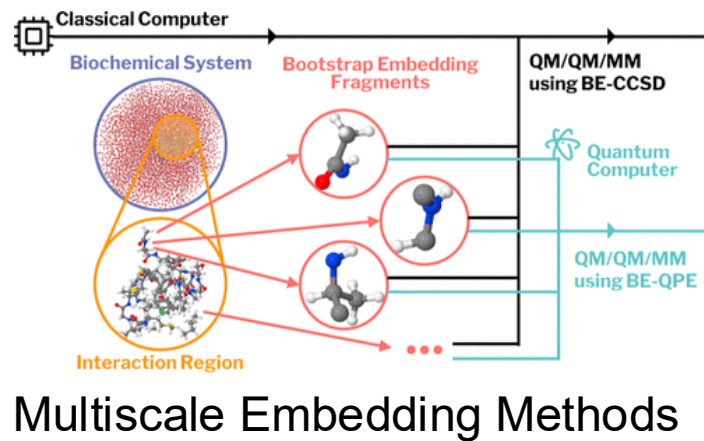
Example Project 1: Exploring the Soai Reaction



- We explored the catalytic cycle (starting point marked with red dot)
- We develop our own software called SCINE Chemoton to explore complex reaction networks
- In this project, we discovered 15'148 reactions and 8'188 compounds
- Such studies can lead to a more complete understanding of the Soai reaction

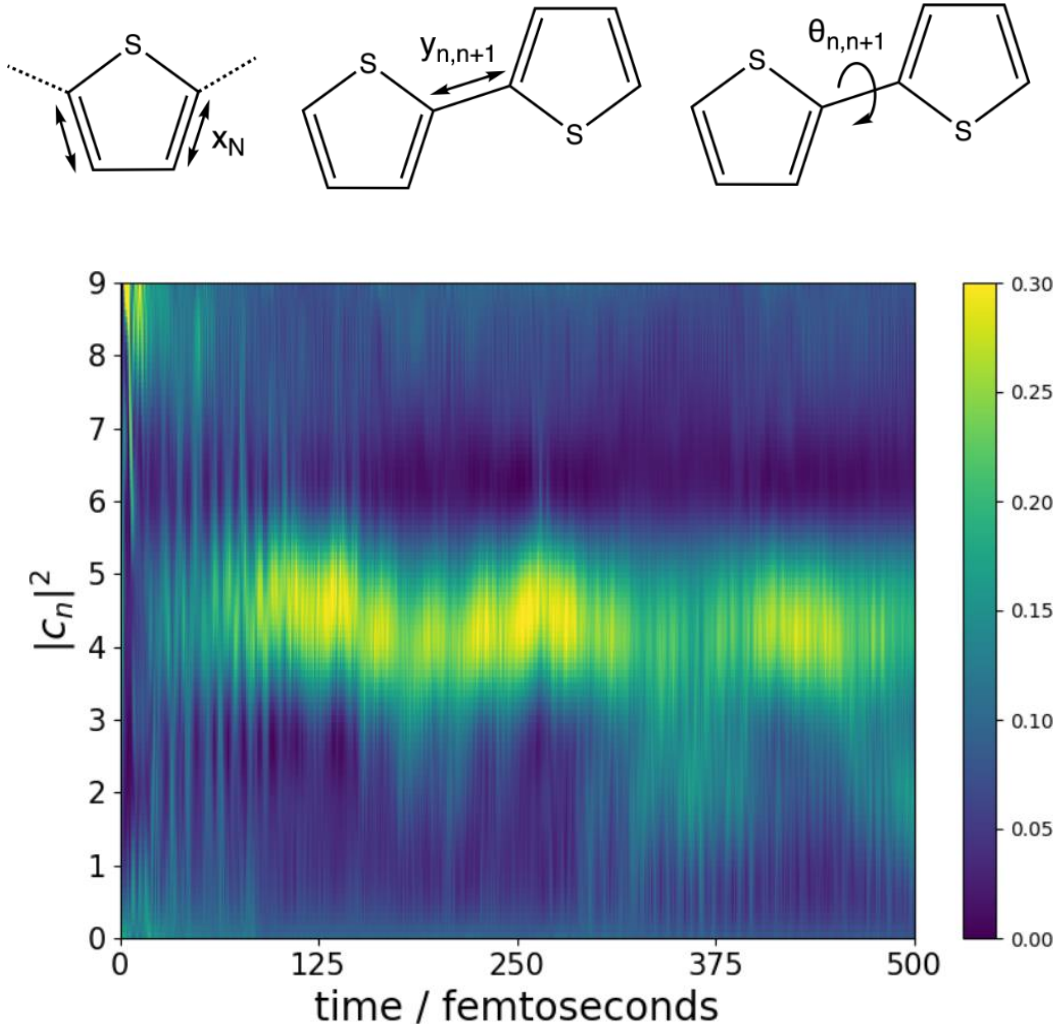
Quantum Computing for Quantum Chemistry

- Theoretical chemistry is a killer application for quantum computers
- Goal: Make Quantum Computers Useful for Chemistry



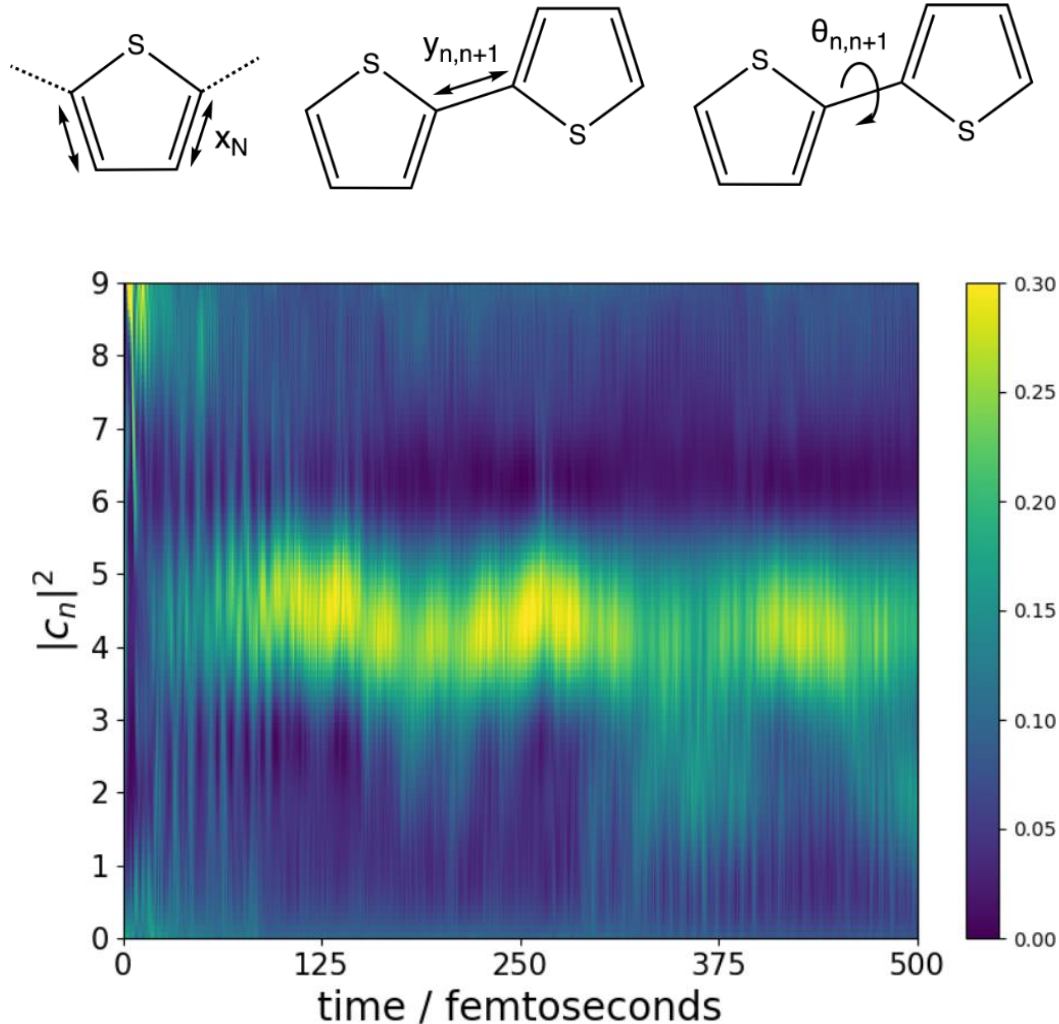
Molecular Property Evaluation

Example Project 2: Exciton Dynamics with TD-DMRG



- Implementing a new model Hamiltonian in our tensor network software "QCMaquis" and running time-dependent calculations with it on a chemically relevant system
- Timeline/Tasks
 - Literature review & getting familiar with the code
 - Implementing the new model Hamiltonian
 - Choosing a relevant, feasible and interesting chemical system
 - Run the TD-DMRG calculations
 - Post processing, plotting results
 - Write the report

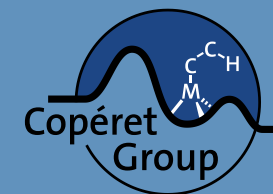
Example Project 2: Exciton Dynamics with TD-DMRG



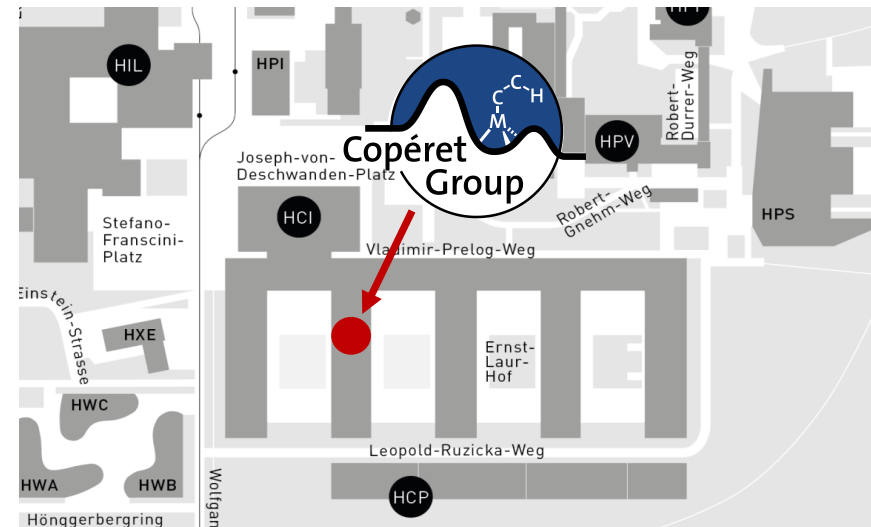
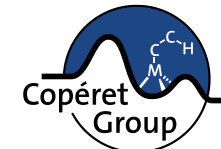
- Implementing a new model Hamiltonian in our tensor network software "QCMaquis" and running time-dependent calculations with it on a chemically relevant system
- Suggested prerequisites
 - Interest in theoretical chemistry
 - Some basic knowledge in theoretical chemistry (e.g., from QC and AQC lectures)
 - Some basic knowledge and interest to program (Python, C++)

Research in the Copéret Group: Catalysis and Sustainable Chemistry using Molecular Principles

Mattia Ciuoli, PhD Student
21st May 2025

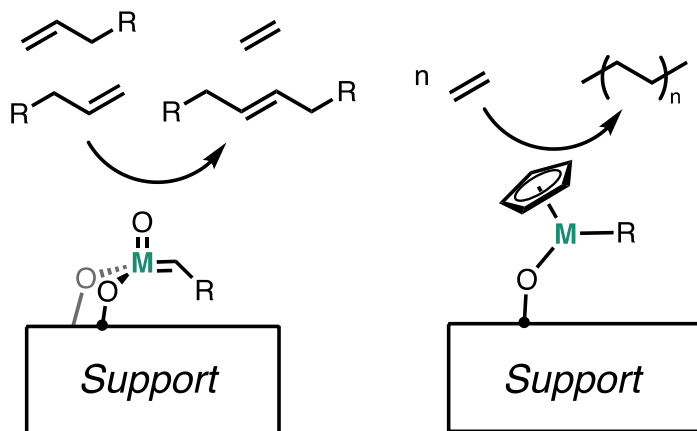


Members of the Copéret Group

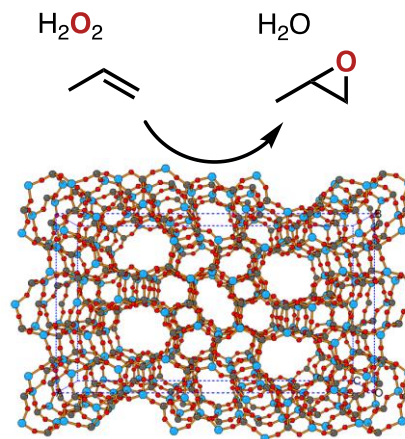


- Prof. Christophe Copéret
- Dr. Alexander Yakimov
- Dr. Millivoj Plodinec
- 8 Postdocs
- 19 PhD Students
- 5-15 Semester students/year
- 2-3 Master students/year
- 2 Visitors

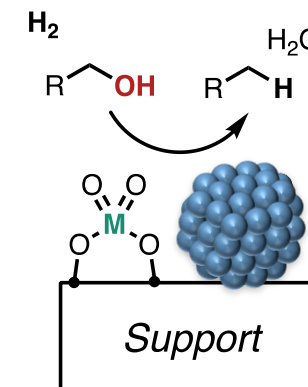
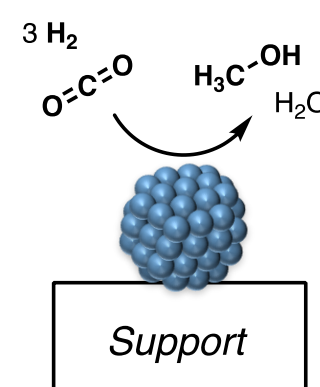
Focus: Reactions with an impact on society and a more sustainable future



Single-Site Catalysts



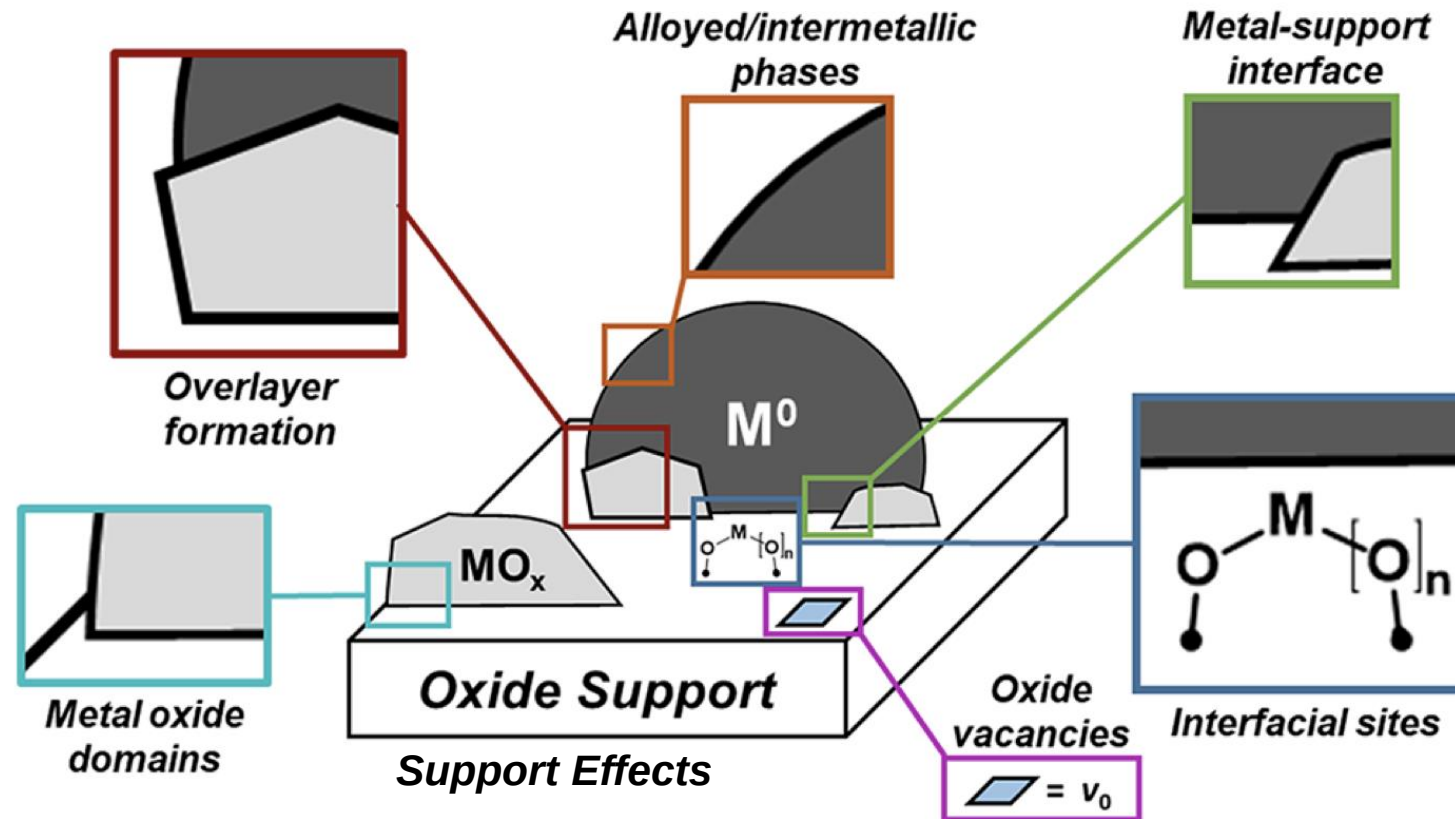
Zeolites

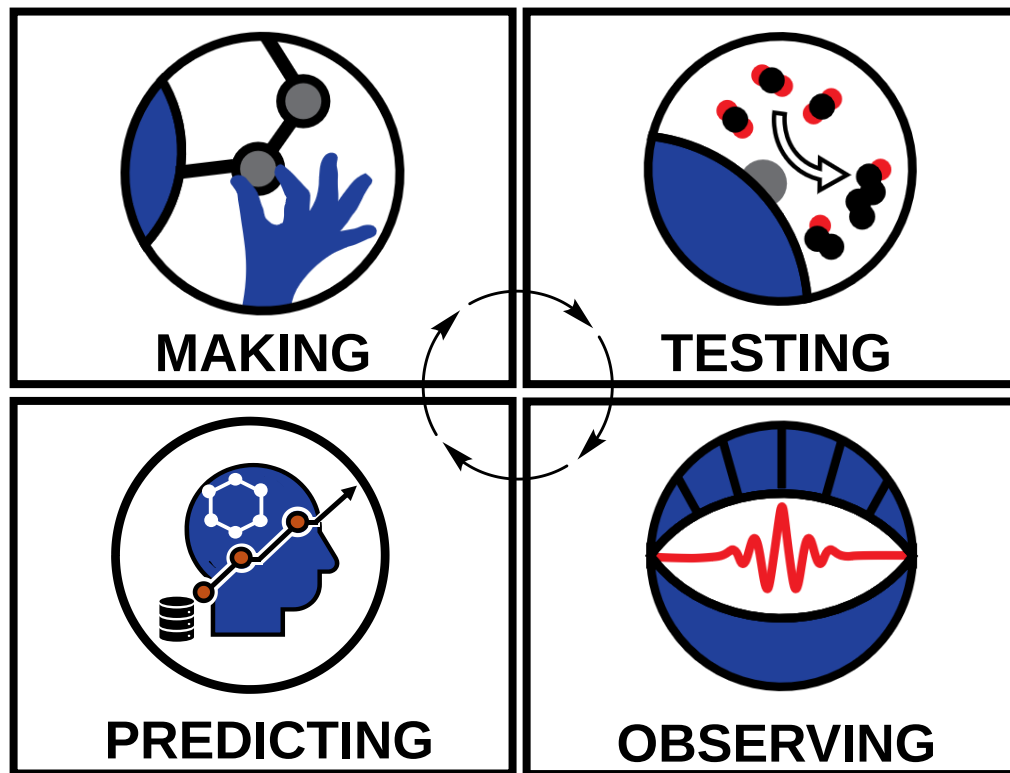


Supported Nanoparticles

Scientific question: what makes a good catalyst – which structural features determine reactivity?

Surfaces are very complex

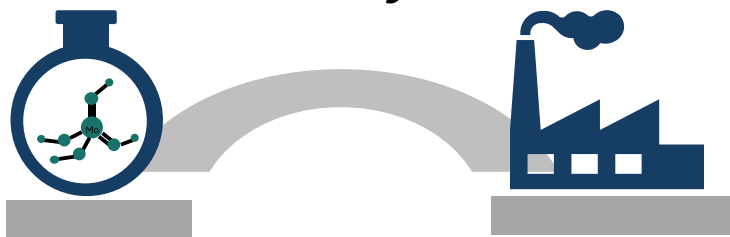




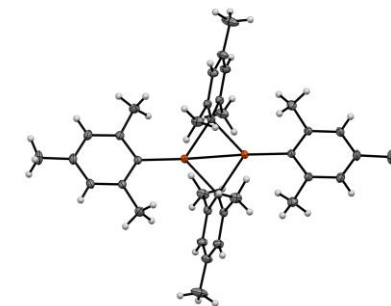
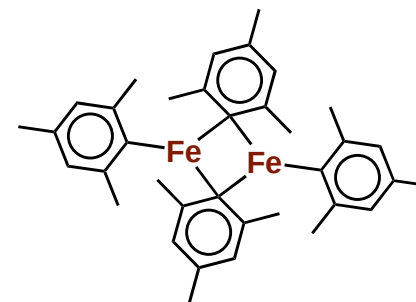
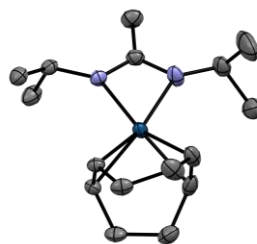
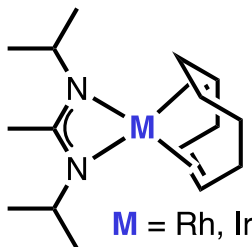
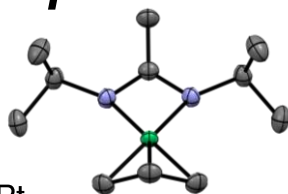
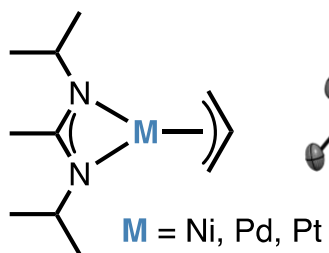


MAKING

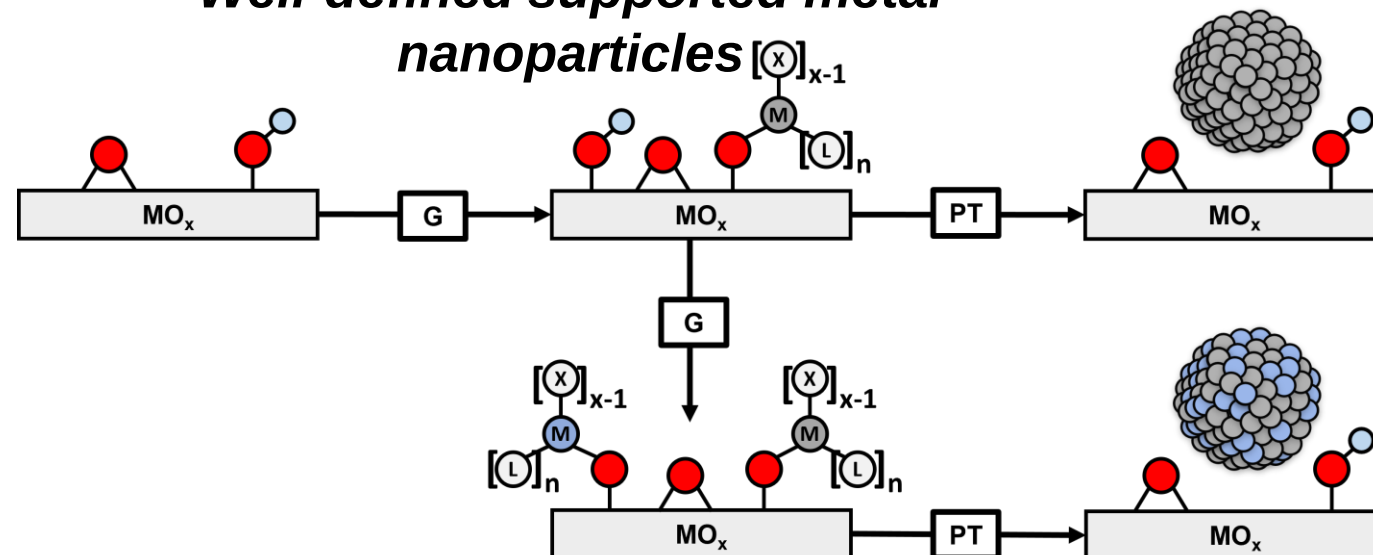
SOMC to bridge the gap between homogeneous and heterogeneous catalysis

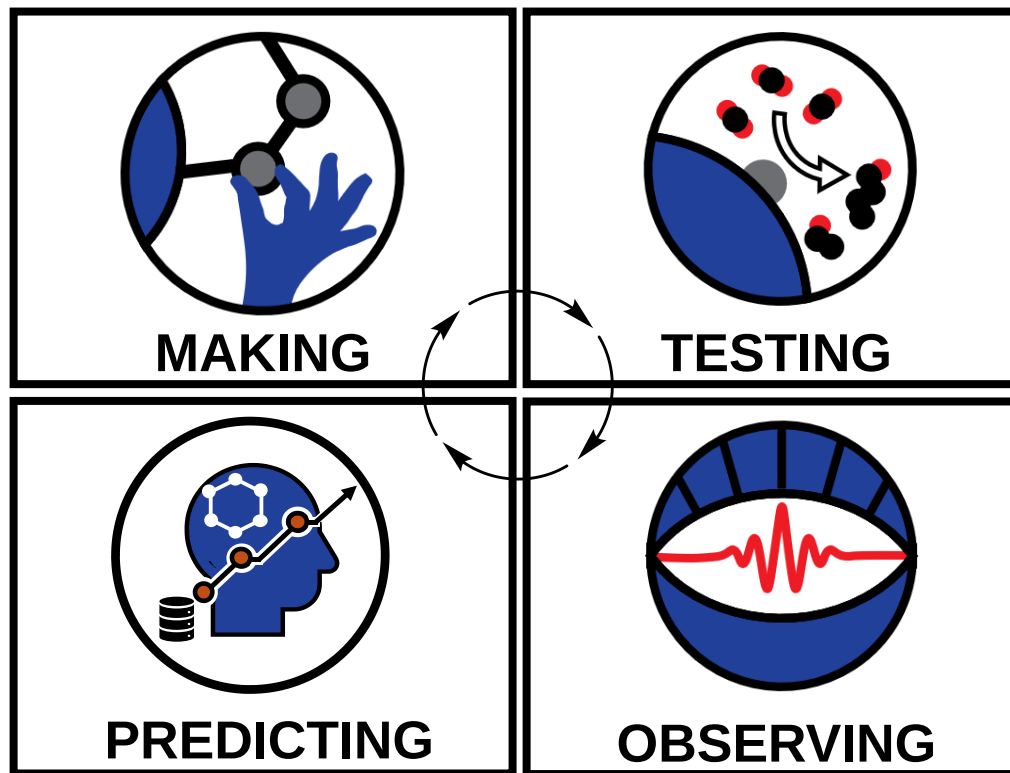


Development of novel molecular precursors

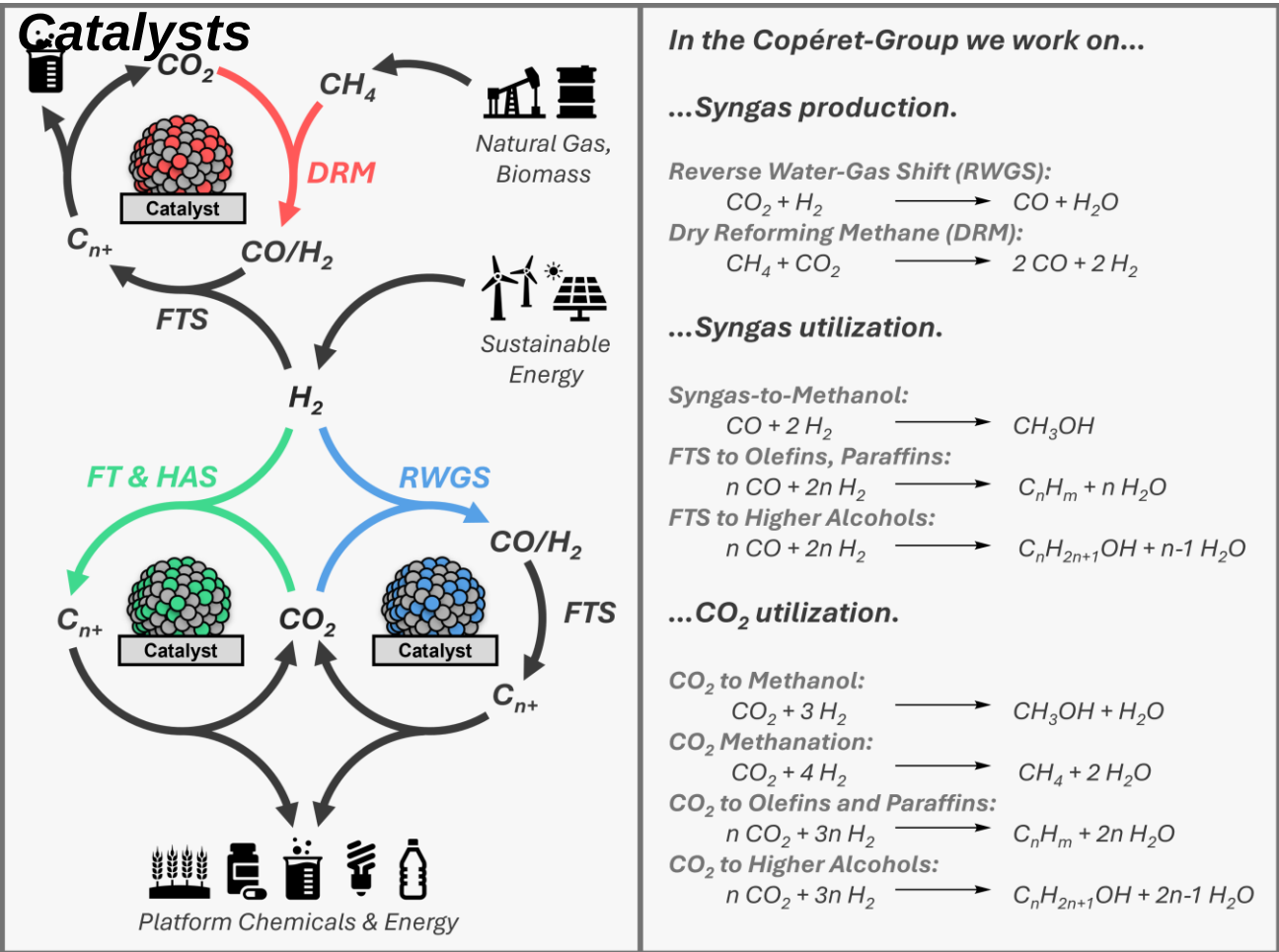


Well-defined supported metal nanoparticles $[(X)_{x-1}]_n$

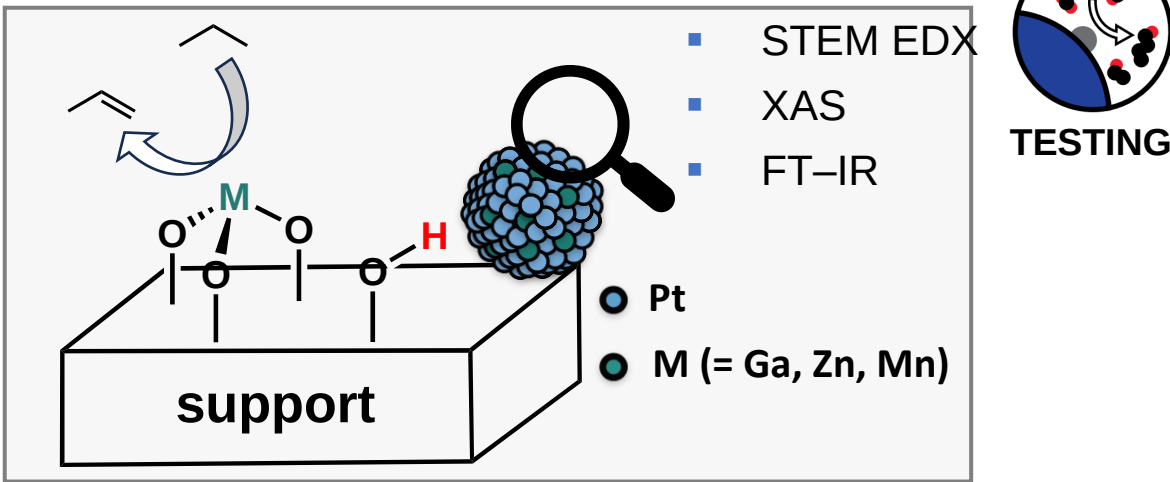




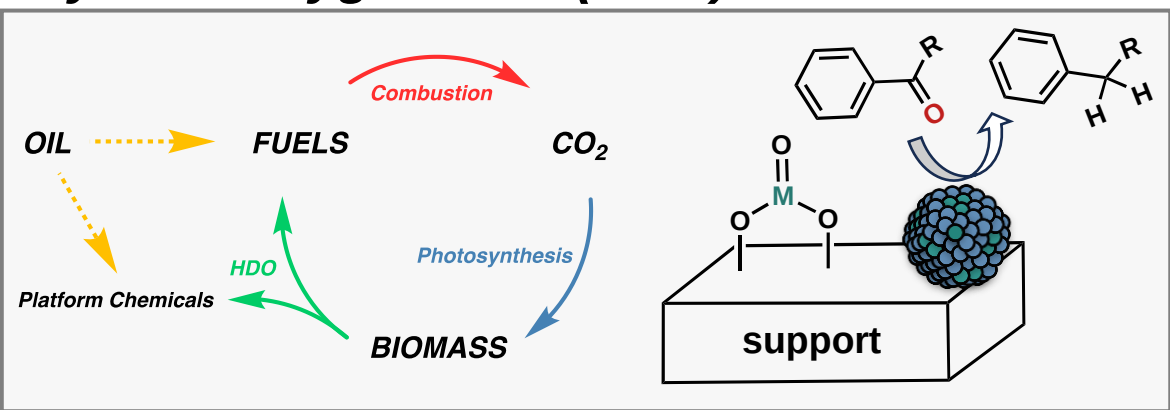
Small Molecule Activation on Heterogeneous Catalysts

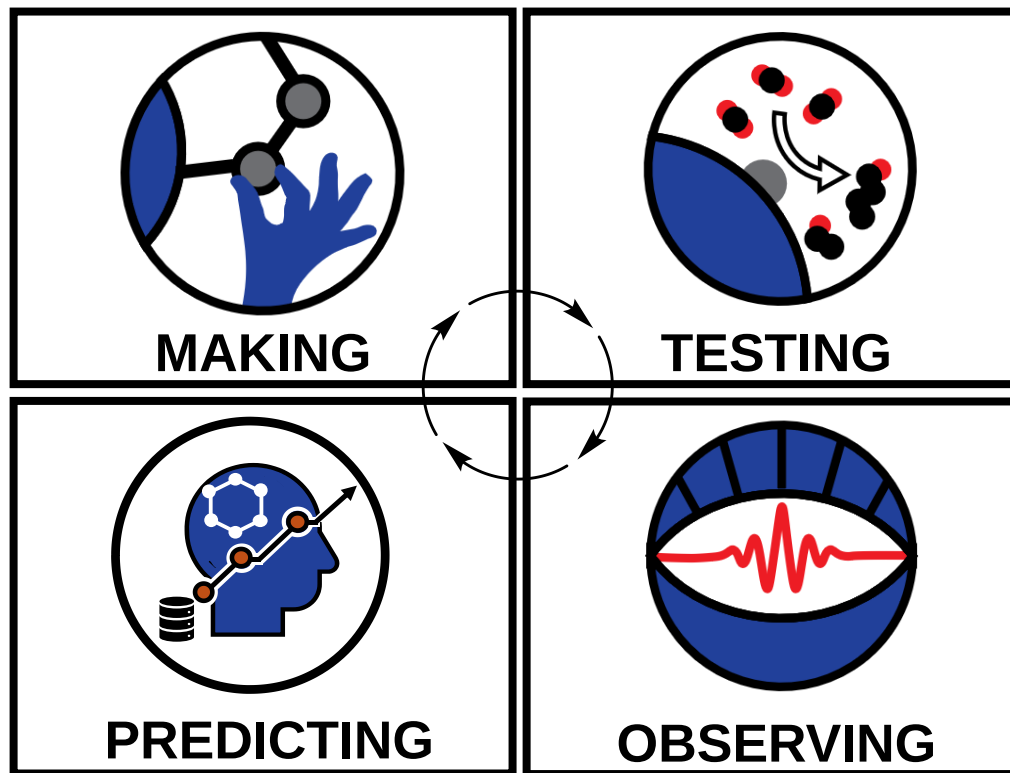


Propene Dehydrogenation

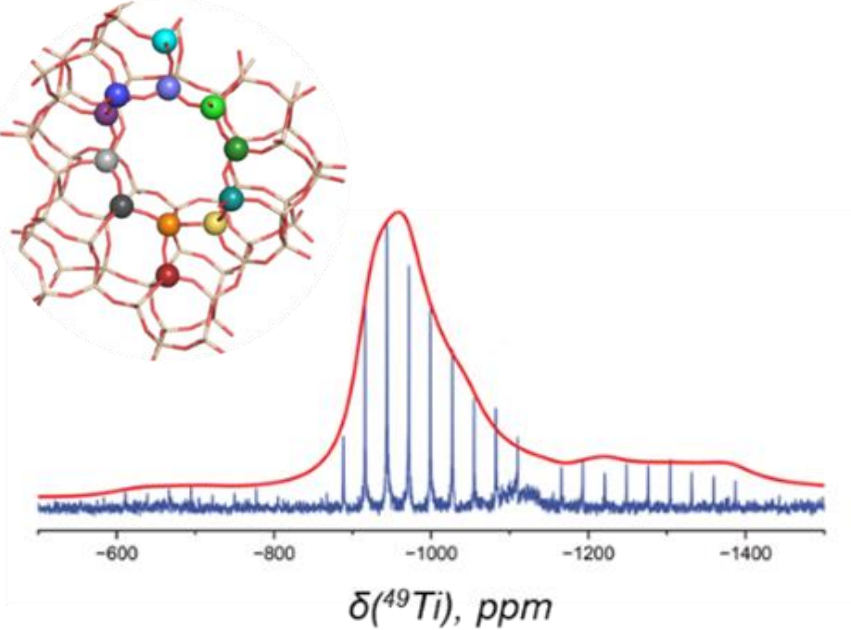


Hydrodeoxygenation (HDO)

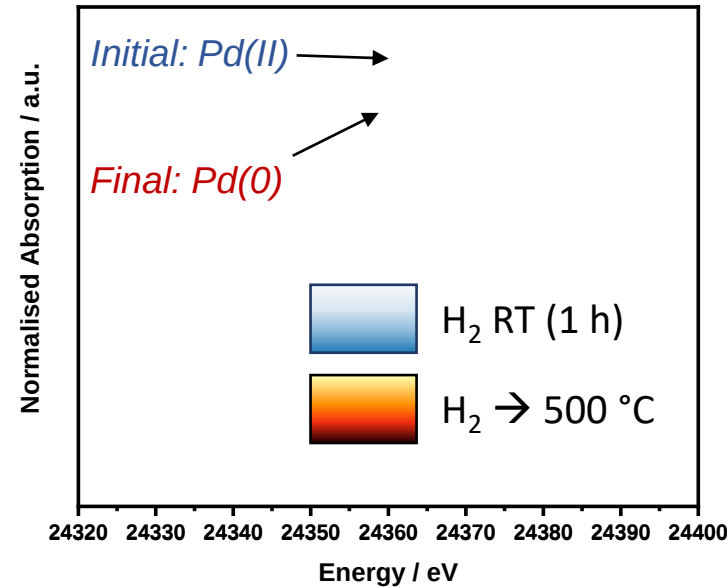




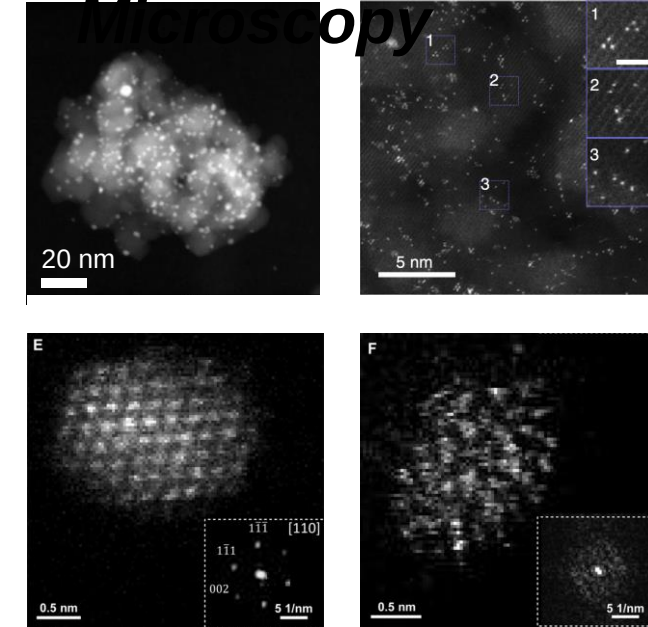
Solid-State NMR



X-Ray Absorption Spectroscopy



Electron Microscopy

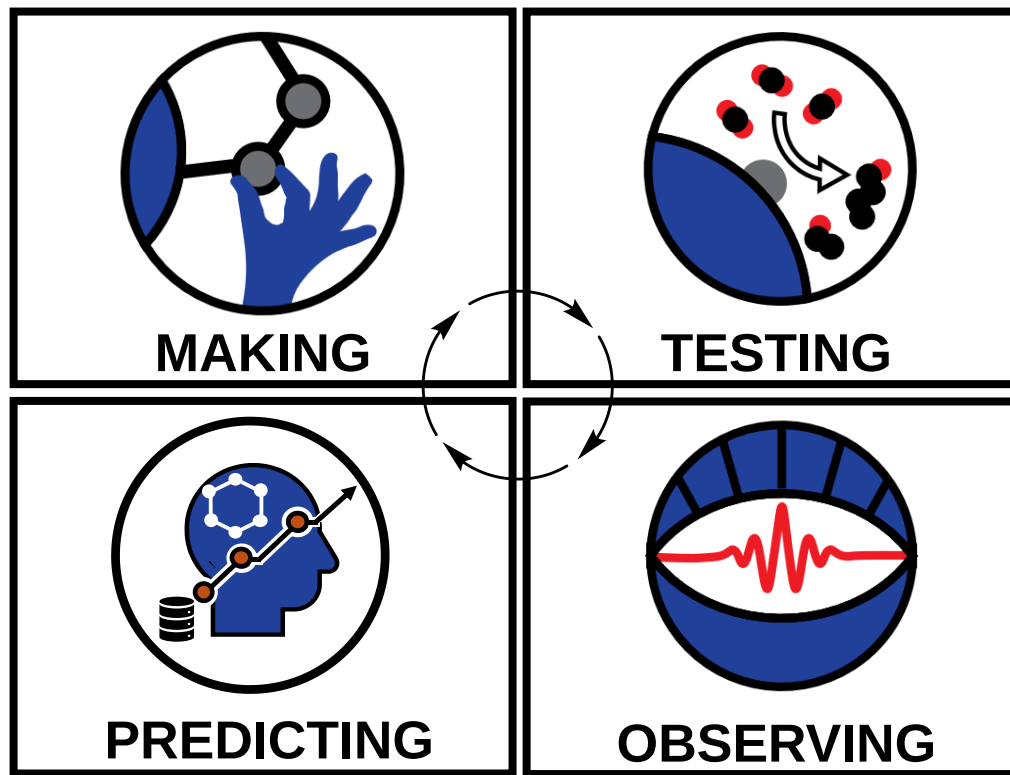


... and IR spectroscopy, probe molecules, chemisorption, physisorption, X-Ray diffraction, cyclic voltammetry, DRIFTS ...

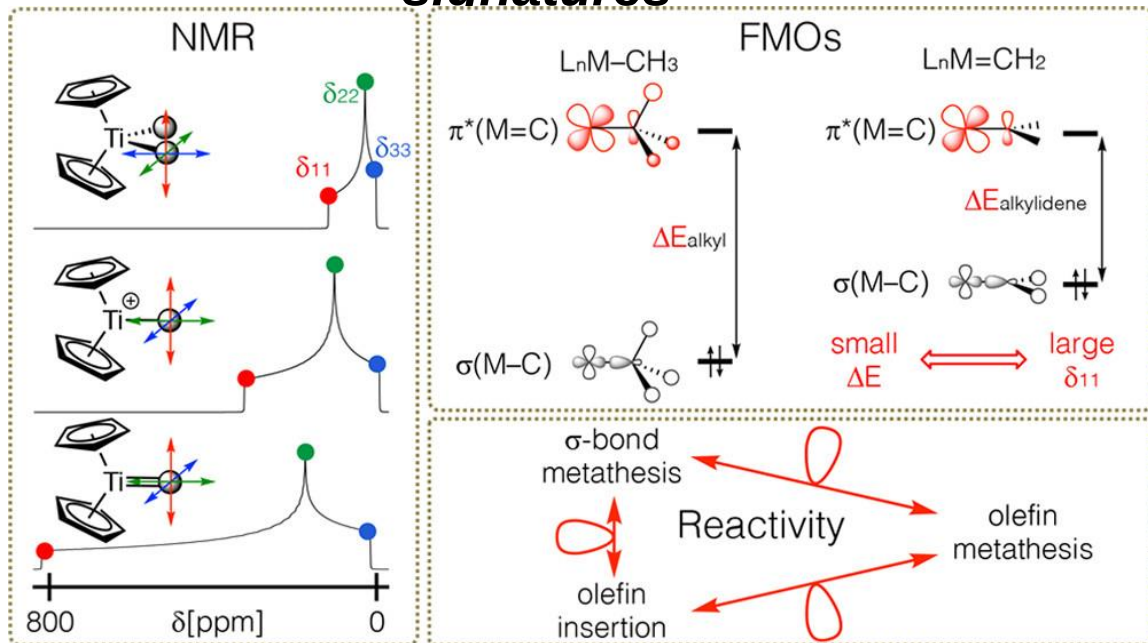
Multiple characterization techniques used to understand surfaces



OBSERVING



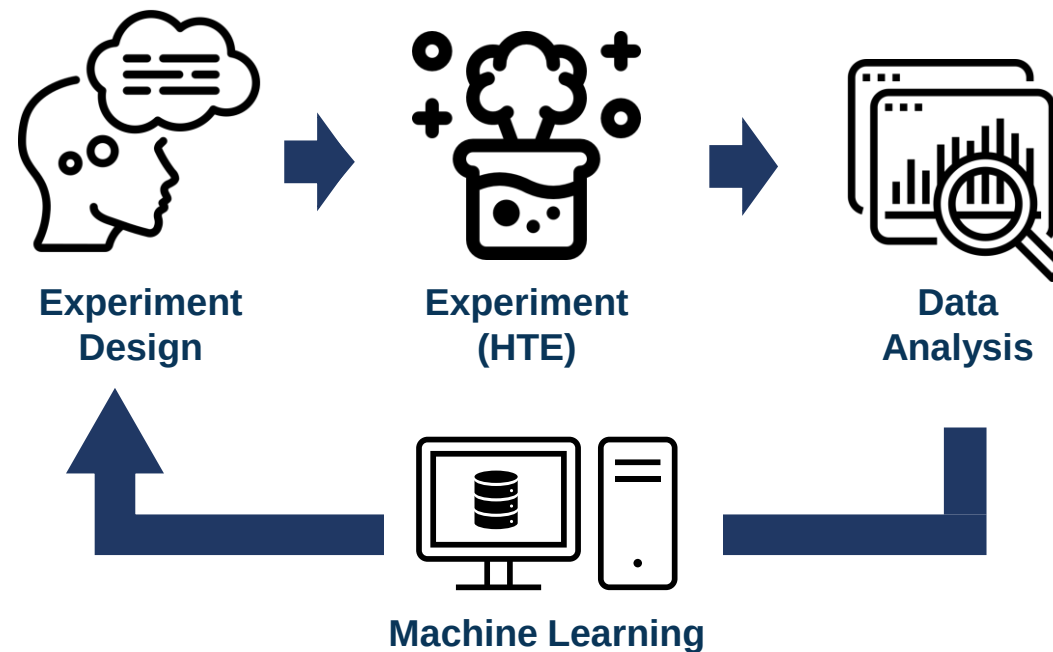
Understanding spectroscopic signatures



PREDICTING

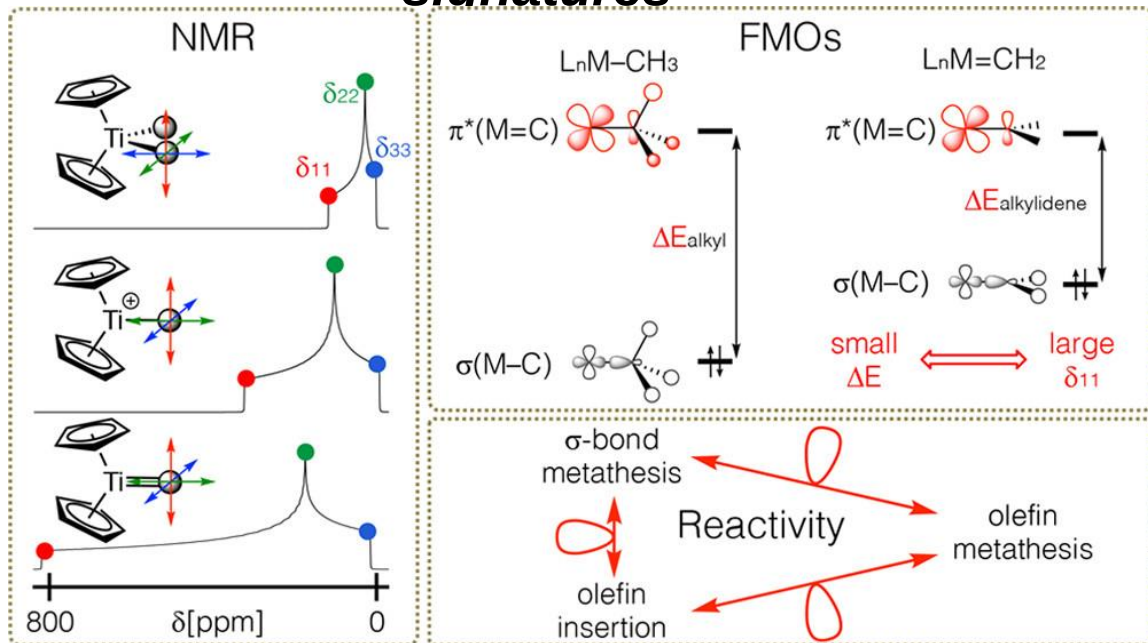
NMR signature = Reactivity descriptor

High-throughput experimentation



Accelerated discovery and automatization

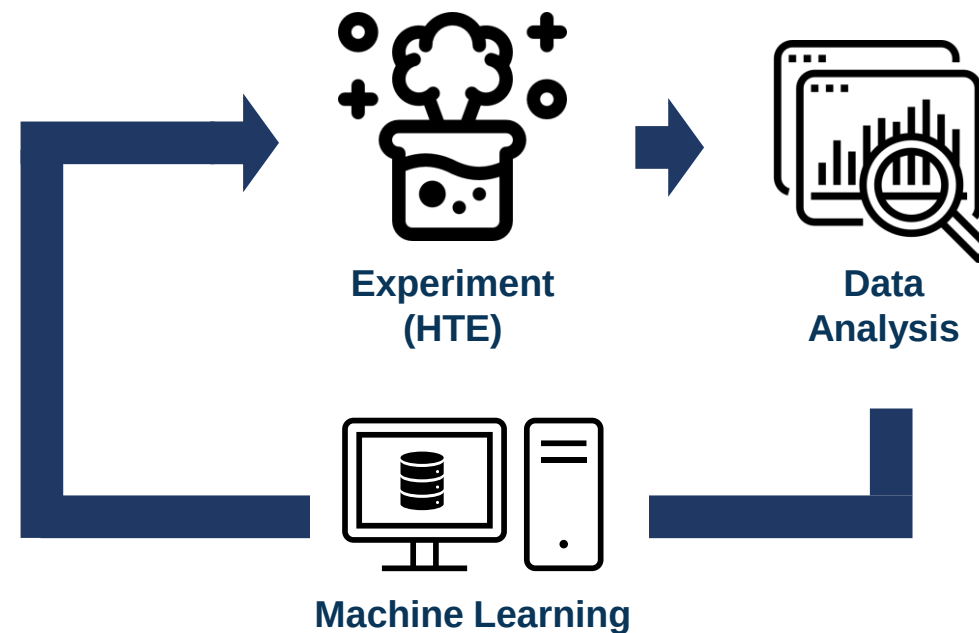
Understanding spectroscopic signatures



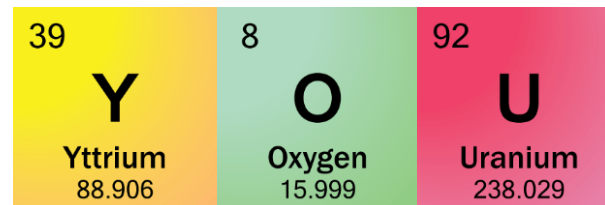
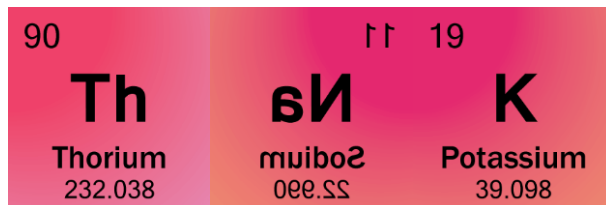
NMR signature = Reactivity descriptor

PREDICTING

High-throughput experimentation



Accelerated discovery and automatization



For further questions:

Mattia Ciuoli

ciuolim@student.ethz.ch

Interested? Reach out directly to:

Prof. Christophe Copéret

ccoperet@ethz.ch



coperetgroup.ethz.ch



Research projects in the Merkt group

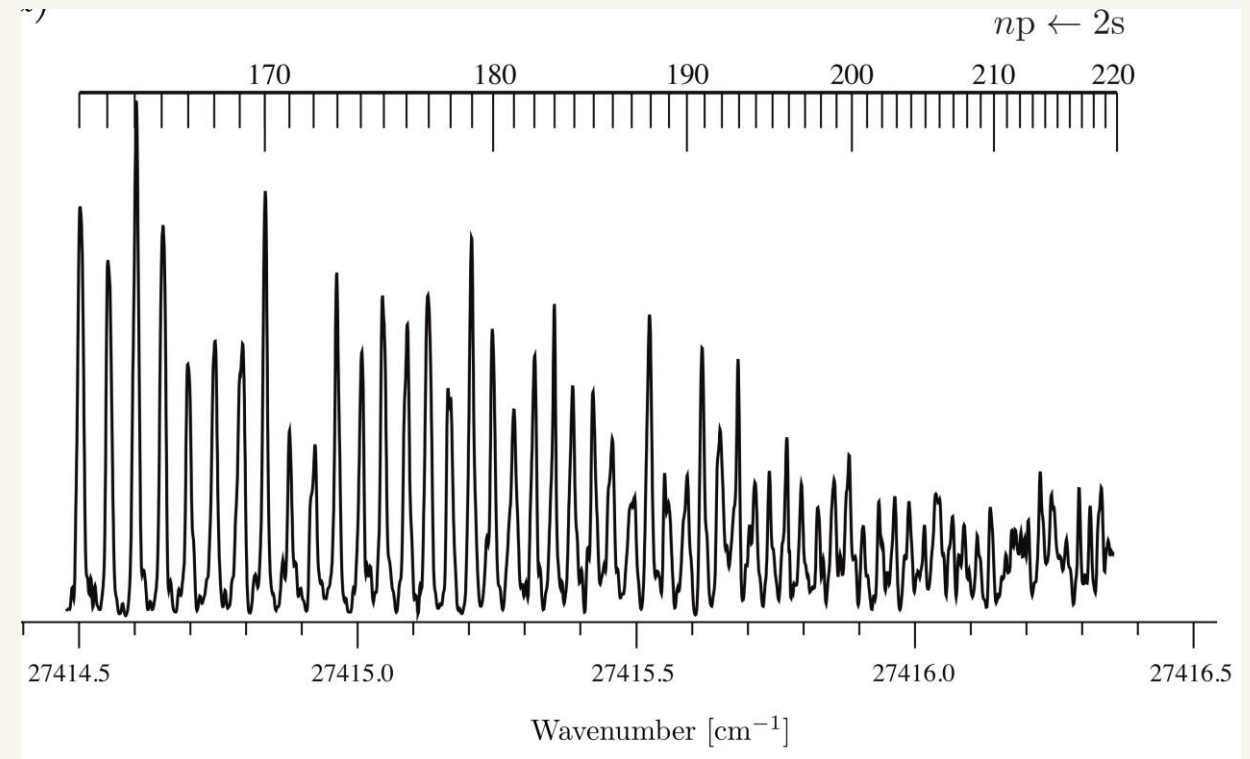
Maxime Holdener, David Schlender
May 21, 2025



(High) Rydberg states

- All experiments rely on unique properties of high Rydberg states
- $15 \leq n \leq 250$
- Some properties

Property	n -scaling	Rb (50p)
Binding energy	n^{-2}	6.2 meV
Energy between adjacent n states	n^{-3}	0.22 meV
Radiative lifetime	n^3	106 μ s
Fine-structure interval	n^{-3}	-0.9 MHz
Orbital radius	n^2	0.17 μ m
Dipole moment $\langle np er nd \rangle$	n^2	3200 ea_0
Geometric cross-section	n^4	0.096 μ m ²
Scalar polarizability	n^7	$\sim$ GHz cm ² /V ²

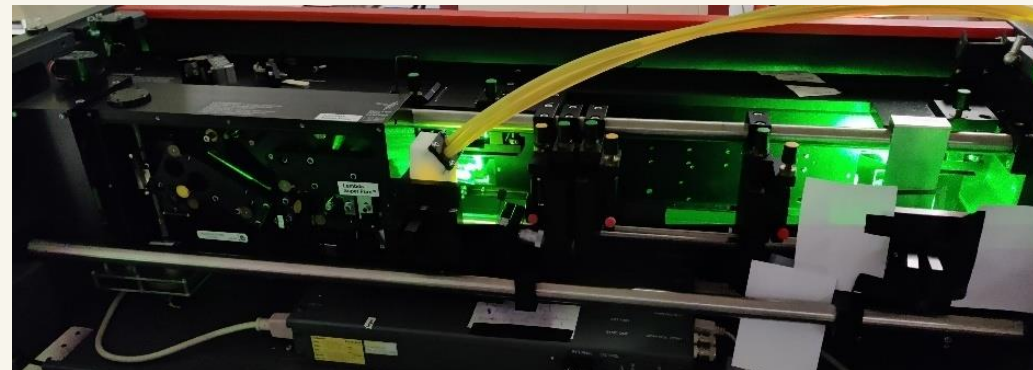
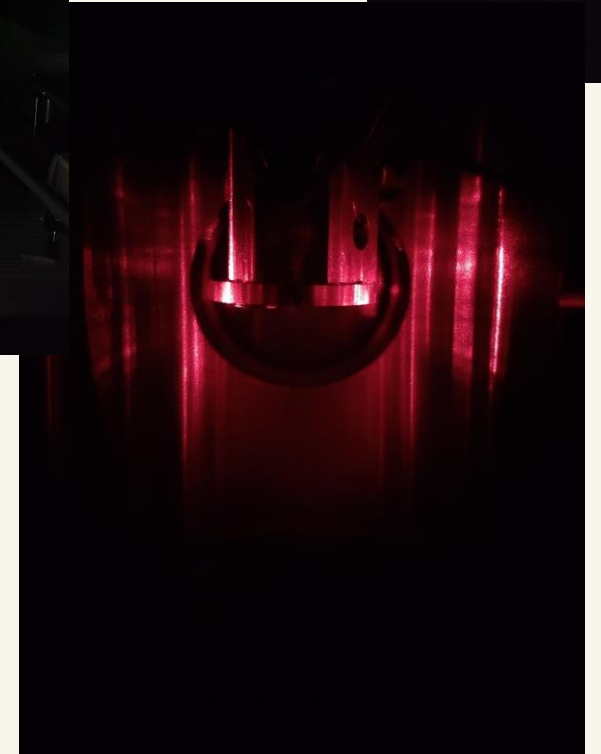


Scheidegger, S. Precision Spectroscopy of Rydberg States of the Hydrogen Atom, ETH Zurich, 2023

Water: 0.730 ea_0

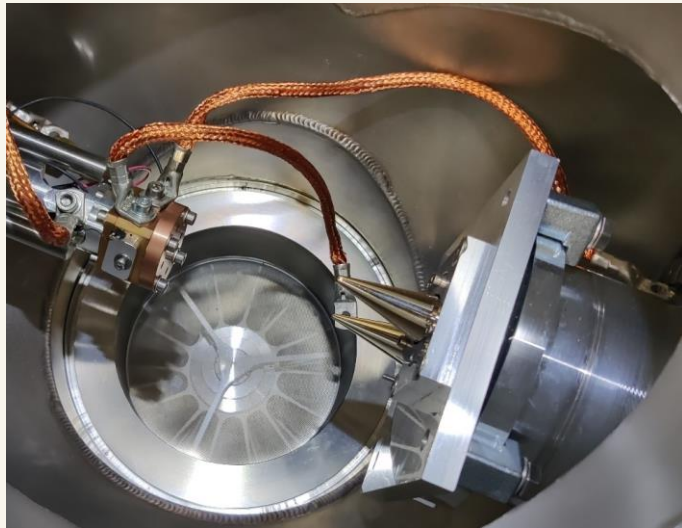
Lasers

- Using Nd:YAG-pumped dye lasers and diode lasers to excite Rydberg states
- Aligning and optimising lasers
- Choosing optics and setting up optical systems



Vacuum

- We investigate isolated atoms and molecules in the gas phase
 - At 10^{-7} mbar mean free path is ~ 700 m (compared to 70 nm at 1 bar)
- Using turbomolecular pumps, working cleanly



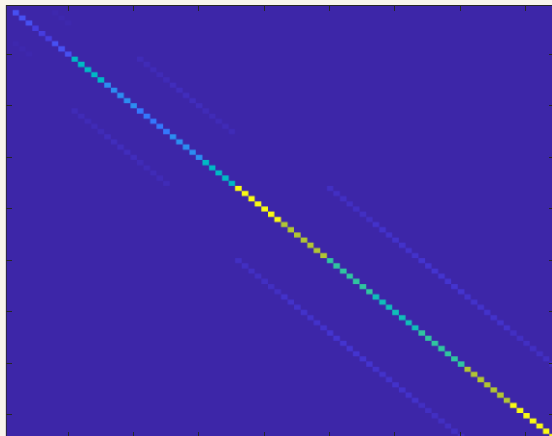
Theory and data evaluation

- Evaluation and understanding of experimental data often requires modelling

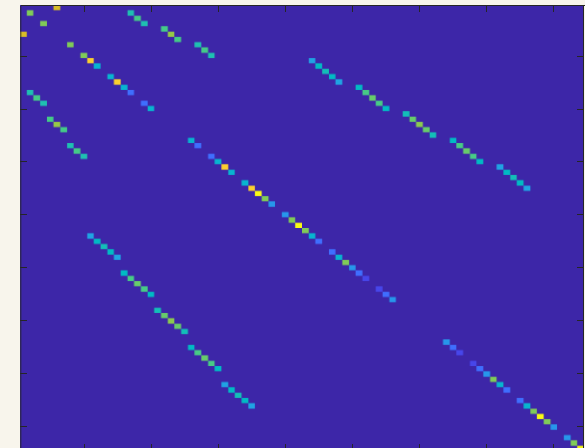
$$\hat{H}(R) = \hat{H}_{Stark}(R) + \hat{H}_{rot}$$

- Programming in Python, R or MATLAB

$$\hat{H}_{rot} = h \left(B \frac{\hat{J}_x^2}{\hbar^2} + C \frac{\hat{J}_y^2}{\hbar^2} + A \frac{\hat{J}_z^2}{\hbar^2} \right)$$

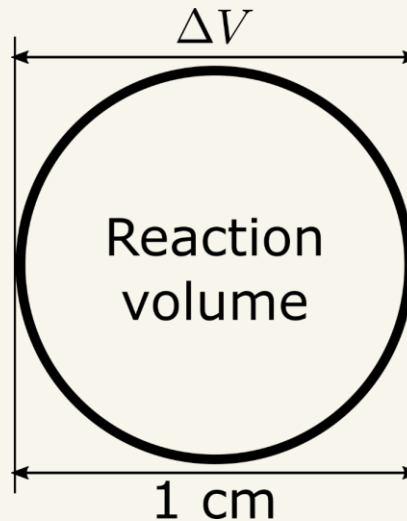


$$\langle J' K' M' | \hat{H}_{Stark}^{(\lambda)}(R) | J K M \rangle = \frac{\mu_{\lambda} q}{4\pi\epsilon_0 R^{\lambda+1}} (-1)^{M'-K'} \sqrt{(2J+1)(2J'+1)} \times \\ \begin{pmatrix} J & \lambda & J' \\ M & 0 & M' \end{pmatrix} \begin{pmatrix} J & \lambda & J' \\ K & 0 & K' \end{pmatrix}$$



Collisions: Cold ion-molecule reactions

- Low-temperature gas-phase ion-molecule chemistry: $E_{\text{coll}} \lesssim k_B \cdot 50 \text{ K}$
 - Relevant for atmospheric chemistry, astrophysics and plasma physics
- Challenges
 - Stray electric fields accelerate ions

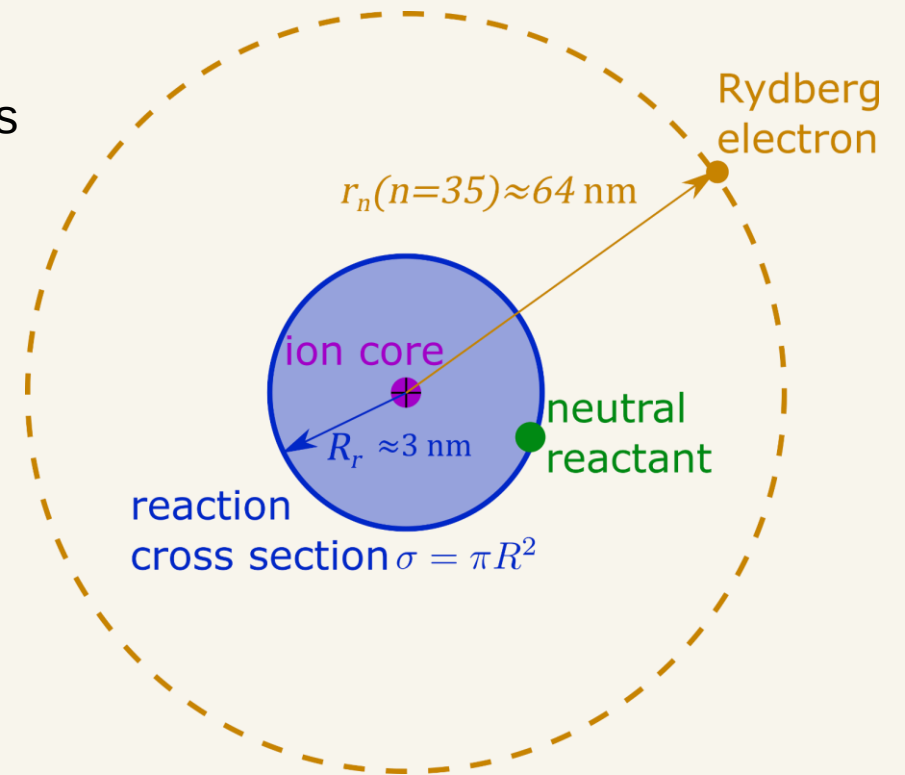


$$\Delta V = 1 \text{ mV} \rightarrow 12 \text{ K}$$

Collisions: Cold ion-molecule reactions

- Replace ionic reactant with high Rydberg state^[1], e.g., $\text{H}_2^+ \rightarrow \text{H}_2(n \gtrsim 25)$

- Rydberg e^- shields reaction volume from stray electric fields
- Reaction takes place within the Rydberg- e^- orbit
- Rydberg e^- is spectator^[2-3]

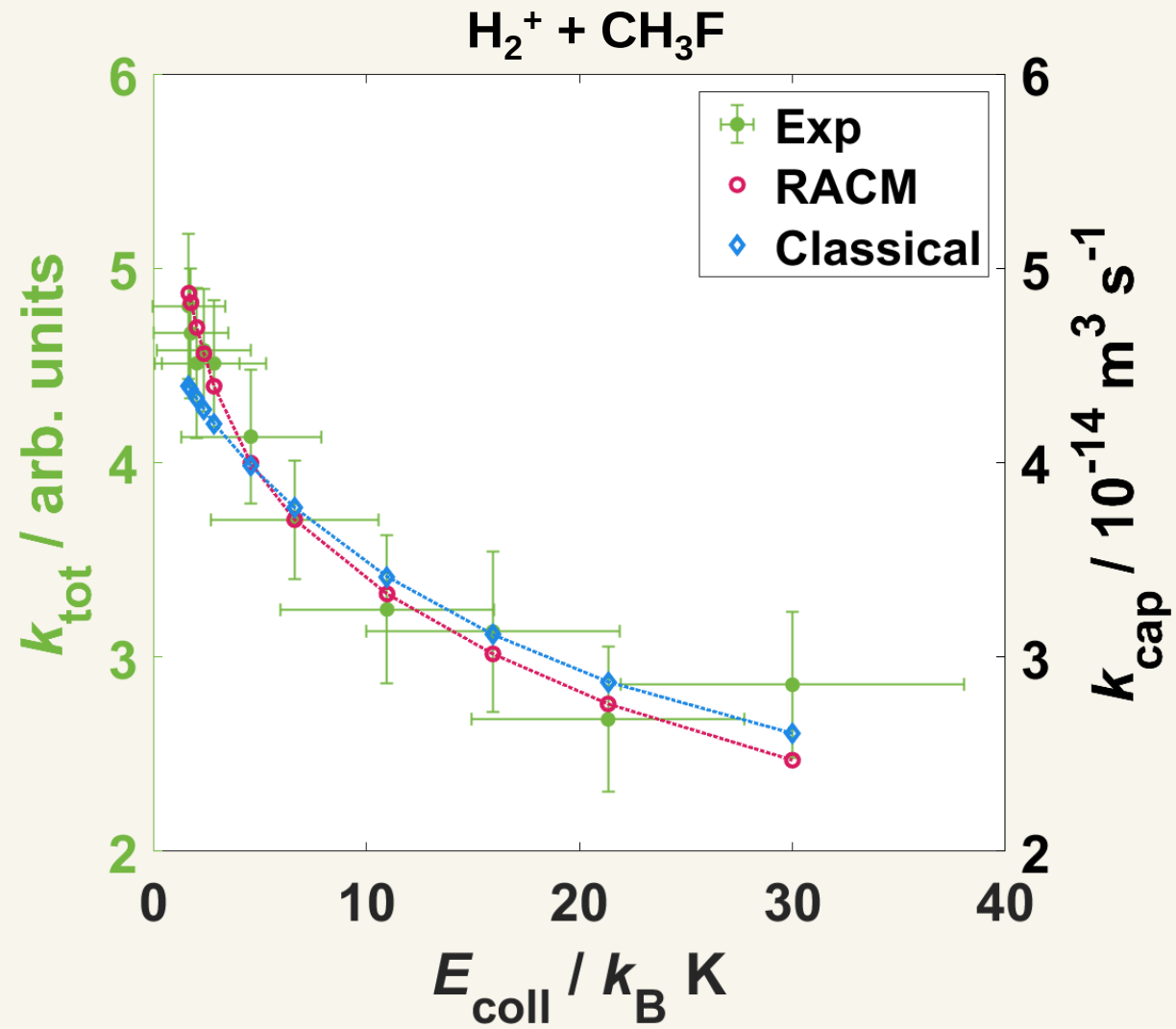


[1] Allmendinger, P.; Deiglmayr, J.; Höveler, K.; Schullian, O.; Merkt, F. *J. Chem. Phys.* **145**, 244316 (2016).

[2] Allmendinger, P.; Deiglmayr, J.; Schullian, O.; Höveler, K.; Agner, J. A.; Schmutz, H.; Merkt, F. *ChemPhysChem* **17**, 3596 (2016).

[3] B.V. Martins, F.; Zhelyazkova, V.; Seiler, Ch.; *New J. Phys.* **23** 095011 (2021).

Collisions: Cold ion-molecule reactions

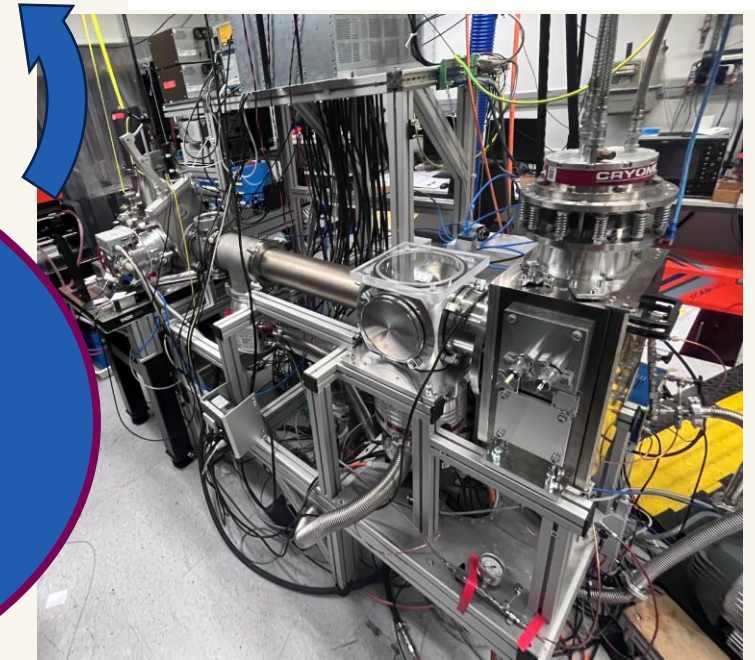
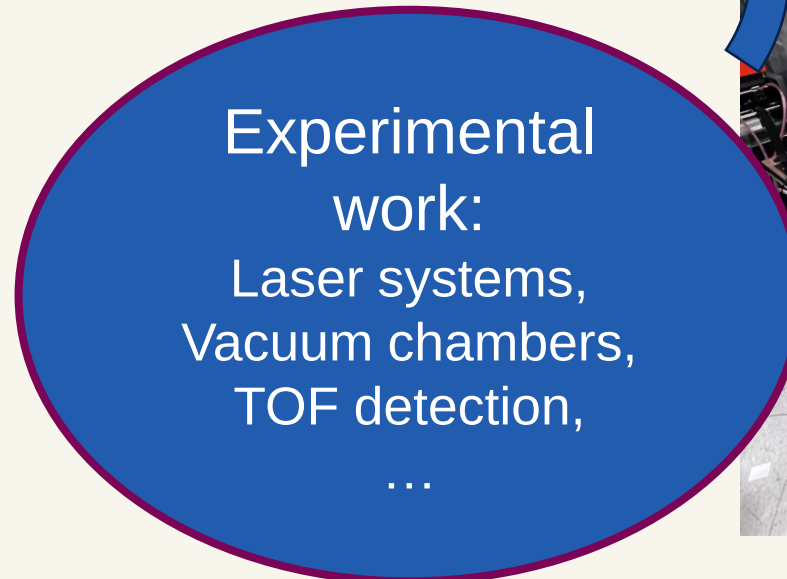
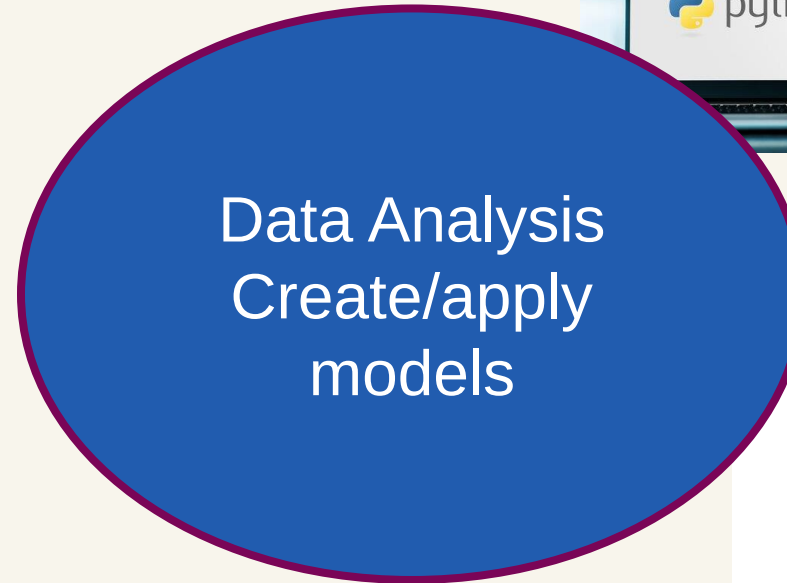
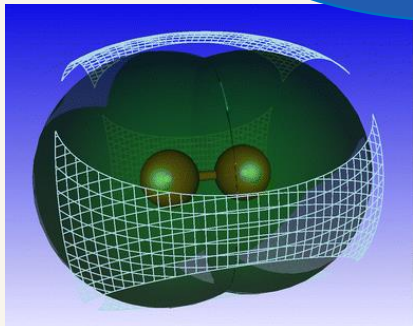
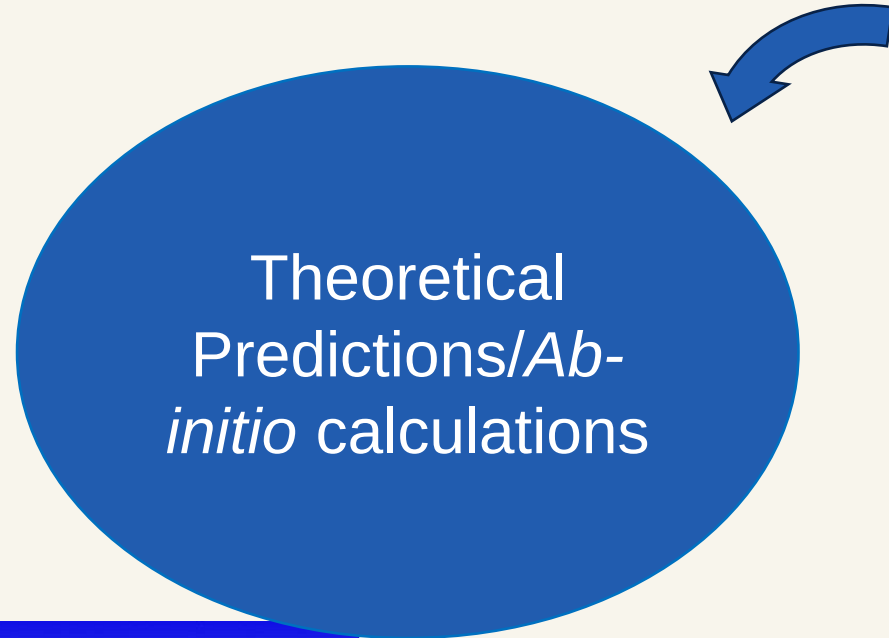


Spectroscopy of atoms and small diatomic molecules

H, H₂, He, He₂, Ne, ... , Yb, BaH, CaO

1. Experiments on these small system gave rise to the Quantum Theory, it's basic principles, the different rules, ...
2. Interface between Physics and Chemistry, electron-core intraction, molecular bond
3. Applying the knowledge of PC III and PC V one to one

Modus Operandi



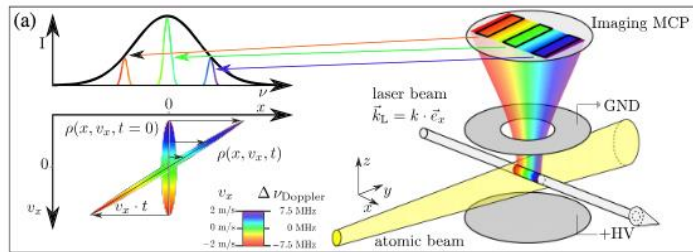
The different projects

Metrology

H, He

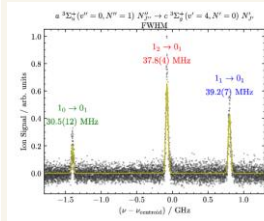
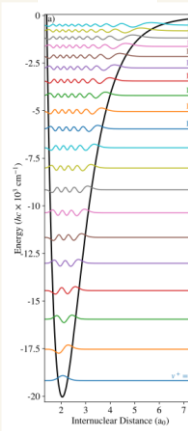


$E_I(2^3S_1)/h = 1\,152\,842\,742.7082$
MHz
 $1\,152\,842\,742.231(52)$
MHz

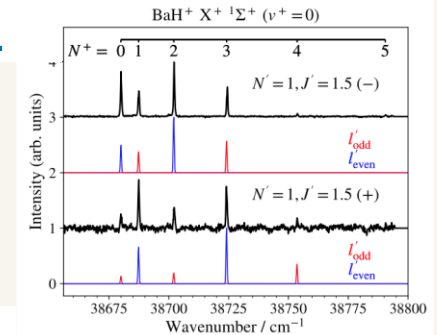
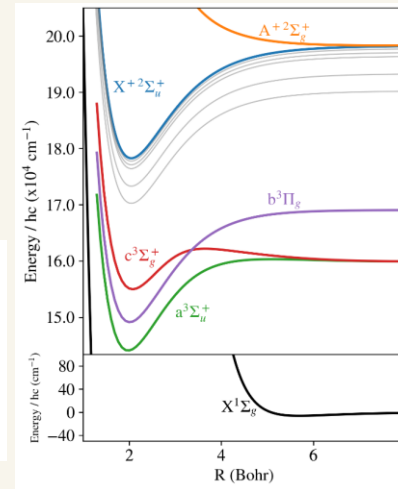


Explorative Spectroscopy, Method Developpement

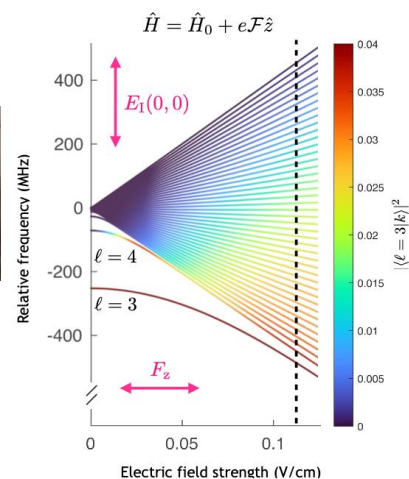
He₂



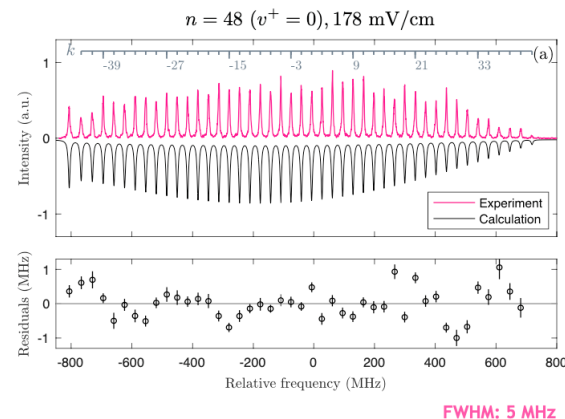
BaH, CaO,



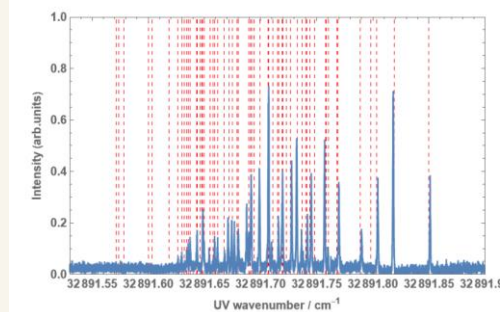
H₂



Fit of line positions with 2 parameters: $E_I(0,0)$ and $\mathcal{F}$

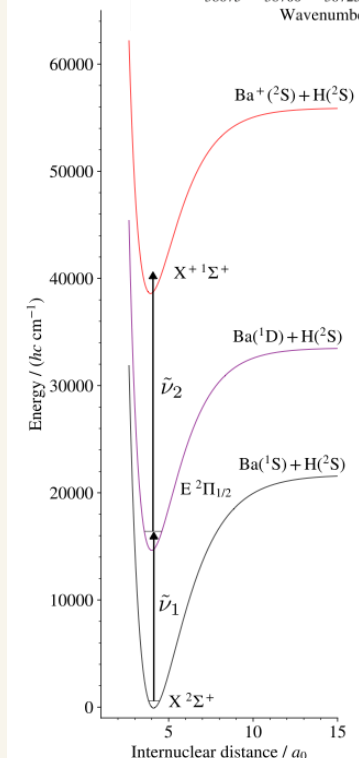


Rare gases, Yb



$$E_n(a^+) = E_{\infty, a^+} - \frac{hcR_M}{(n - \delta_l)^2}$$

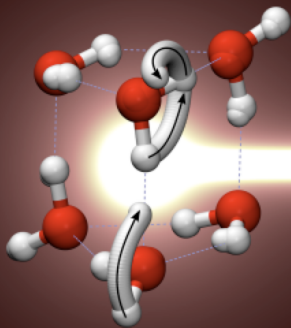
Quantum defect



How to get on board

1. Also contacts with Amsterdam, Paris, London
2. Email:
mholdener@ethz.ch
dschlander@ethz.ch
3. Email Prof. Merkt with an idea of a project
merkt@ethz.ch
4. Come to the apéro and chat with us





Projects in the Richardson group

Jindra Dušek (they/them)
VCS Info Event

Introduction

- Basic info:
 - www.richardson.ethz.ch
 - HCI D 267.3
 - Cca. 10 permanent members at the moment.
 - Looking for: bachelor or master semester projects or semester theses (so any kind of project)

Introduction

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- **Theoretical molecular quantum dynamics**

Introduction

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 - HCI D 267.3
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 - Looking for: bachelor or master semester projects or semester theses (so any kind of project)
- **Theoretical molecular quantum dynamics**
- Intersection between: **physics**, **chemistry**, **math** and **informatics**

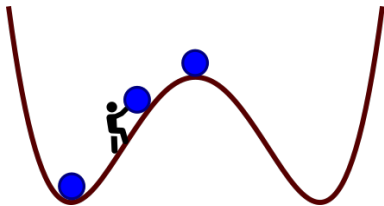
Quantum tunnelling



Quantum tunnelling

- Arrhenius and activation energy (for rate problems)

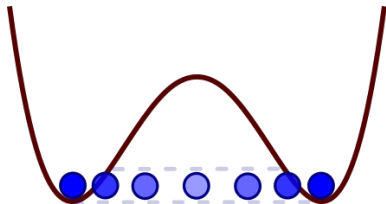
$$k = A \exp(-E_a/RT) .$$



Quantum tunnelling

- Arrhenius and activation energy (for rate problems)

$$k = A \exp(-E_a/RT) .$$

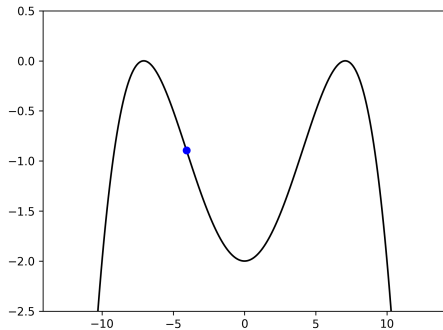


Imaginary time

- Forbidden region $\Rightarrow$ Imaginary time $\Rightarrow$ Upside-down potential

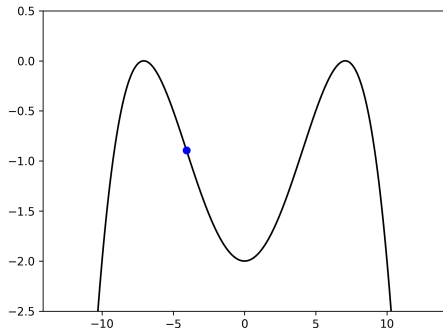
Imaginary time

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Imaginary time

- Forbidden region $\Rightarrow$ Imaginary time $\Rightarrow$ Upside-down potential



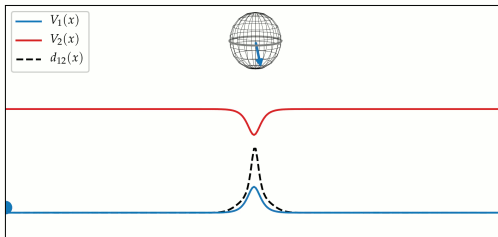
$$i\hbar \frac{\partial}{\partial t} |\psi\rangle = \hat{H} |\psi\rangle$$

vs.

$$K(x_i, x_f, \tau) = \int \mathcal{D}\mathbf{x} \exp(-S[\mathbf{x}])$$

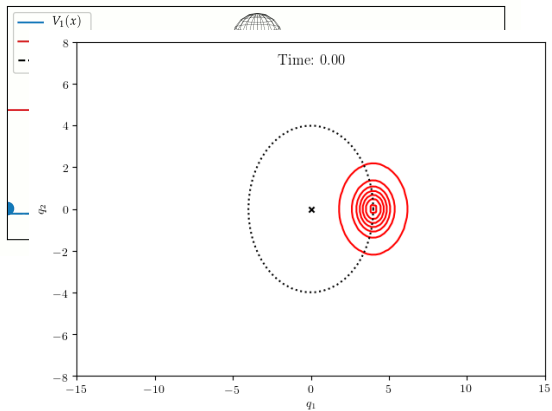
Nonadiabatic dynamics

- Multiple electronic levels, adiabatic representation

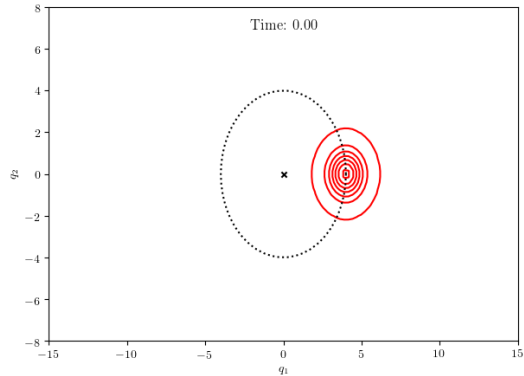


Nonadiabatic dynamics

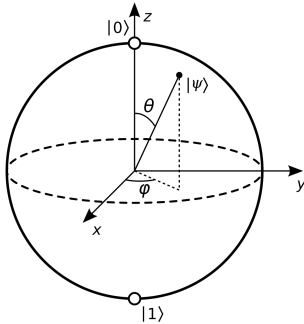
- Multiple electronic levels, adiabatic representation



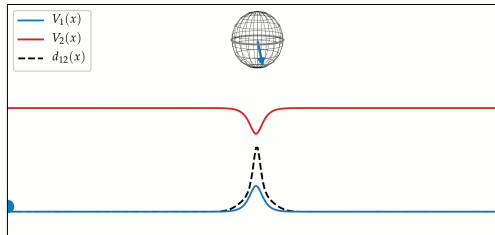
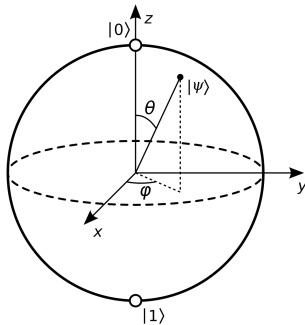
Nonadiabatic dynamics



Nonadiabatic dynamics

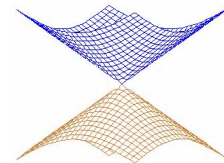


Nonadiabatic dynamics



Topics

- Chemistry
 - Nuclear quantum effects in all kinds of reactions and processes
 - Nonadiabatic dynamics
 - Polariton chemistry (/quantum optics)
 - ...



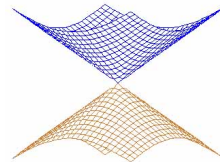
Topics

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- Nuclear quantum effects in all kinds of reactions and processes
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- ...

- Math/Physics

- Path integrals
- Asymptotic methods
- Monte Carlo
- Hierarchical equations of motion
- ...



$$\langle x_t | e^{-i\hat{H}t/\hbar} | x_0 \rangle =$$


<http://www-stuart.ch.cam.ac.uk/img/paths.jpg>

Topics

- Chemistry

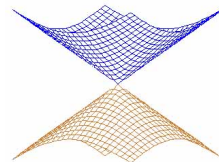
- Nuclear quantum effects in all kinds of reactions and processes
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- ...

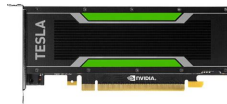
- Informatics

- Python, Git
- GPU computing
- ...



$$\langle x_t | e^{-i\hat{H}t/\hbar} | x_0 \rangle =$$


<http://www-stuart.ch.cam.ac.uk/img/paths.jpg>



What to expect

- Typical research stages
 - Chemical problem (chemistry) $\rightarrow$ Theory (math) $\rightarrow$ Validation (computer simulations)

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 - Chemical problem (chemistry) $\rightarrow$ Theory (math) $\rightarrow$ Validation (computer simulations)
- In our group, you will join us in this process.

What to expect

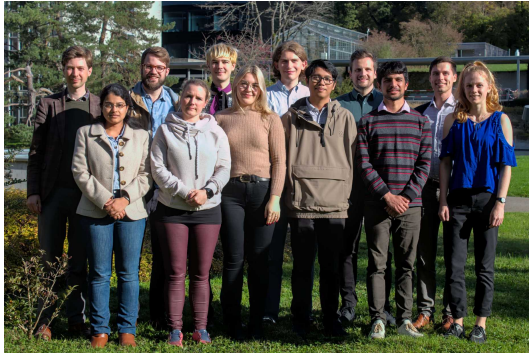
- Typical research stages
 - Chemical problem (chemistry) $\rightarrow$ Theory (math) $\rightarrow$ Validation (computer simulations)
- In our group, you will join us in this process.
- Choose your project to tailor it to your strengths!

Curious?

- Try working with Python
- Visit the Advanced Kinetics lecture (529-0442-00L)

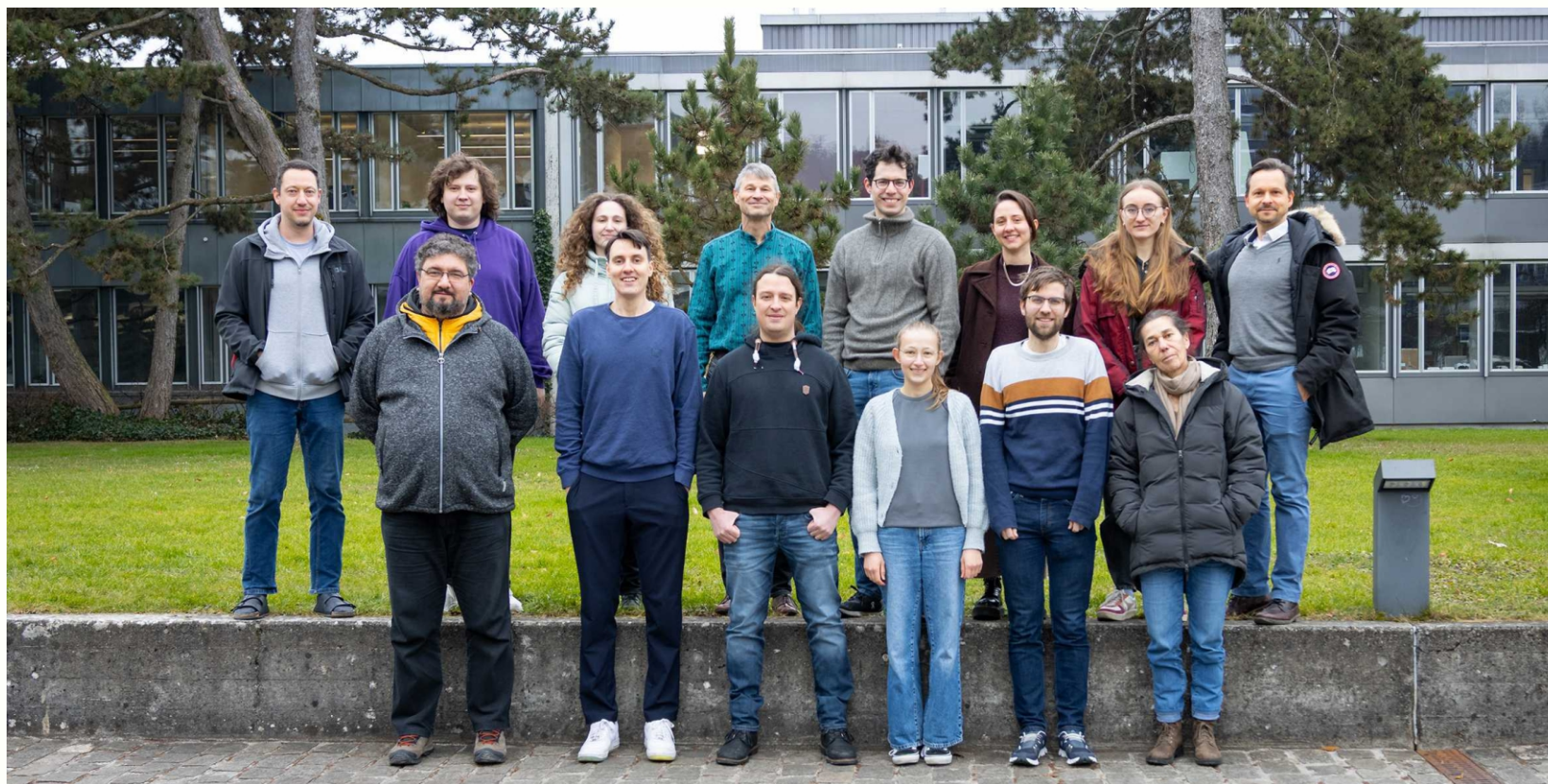
Get in touch

- Just come to our office at HCI D 267.3!
- www.richardson.ethz.ch/group/open-positions.html
- jindra.dusek@phys.chem.ethz.ch
- rjeremy@ethz.ch

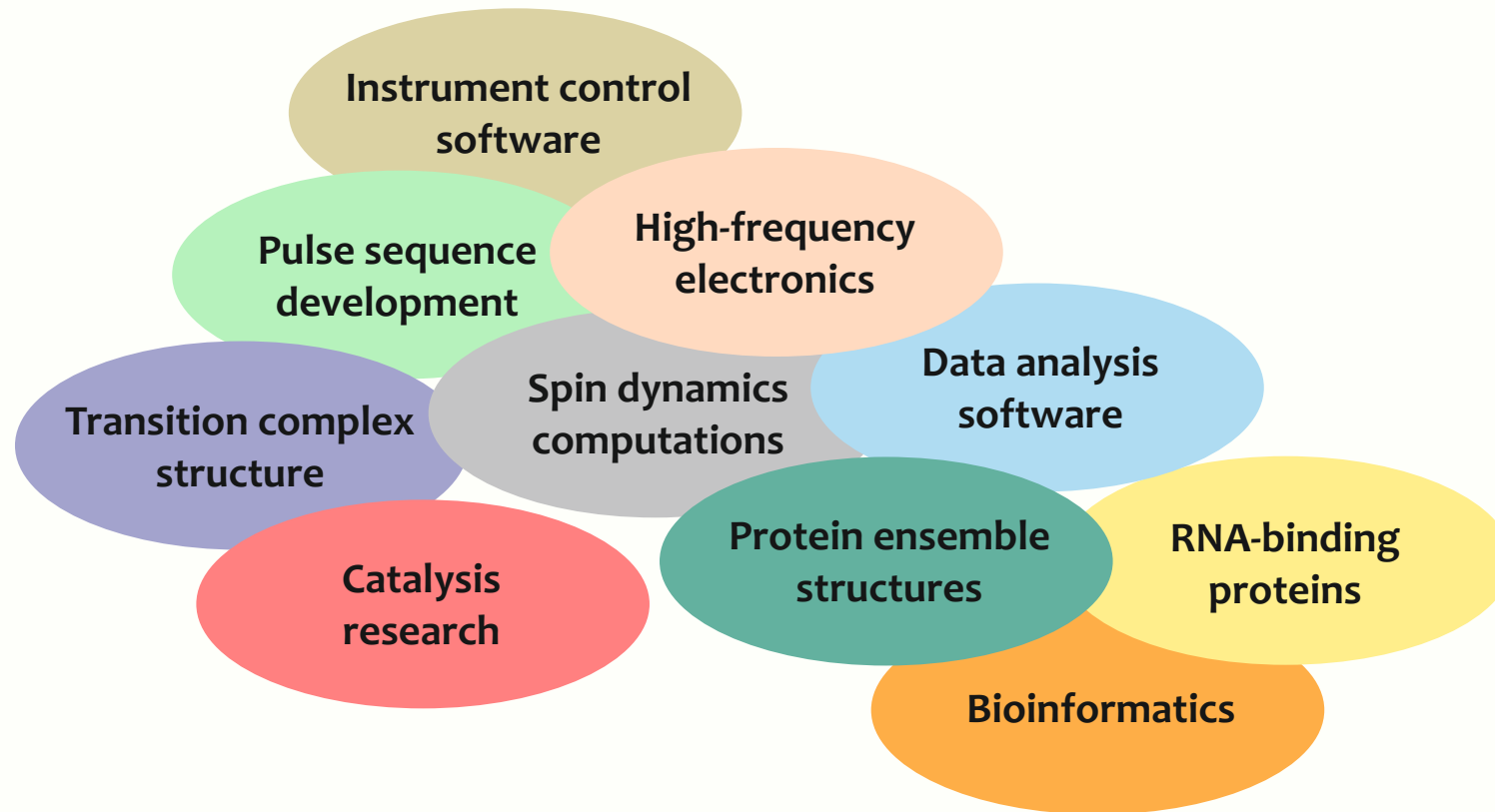


The Electron Paramagnetic Resonance Group

G. Jeschke, ETH Zürich, Department of Chemistry and Applied Biosciences



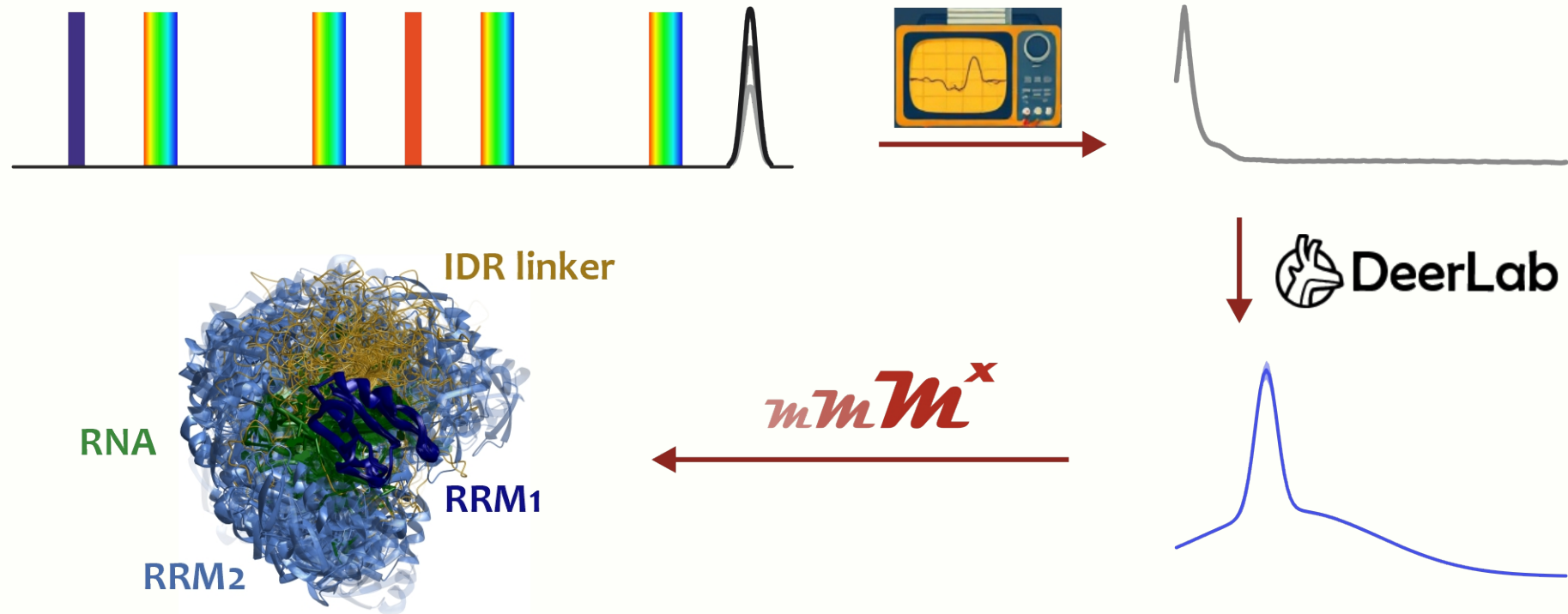
What are we doing



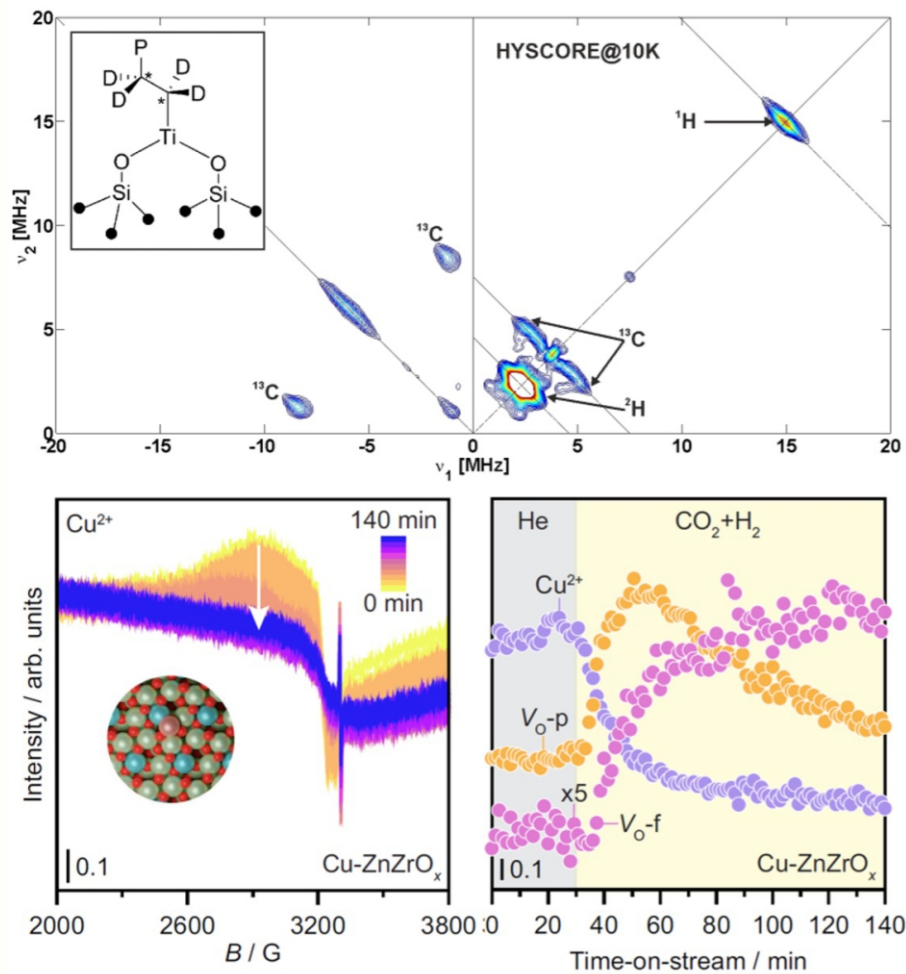
The research matrix

	Bio wetlab	Spin dynamics	Data analysis	Instrumen- tation	Pulse sequences	Ensemble structure	DEER/PDS	hyperfine	DNP	Spin trapping	Proteins	Dietary fibers	Catalysis
Katya	●					●	●				●		
Katja			●	●				●					●
Élise	●					●	●				●		
Olga	●					●	●				●		
Julian				●	●			●					●
Hugo		●	●	●			●						
Gian-Marco		●	●		●				●				
Laura	●					●	●				●		
Mikhail			●	●				●		●			●
Daniel	●		●	●	●		●	●			●		●
Maxim		●	●	●	●		●	●	●		●	●	●
Gunnar		●	●	●	●	●	●	●	●	●	●		●

Method development



Catalysis

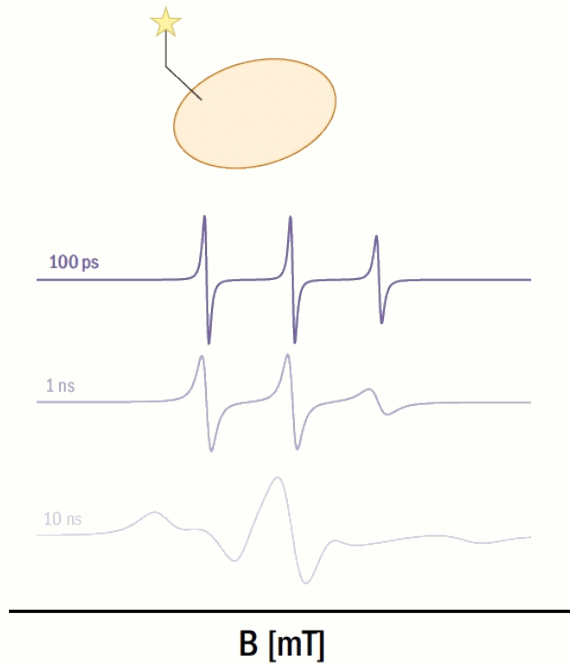


- operando EPR, also with modulation excitation, coupled to MS
- kinetics of paramagnetic active sites
- electronic and spatial structure of paramagnetic active sites
- speciation and its dynamics

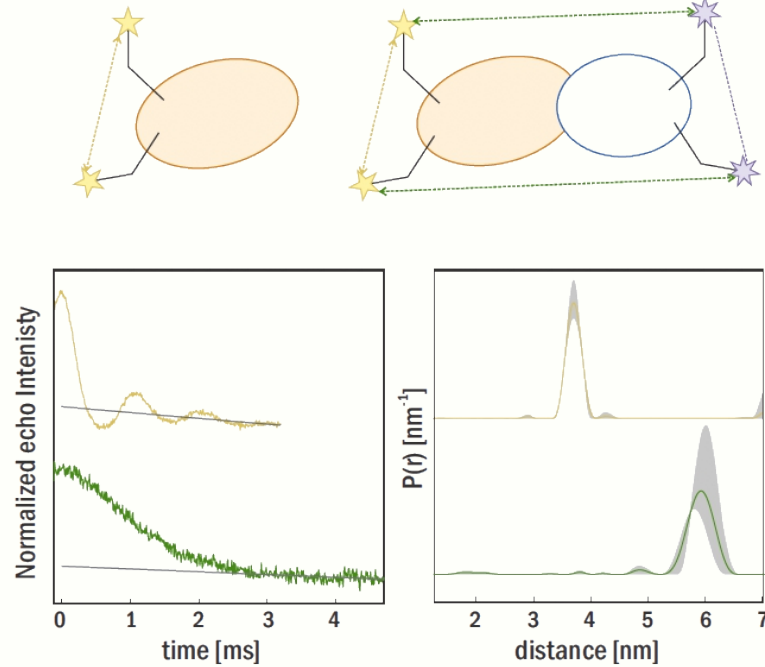


Biological applications

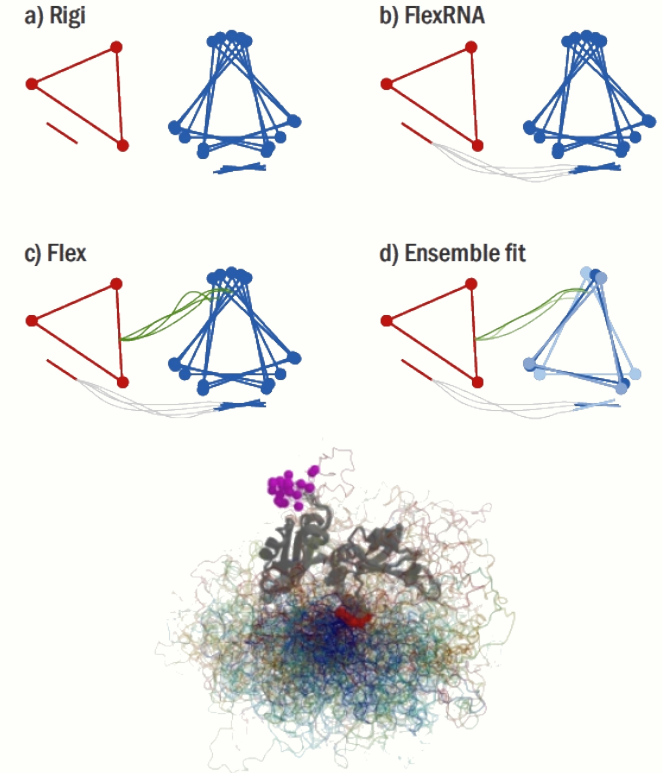
Continuous-wave EPR



Pulsed Dipolar Spectroscopy (Frozen solution)



Ensemble modelling



Any questions?



Ultrafast Spectroscopy and Attosecond Science group ETHZ



Group Leader



Prof. Dr. Hans Jakob Wörner

Head of Laboratory of Physical Chemistry



Chasing Ultrafast Molecular Dynamics with Attosecond Pulses:
from XUV to soft-X-Ray

Dr. Federico Vismarra

Measuring “time” in Quantum Mechanics

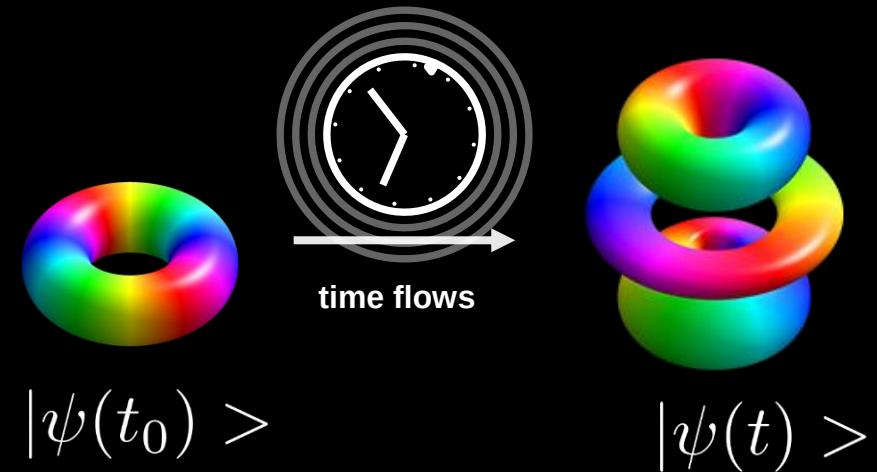
$$\hat{H}|\psi(t)\rangle = i\hbar|\dot{\psi}(t)\rangle$$

Time of a system is a **parameter** in QM
→ It cannot be measurable directly.



"I think I can safely say that
nobody understands quantum mechanics"
R.P. Feynman

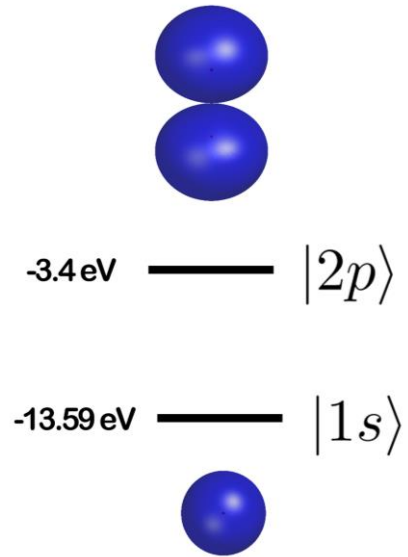
$$|\psi(t)\rangle = e^{-i \int_{t_0}^t \hat{H} dt'} |\psi(t_0)\rangle$$



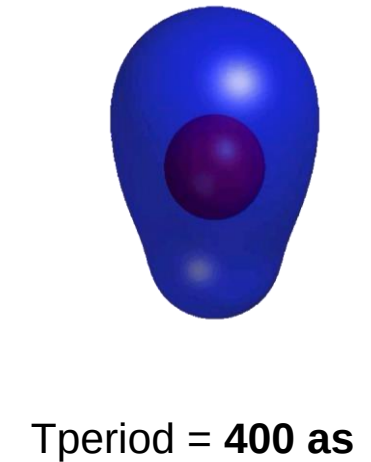
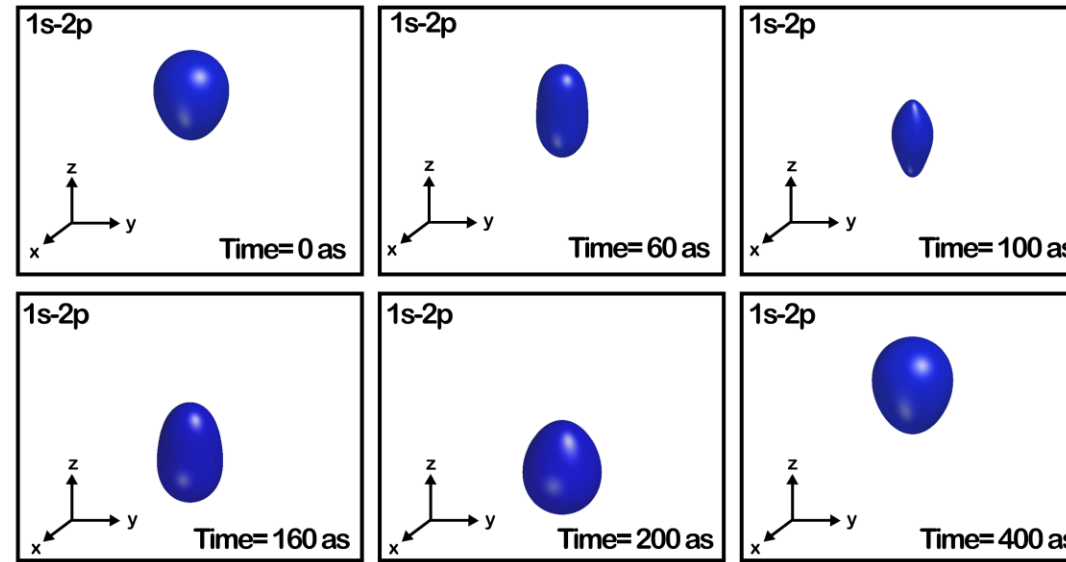
Assuming that **time flows** and knowing the starting point $|\psi(t_0)\rangle$
we can tell what will happen to the wavefunction.

Electronic motion in matters

Hydrogen **ATOM** 1s 2p states



A superposition of *states* create motion in quantum mechanics.

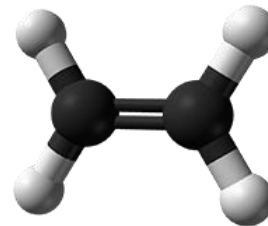


The **energy** of the *states* define the **timing** of the quantum process

$$\Delta T \propto \frac{1}{\Delta E}$$



Micro-biological processes
1 ps (10^{-12} s)



Nuclear motion
1 fs (10^{-15} s)



Electron motion
1 as (10^{-18} s)

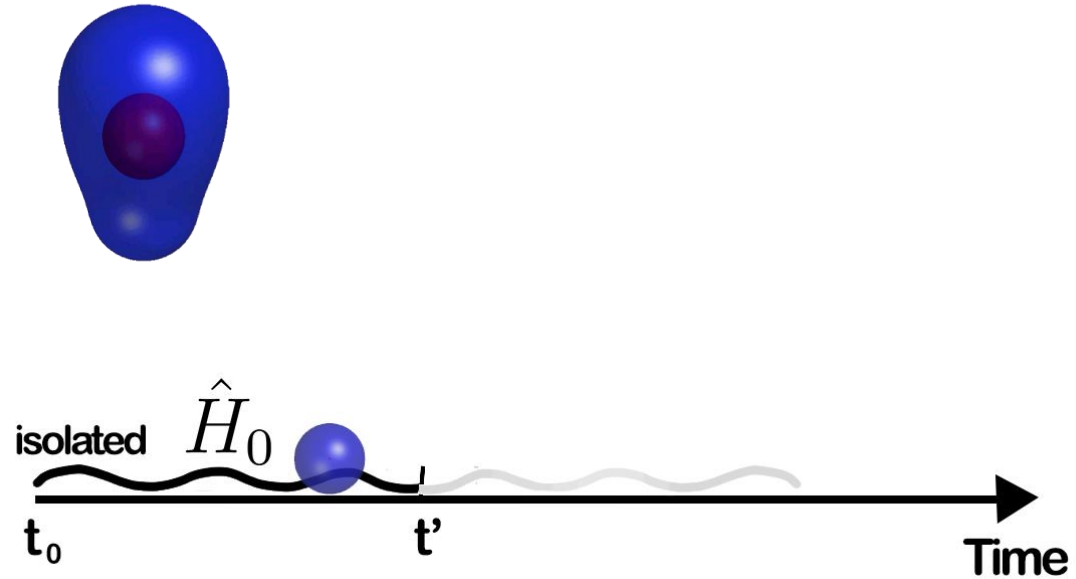
Q: How fast is this?

→ 1 billion times faster than your computer CPU (ns - 10^{-9} s)!



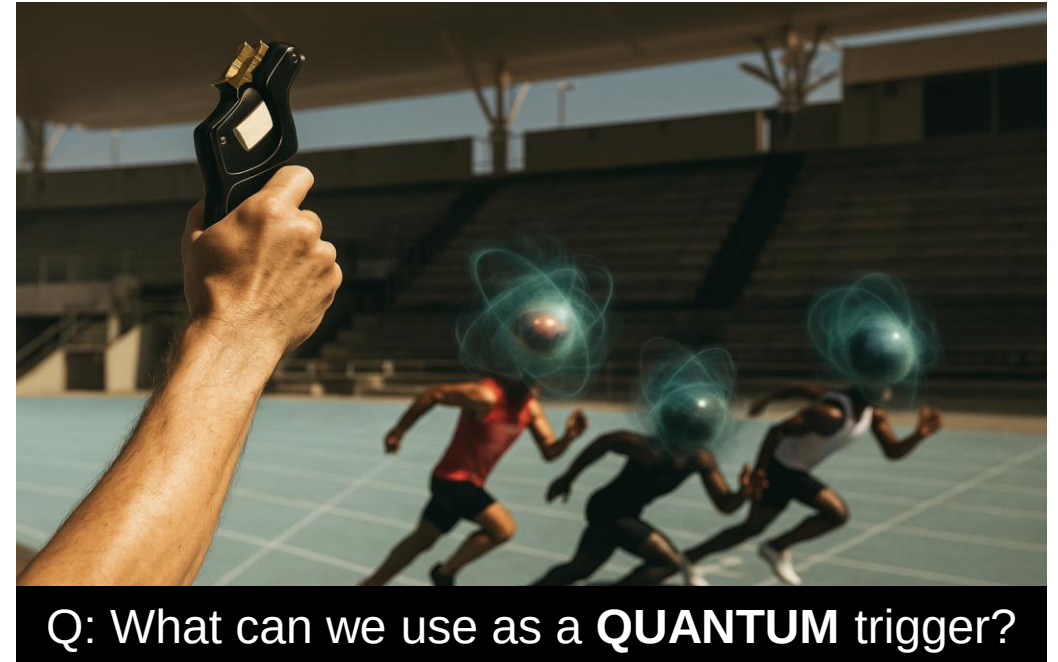
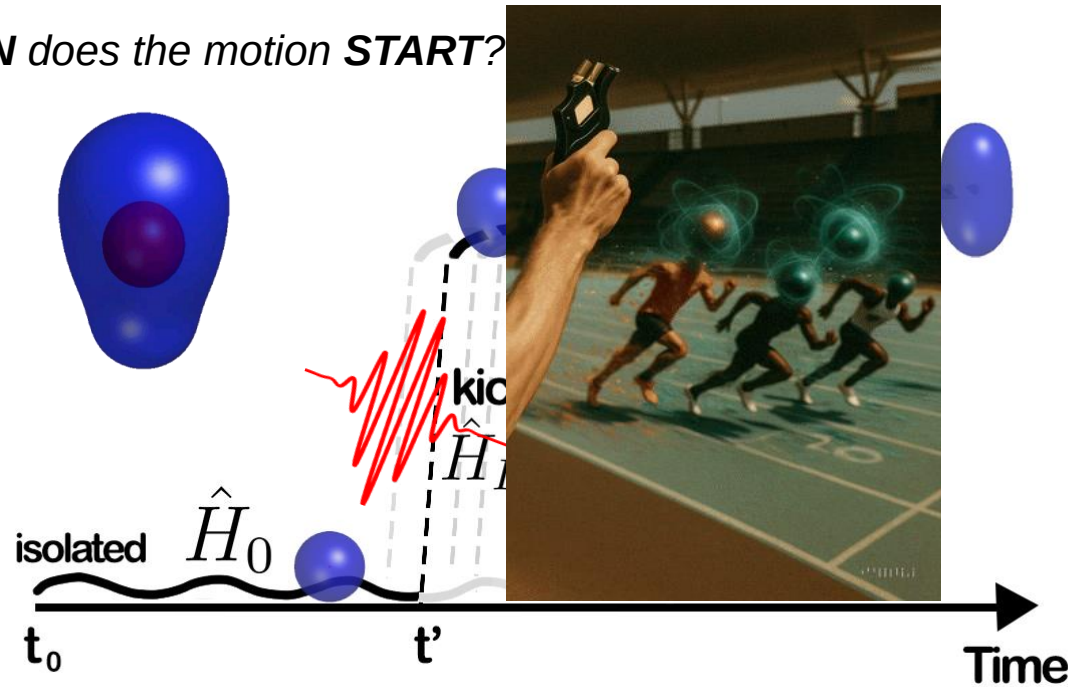
Electronic motion in matters

Cool... but **WHEN** did the motion **START**?



Electronic motion in matters

But **WHEN** does the motion **START**?



A **temporally confined** electromagnetic field (i.e. a **PULSE**)



LASER is great!

Pulse duration



10^{-15} s (femtosecond)

down to

10^{-18} s (attosecond)

with some tricks...

ETH zürich



Q: **who** has the record for the shortest pulse?

Spoiler: it is only **43 attoseconds** ...and it likes founde..

Nobel Prize to Attosecond Physics (2023)

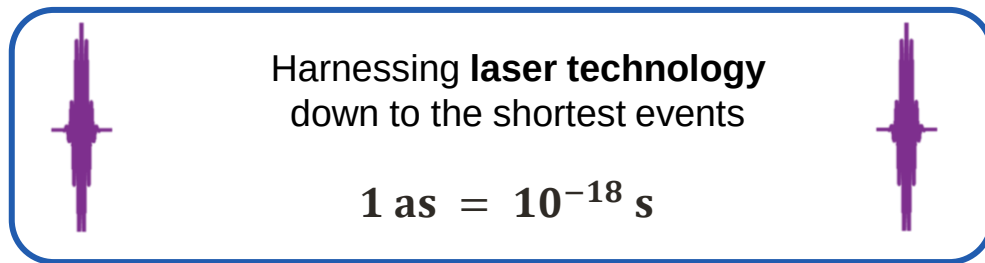


- **Ferenc Krausz**
Max Planck Institute of Quantum Optics, München, Germany
- **Anne L'Huillier**
Lund University, Sweden
- **Pierre Agostini**
The Ohio State University, Columbus, USA



*“for experimental methods that
generate **attosecond pulses** of light for the study of **electron dynamics** in matter”*

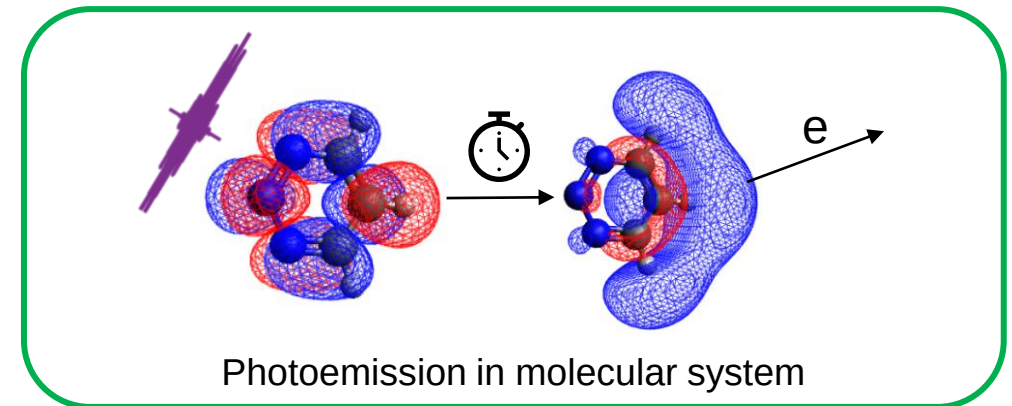
Attosecond Technology



XUV to **Soft-X-Ray** with compact tabletop setup

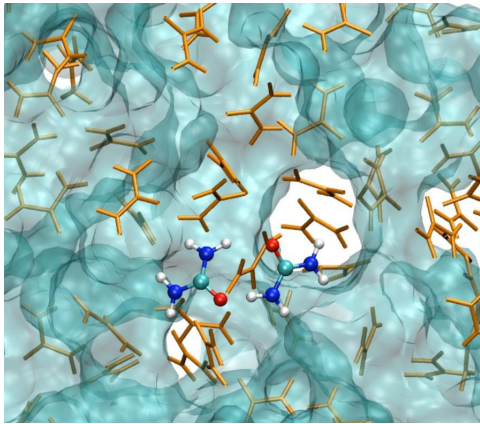


Electron dynamics in matter

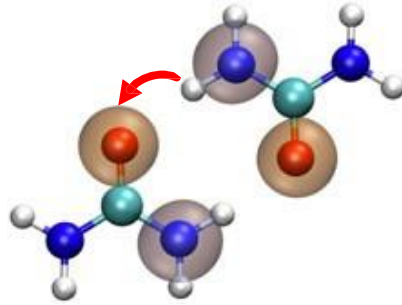


Investigating **natural processes** with the
ultimate **time-resolution** of **chemistry**

Ultrafast Chemistry of Liquids and Solutes

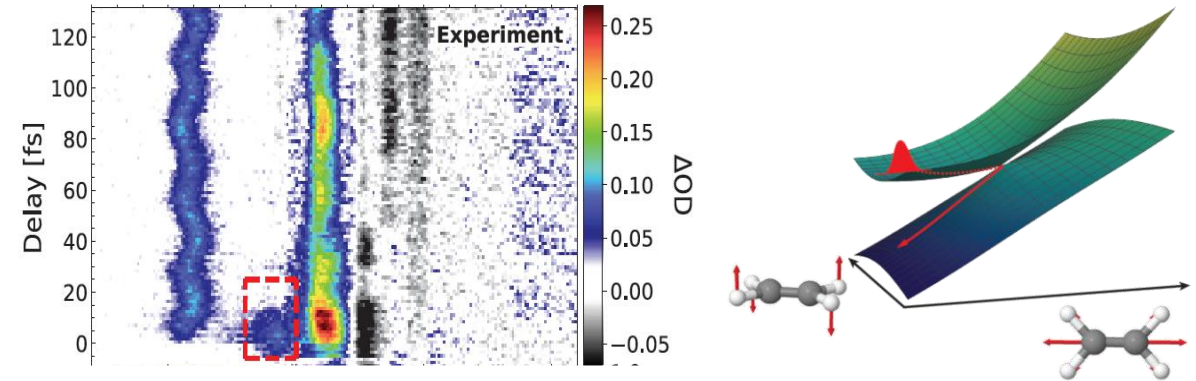


Z. Yin, et al. *Nature* **619**, 749 (2023)



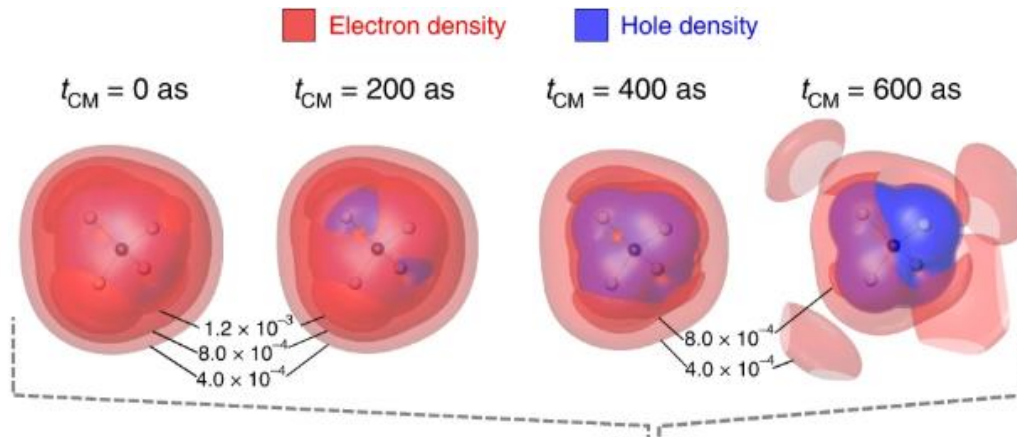
Attosecond X-ray Absorption Spectroscopy

non-adiabatic electron dynamics



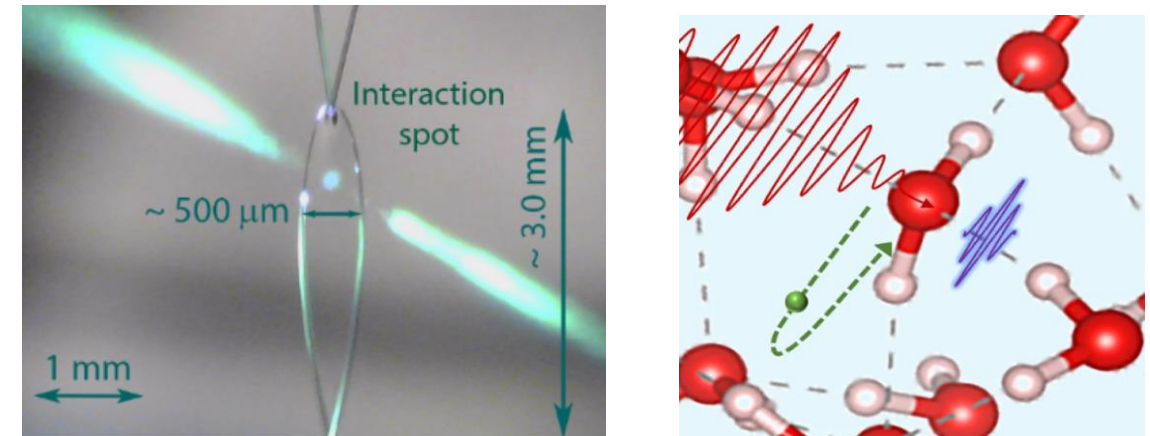
K. S. Zinchenko et al. *Science* **371**, 489-494 (2021).

Time-resolved Ultrafast Spectroscopy in gas-phase molecule



Matselyukh, D.T., et al. *Nat. Phys.* **18**, 1206-1213 (2022)

Generation of coherent extreme ultraviolet radiation in liquids



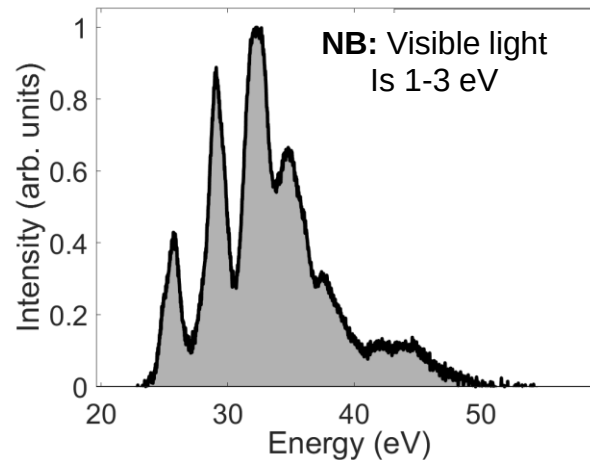
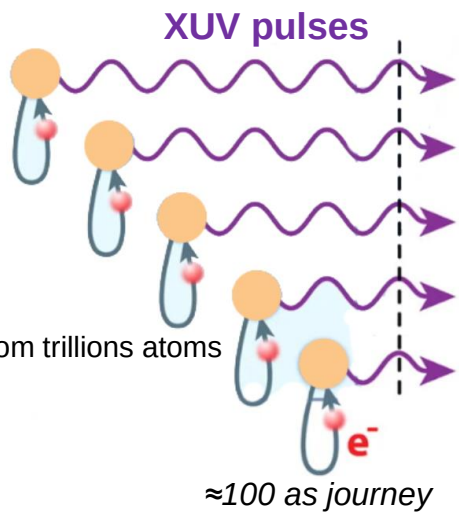
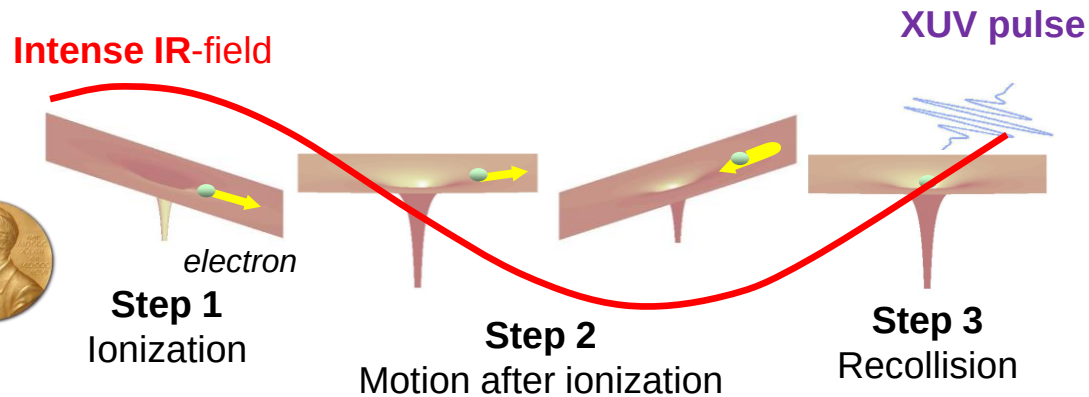
Mondal, A et al. *Nat. Phys.* **19**, 1813-1820 (2023).

Generation of coherent **extreme** ultraviolet radiation in liquids

High-order harmonics generation... in **liquids**

The recipe for generating **attosecond pulses**... and a **Nobel Prize** :

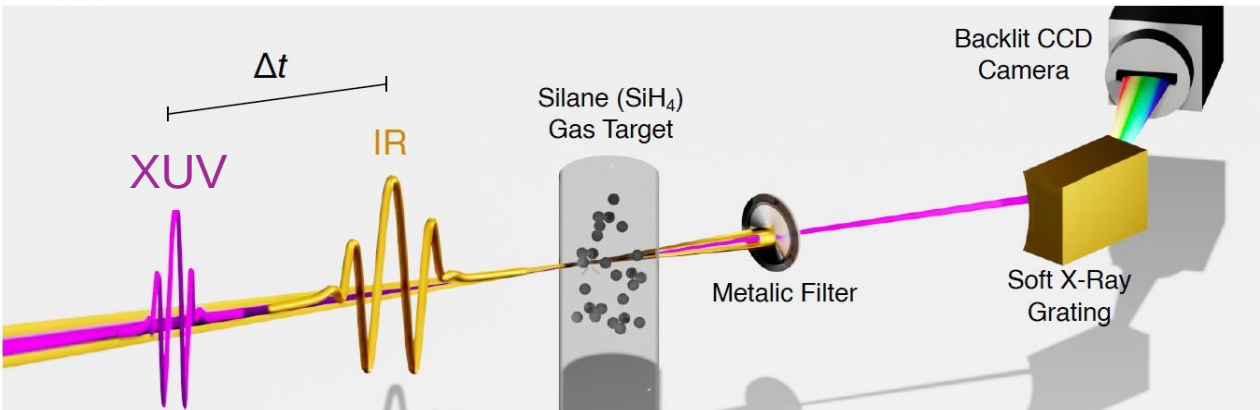
(standard) High-order harmonics generation ...in **atoms**



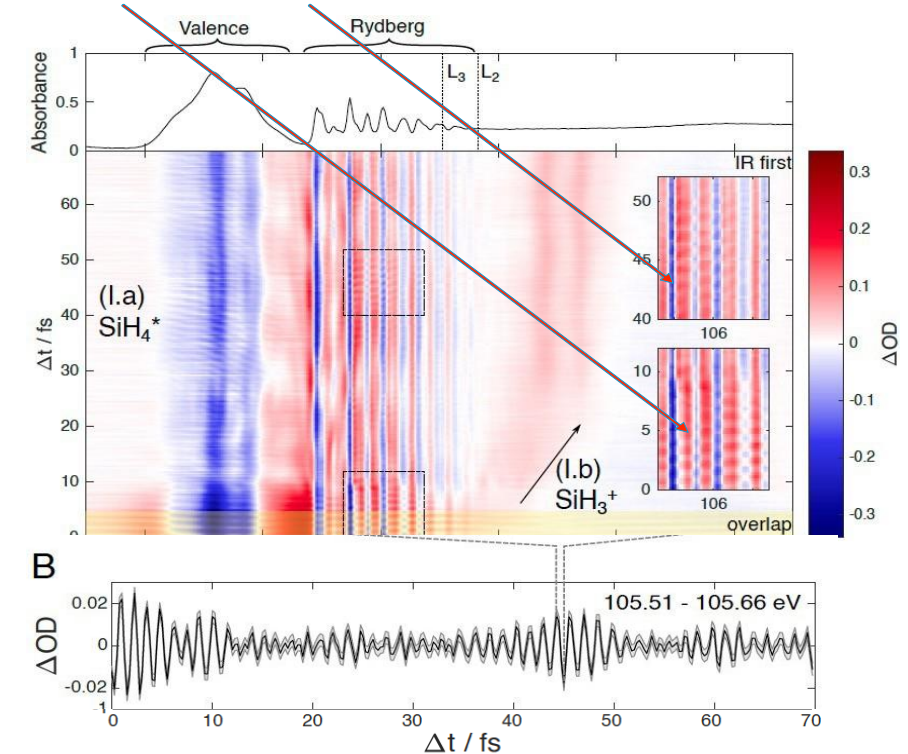
Q: What will happen in complex liquid environment with multiple molecular species?

This is how you generated **coherent XUV PULSES!!**

Time-resolved **Ultrafast Spectroscopy** in gas-phase molecules



Decoherence and revival of a 1.3-fs electronic wavepacket



Nat. Phys. **18**, 1206-1213 (2022)

Why is cool:

Exploring the coupling between **electronic coherence** and **ultrafast structural relaxation** processes, at the heart of molecular Quantum Mechanics

Q: Can electronic coherence survive in larger system?



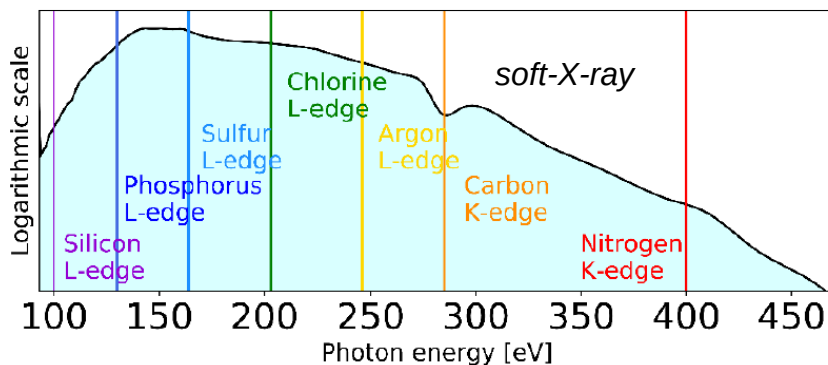
time resolution < 1 fs

ETH zürich

Attosecond X-ray Absorption Spectroscopy

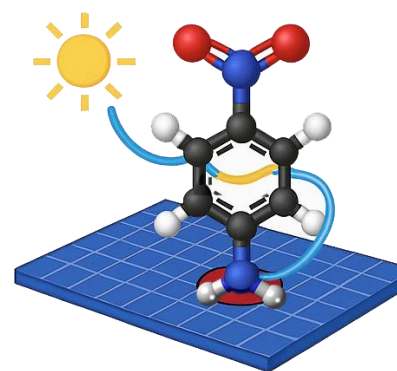
The ultimate experiment in **photochemistry** / **photovoltaic**/ **molecular optoelectronics**

Time resolution and **atomic** resolution!



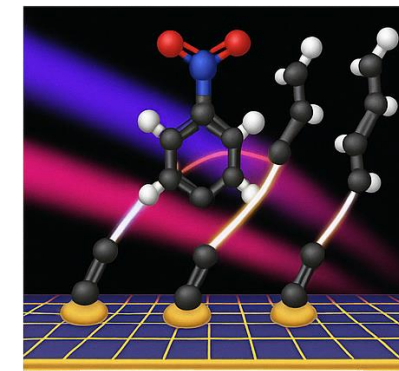
Sci Rep 13, 3059 (2023).

Initiating and probing **photochemistry** reactions



Photovoltaic

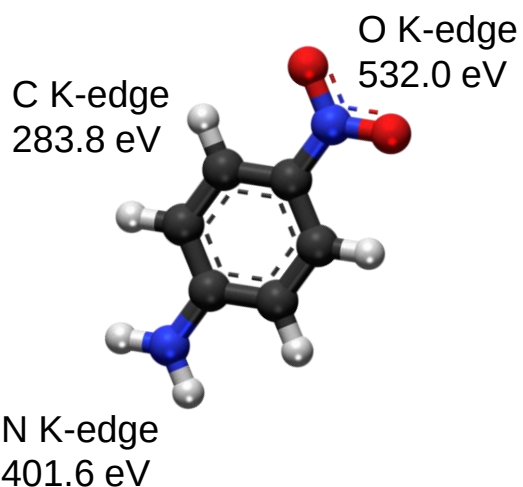
Photoswitching



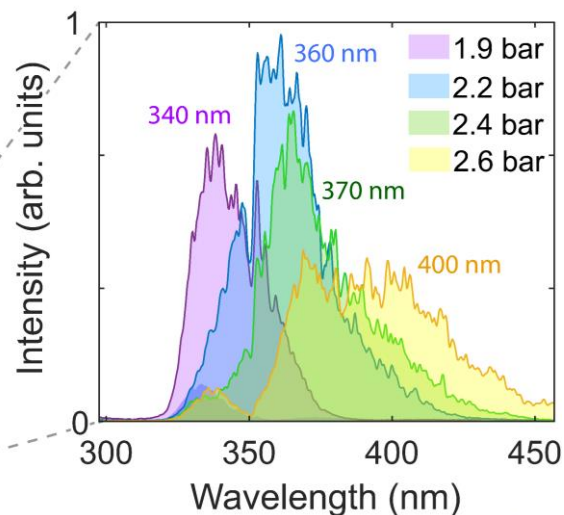
Photocatalysis

Molecular optoelectronics

X-ray Absorption Spectroscopy



Short-tunable-UV-pulses



Why is cool:

Following the charge motion in “real-time” and understand the core physical mechanism behind **photovoltaic** and **optoelectronics**



Q: Can we control **electronic motion** across different site of a molecules on **few-femtosecond time scale**?

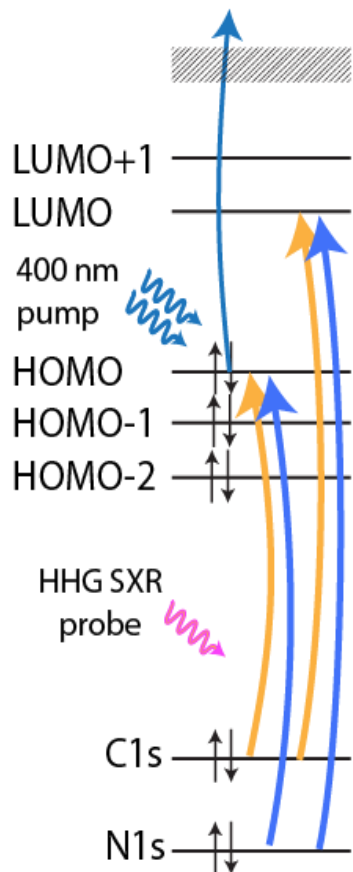
Ultrafast Chemistry of Liquids and Solutes

400 nm pump, ~30 fs

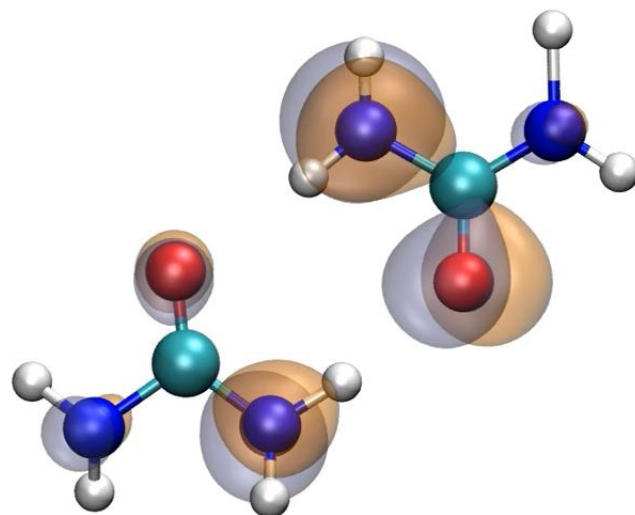
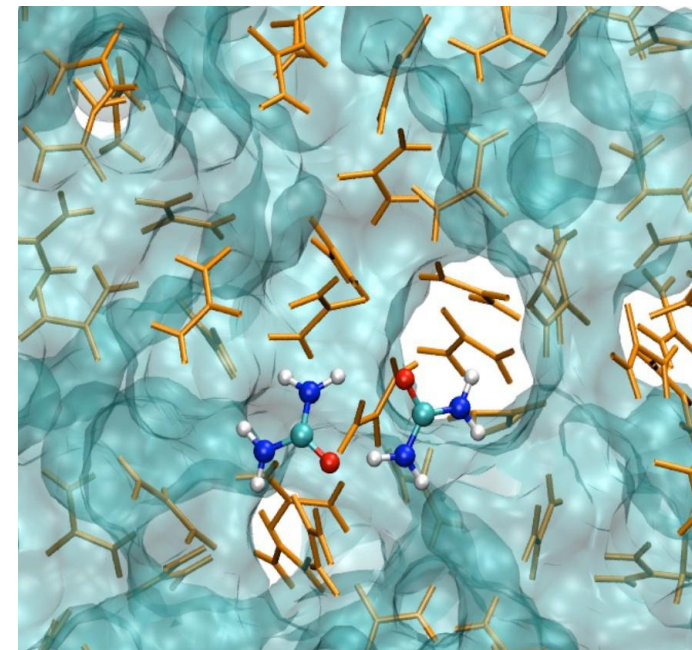
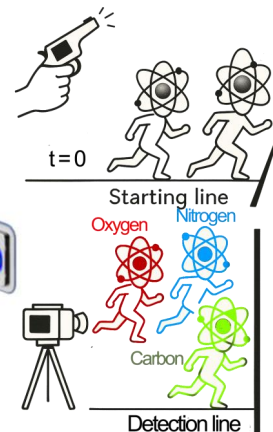
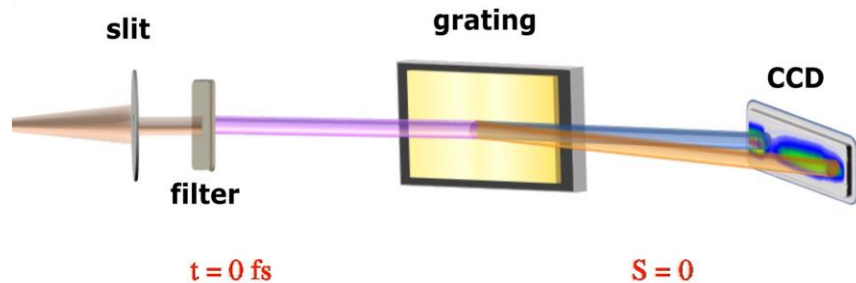
$\sim 1 \times 10^{14} \text{ W/cm}^2$

soft X-ray

mirror



Attosecond X-ray Absorption Spectroscopy



Calculations by: Y. Shaky, L. Inhester, R. Santra

Discovery of first key step
(i.e. proton transfer) in life-precursor molecule
(UREA)

Nature **619**, 749 (2023)

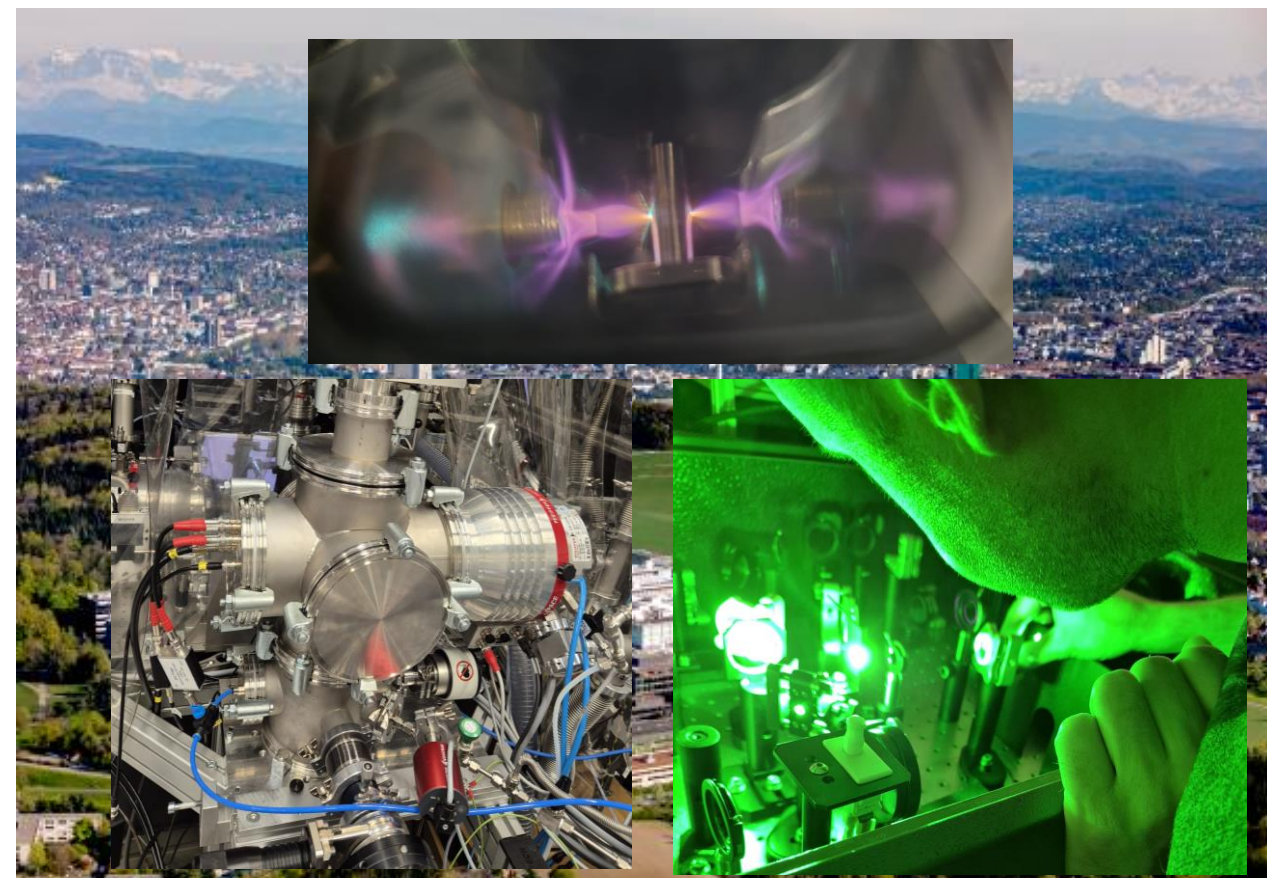
Why is cool:



Understanding **fundamental processes** and chemical reactions in liquid environment with the **ultimate time resolution** of **Chemistry**

Q: What is the *mesoscopic limit* of quantum mechanical process and the impact of **decoherence** on the wavefunction in an actual environment?

Ultrafast Spectroscopy and Attosecond Science group ETHZ



The team + Anne L'Huillier 



For more info contact:

hansjakob.woerner@phys.chem.ethz.ch



You like one of this topic? Looking forward to see you in the lab!

March 2025

Review article

 Check for updates

Ultrafast spectroscopy of liquids using extreme-ultraviolet to soft-X-ray pulses

Hans Jakob Wörner¹✉ & Jean-Pierre Wolf²✉





Shuttle Catalysis & Molecular Editing

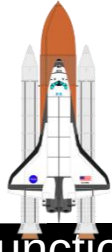
Recent Adventures in the Morandi Group

Yannick Brägger

Our Group



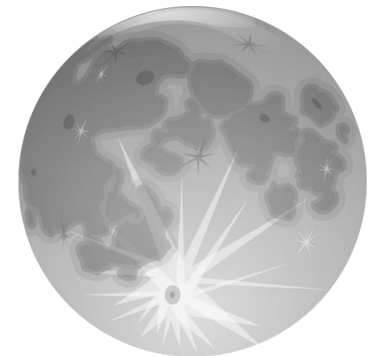
Shuttle Catalysis - Concept



Molecule1

Functional
Group

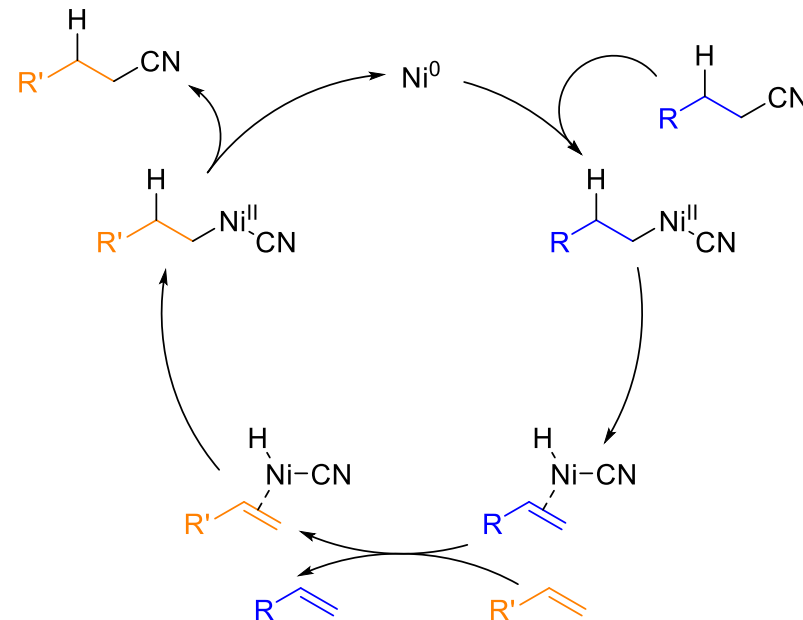
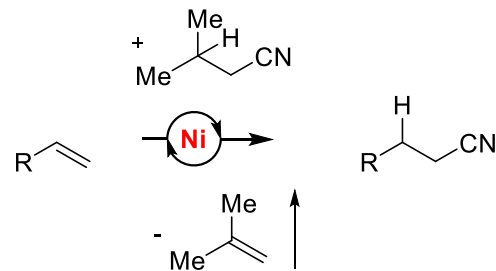
Molecule2



Shuttle Catalysis - Concept

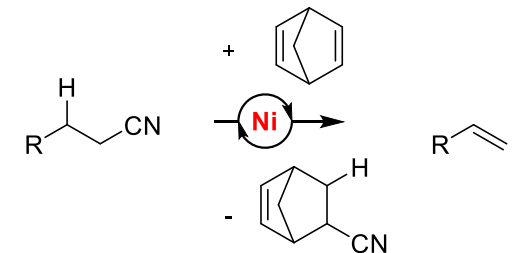


Molecule1



Molecule2

Functional Group



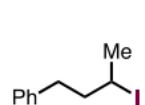
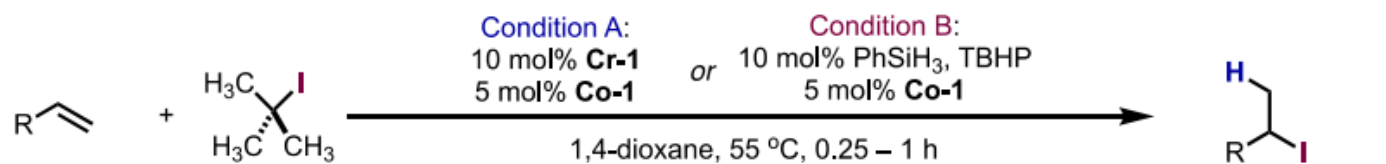
Shuttle Catalysis – Recent Developments

How to overcome limitations of classical approach?

Use 1 e⁻ logic instead!

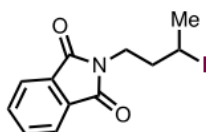


Dr. Tanner Jenkins



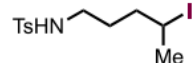
2a

[A] 91% (81%)
[B] 84%



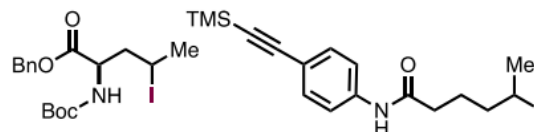
2b

[A] 99% (99%)
[B] 92%



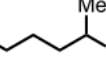
2c

[A] 64% (54%)
[B] 62%



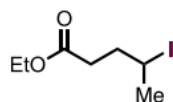
2d

[A] 65% (60%) d.r. 1.9:1
[B] 64%



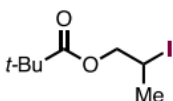
2e

[A] 39% (36%)
[B] 15%



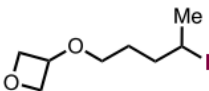
2f

[A] 75% (60%)
[B] 79%



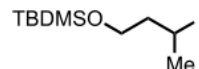
2g

[A] 54% (50%)
[B] 26%



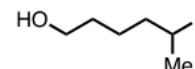
2h

[A] 43% (40%)
[B] 50%



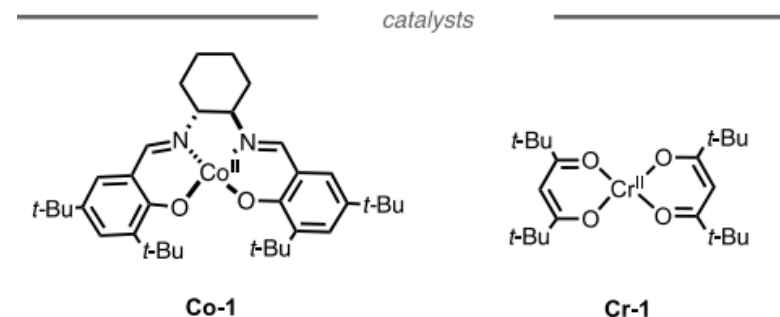
2i

[A] 92% (85%)
[B] 76%



2j

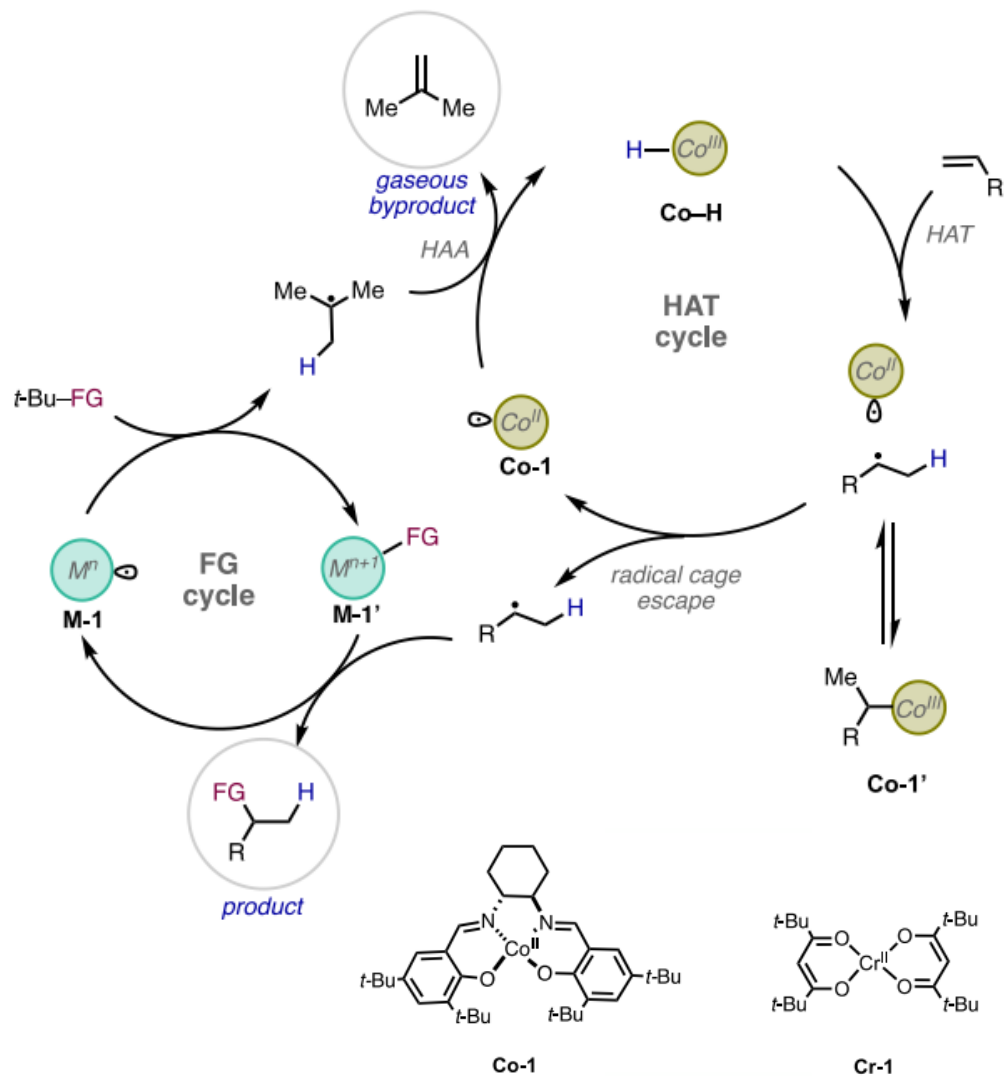
[A] 60% (47%)
[B] 15%



Shuttle Catalysis – Recent Developments

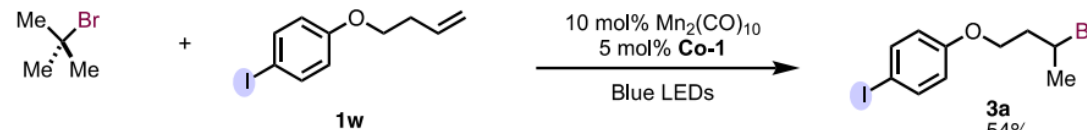


Dr. Tanner Jankins

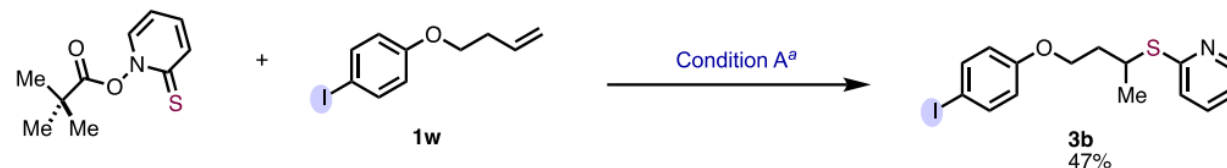


Many different groups transferable!

(E) Transfer hydrobromination



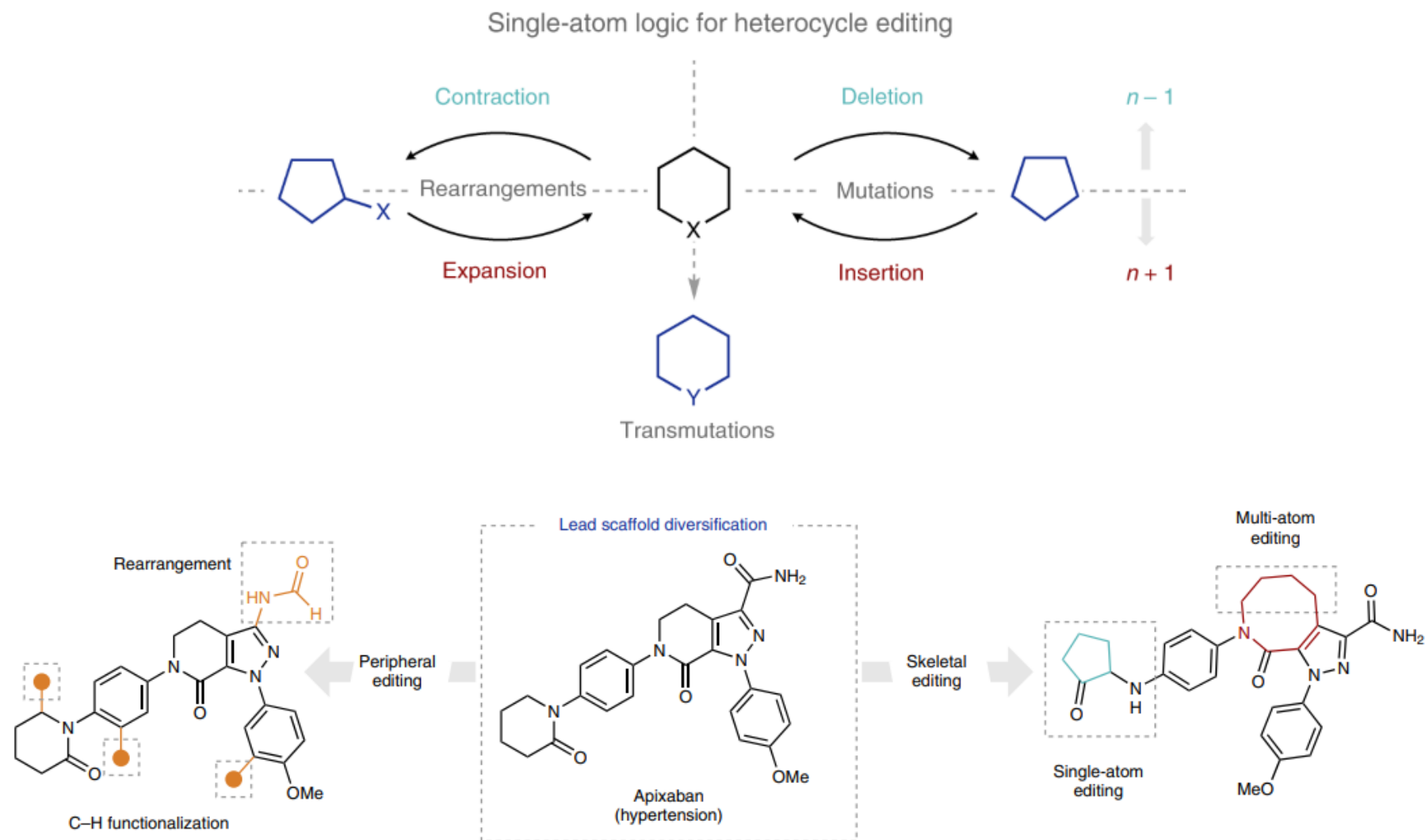
(F) Transfer hydrothiolation



+ ...

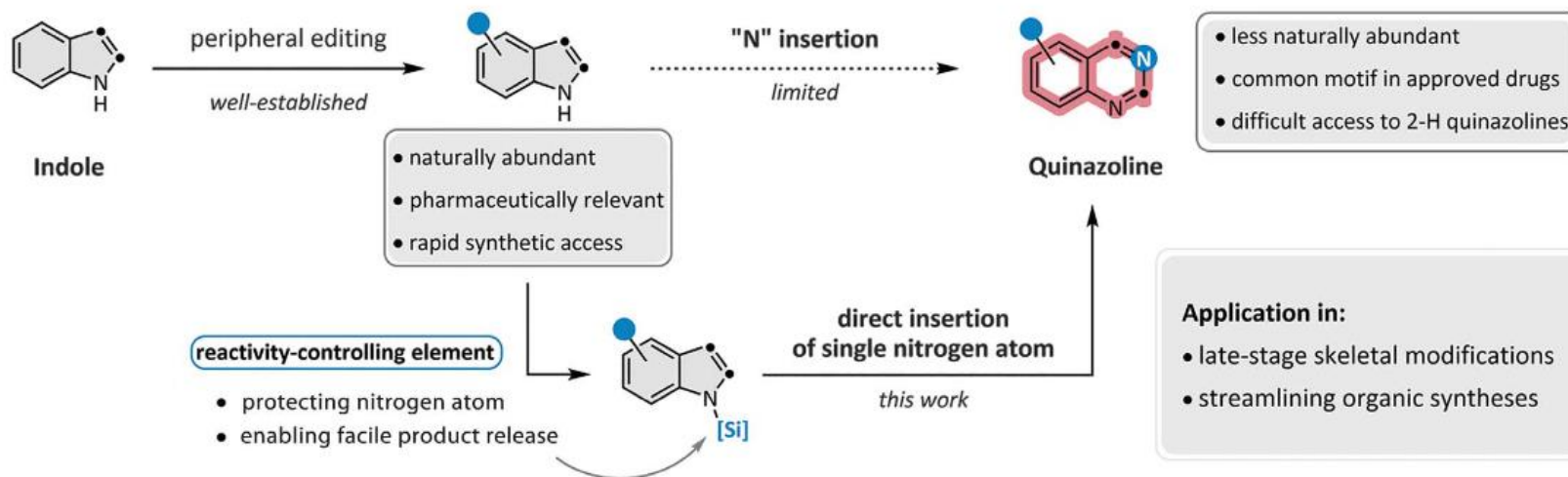
Many ongoing projects in our group

Molecular Editing

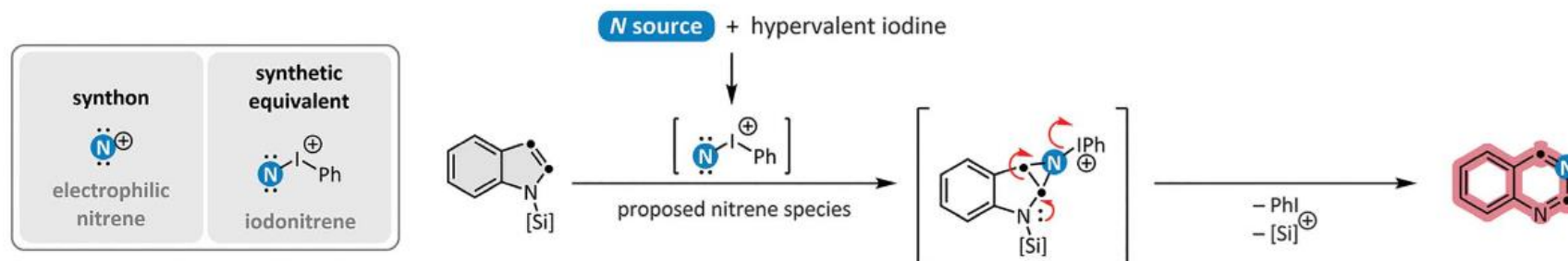


Molecular Editing – Recent Developments

Conceptual outline



Mechanistic design

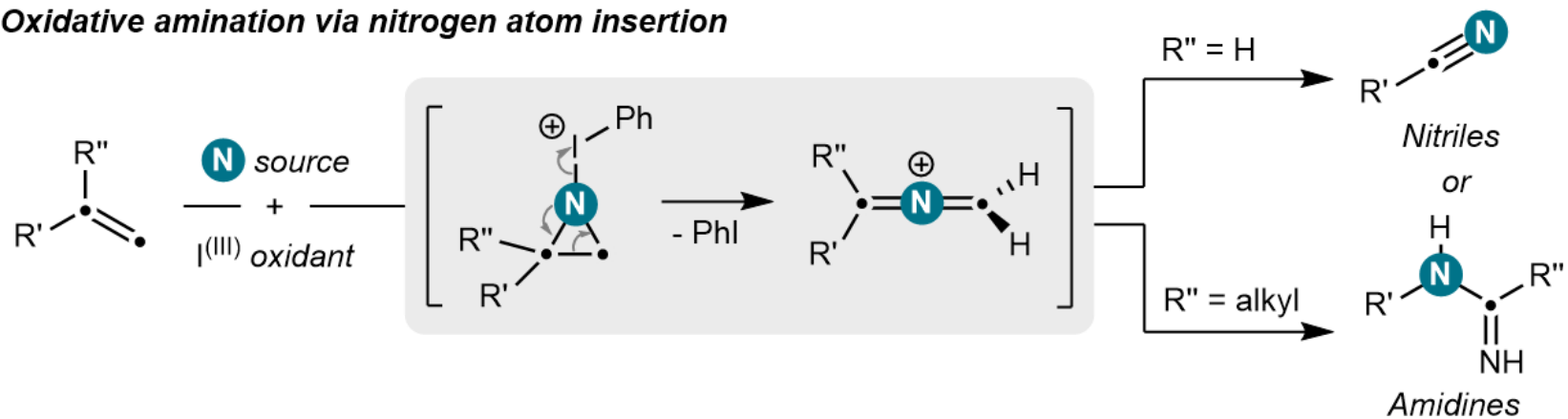


Dr. Julia Reisenbauer

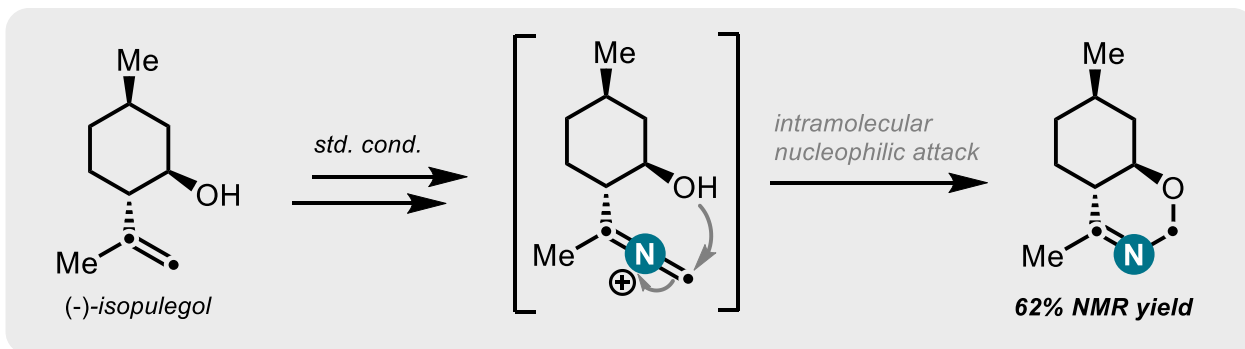
Extremely useful reaction! Can we do something like this with unactivated alkenes?

Molecular Editing – Recent Developments

Oxidative amination via nitrogen atom insertion



Observation during the project:



Can we quench aza-allenium salts intramolecularly in modular fashion?



Ann-Sophie
Paschke



Yannick
Brägger

Real heroes behind this project:



Nima
Nasiri

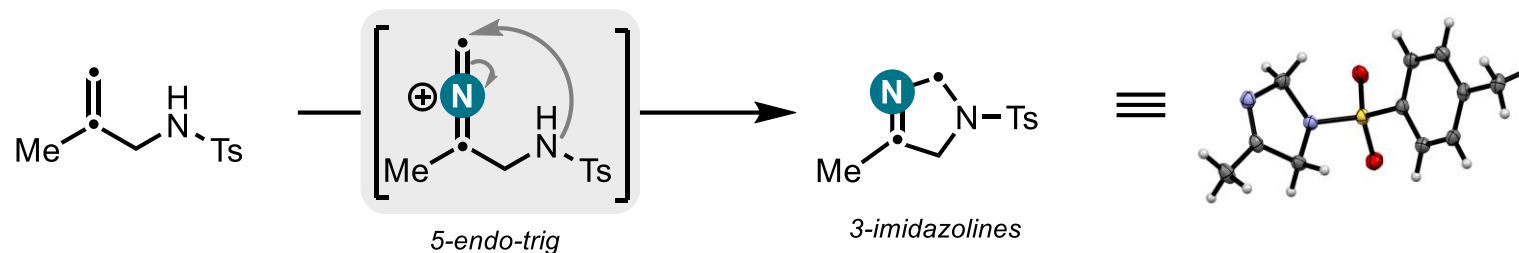


Francesco
Felician

former semester students

Molecular Editing – Recent Developments

Can we quench aza-allenium salts intramolecularly in modular fashion?

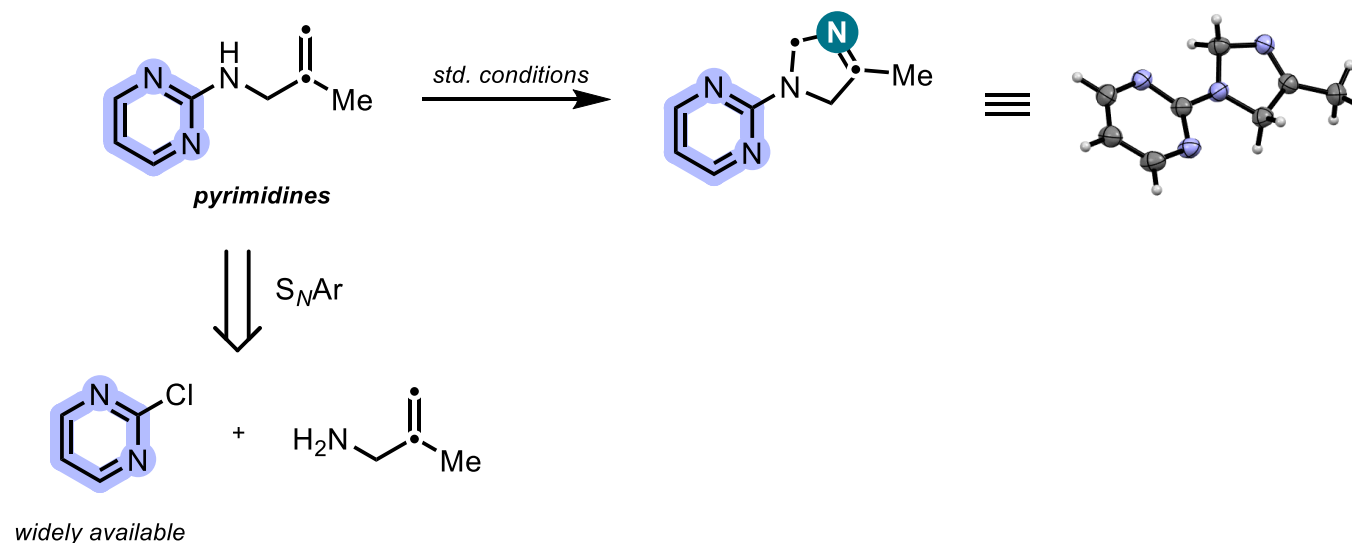


Eleonora
Tufano



Yannick
Brägger

Real heroes behind this project:



Lara
Sorrentino



Matteo
Amberg



Paul
Gärtner

former/current semester students

What kind of work can students expect?

- Organic / organometallic synthesis
- Screening
- Analytical methods (GC-FID, GC-MS, NMR etc.)
- Cool instruments: Glovebox, HPLC
- All electronic lab journals (no manual calculations!)
- Biotage (automated flash column!!)
- Own fumehood or shared with supervisor
- Contributing ideas is encouraged!
- Students have some say in which area they work



Interested?

- Contact Bill directly via E-Mail (have patience)
- Try to be early (one semester in advance)



Morandi Group Website

Thanks for your attention!



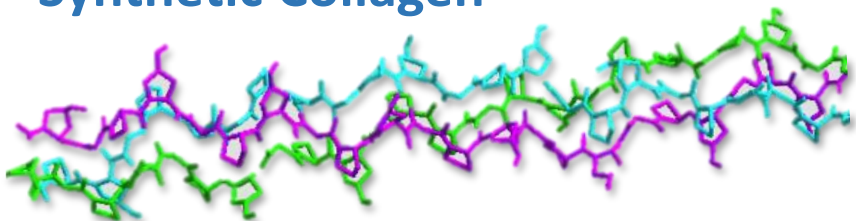
Peptides: From Cell Penetration to Catalysis



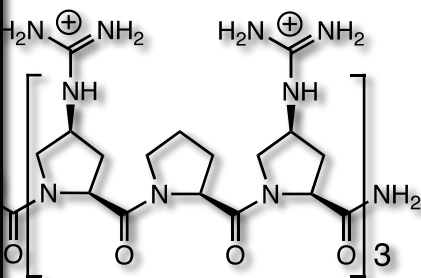
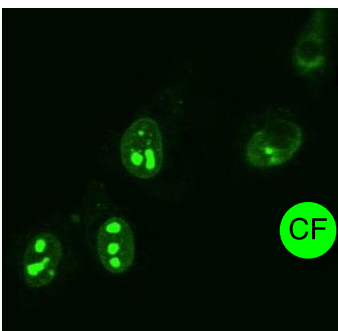
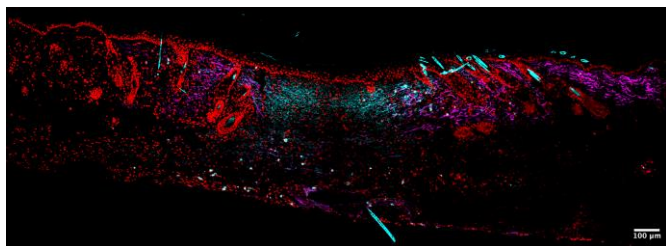
Lena Beiersdörfer - Semesterarbeitsinfoevent, 22.05.2025

Research in the Wennemers Group

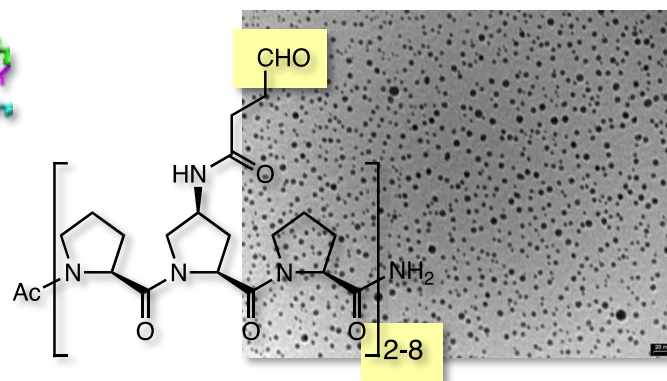
Synthetic Collagen



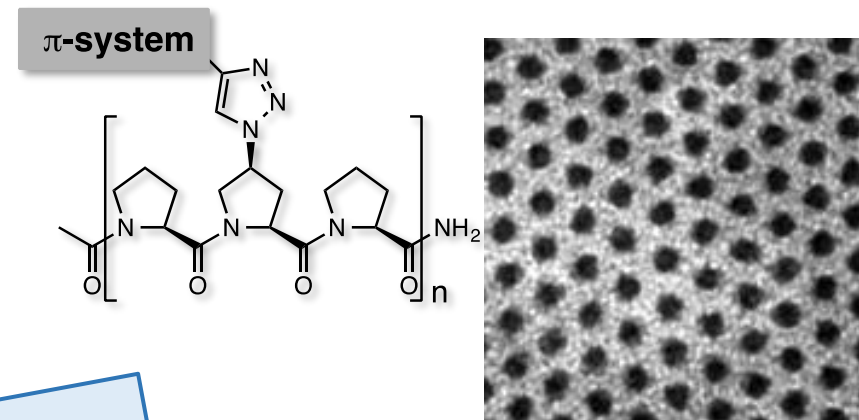
Chemical Biology



Metal Nanoparticles

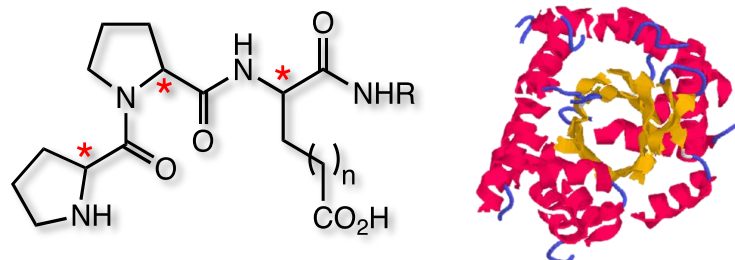


Supramolecular Assemblies

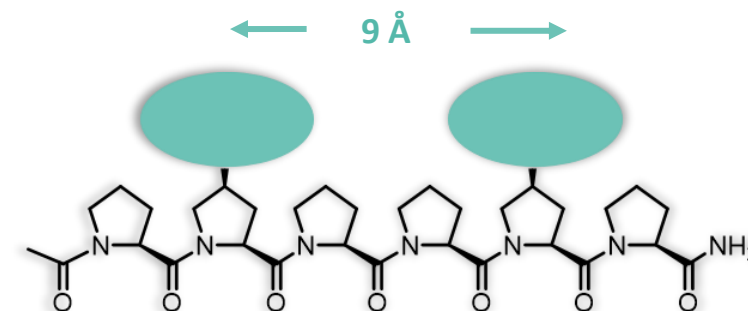


Peptides – Molecular Allrounders

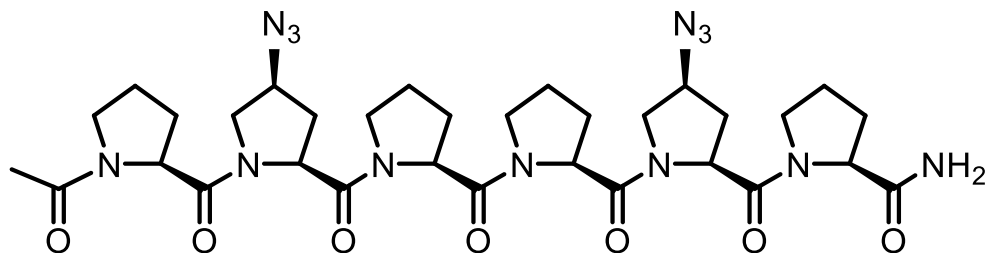
Asymmetric Catalysis



Host-guest Chemistry

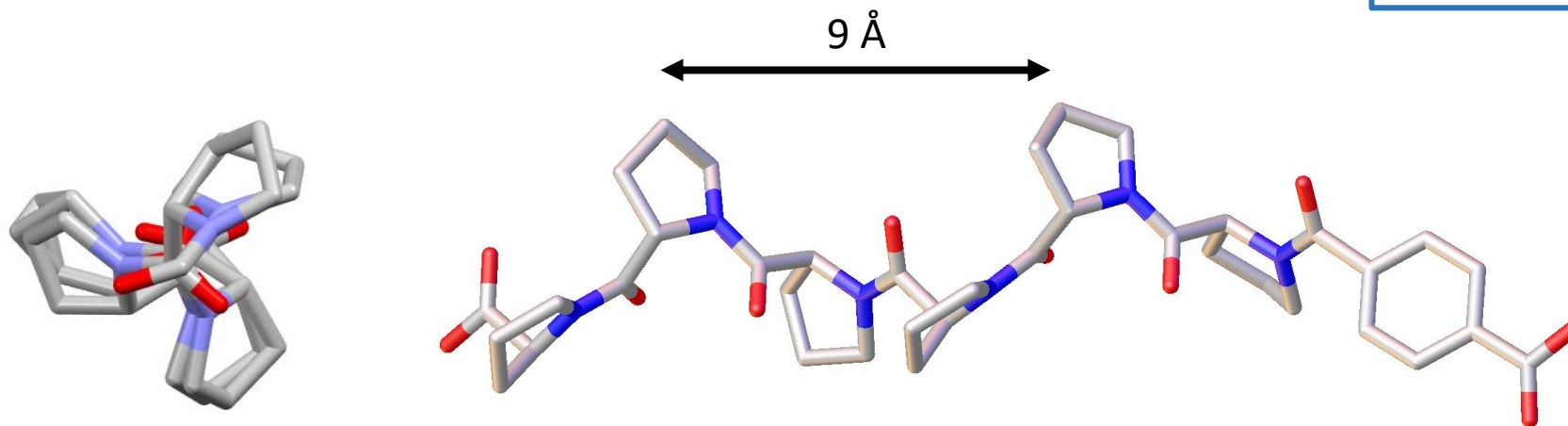


Oligoprolines – Versatile Molecular Scaffolds



Polyproline II helix

- Three residues for one turn
- Distance of 9 Å
- Scaffold is functionalizable by incorporation of azidoproline



A triaxial supramolecular weave



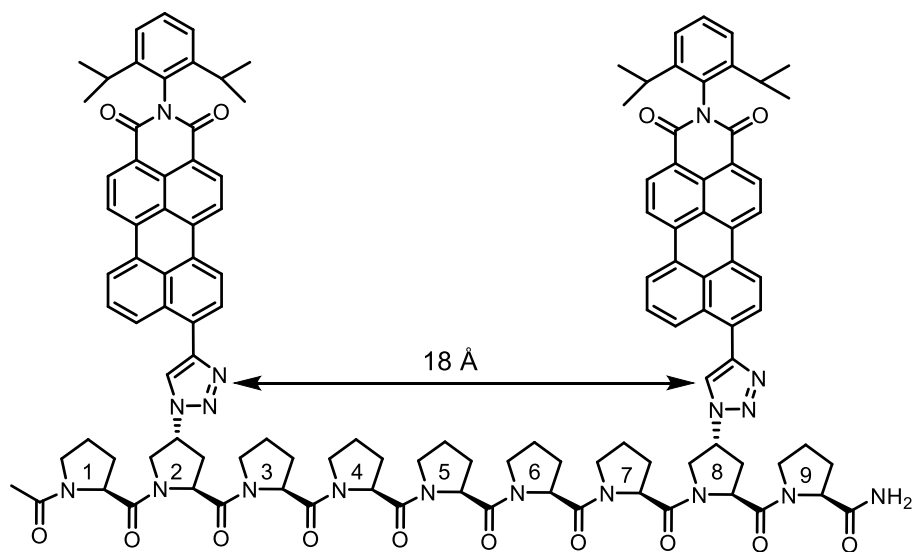
Organic Synthesis



Supramolecular Chemistry

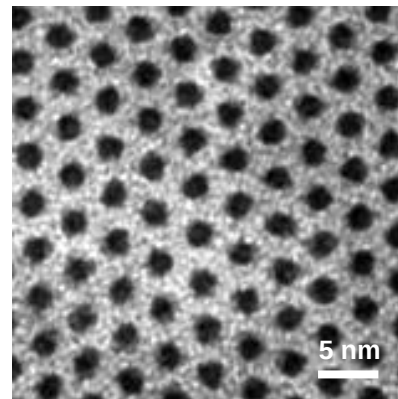


Cool Analytical Techniques

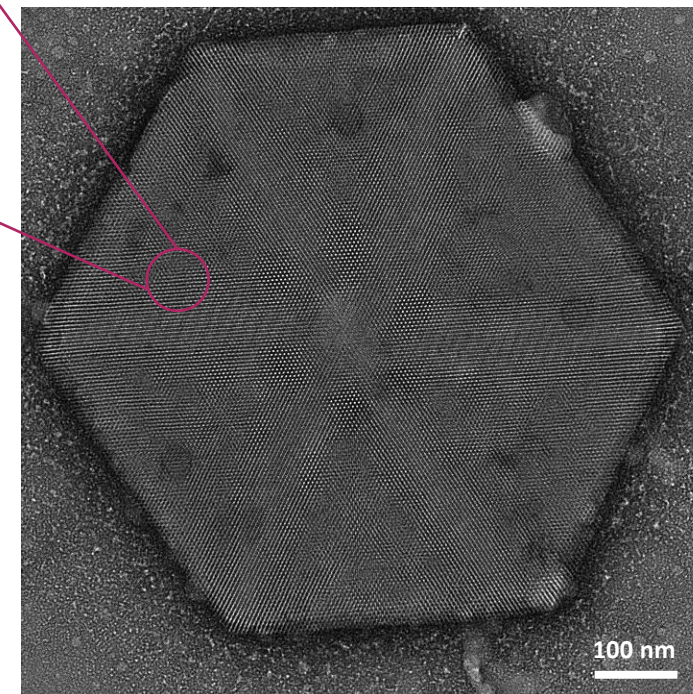


Possible projects

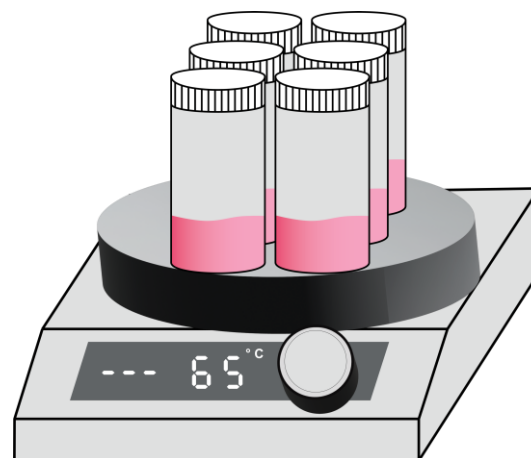
- Organic synthesis of building block (e.g. ^{13}C labelling for solid state NMR, derivatization of standard structure)
- TEM analysis of assemblies



Transmission Electron Microscopy

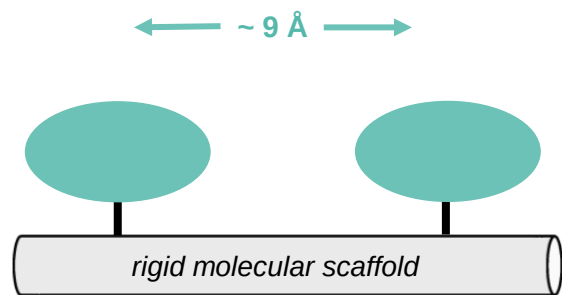


Annealed 65°C, 1h,
3:7 THF/H₂O

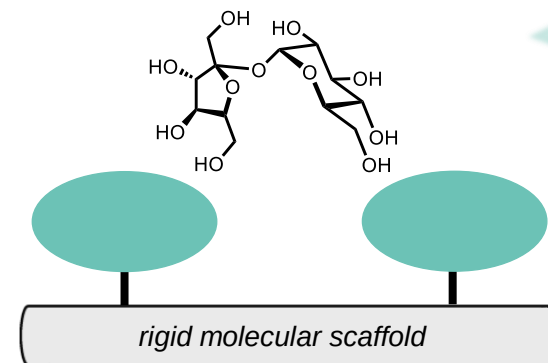
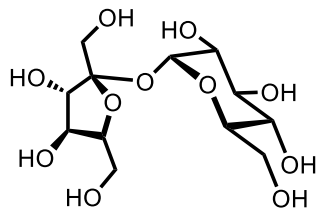


Kagome: 'basket with eyes'

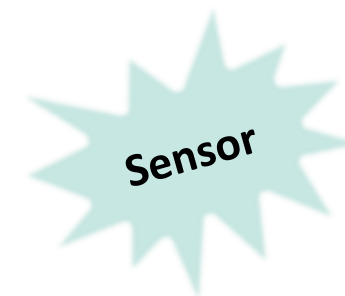
Synthetic Receptors for Carbohydrates



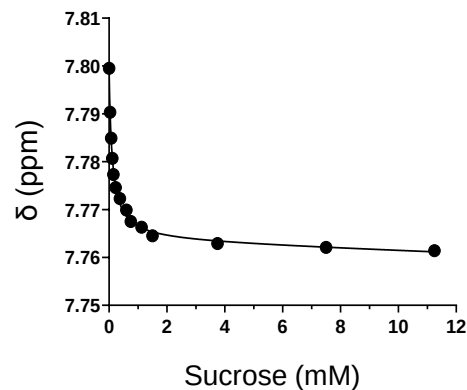
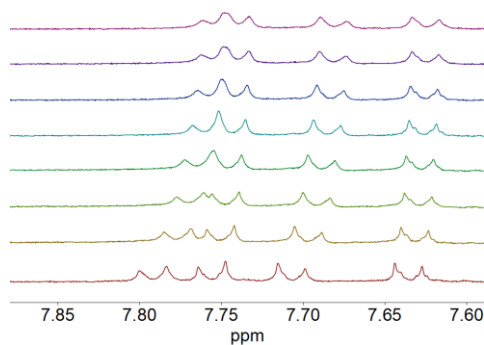
Precise placement of functional groups



Binding of carbohydrates



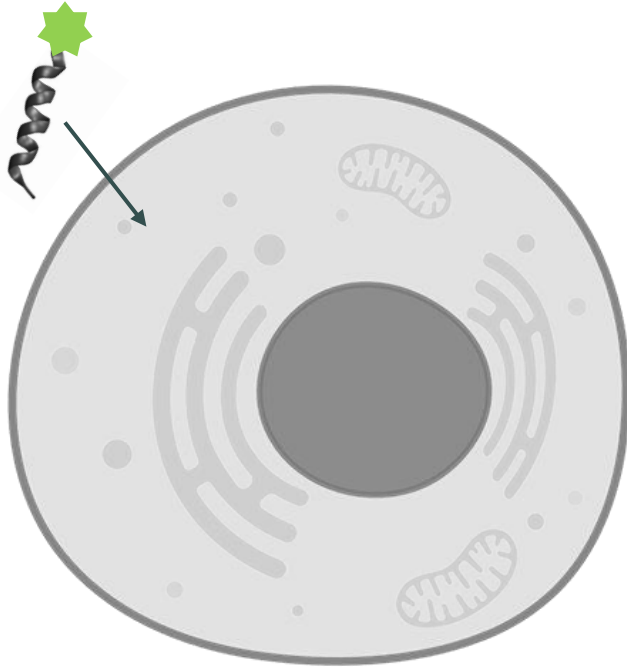
Determination of binding constants



Projects

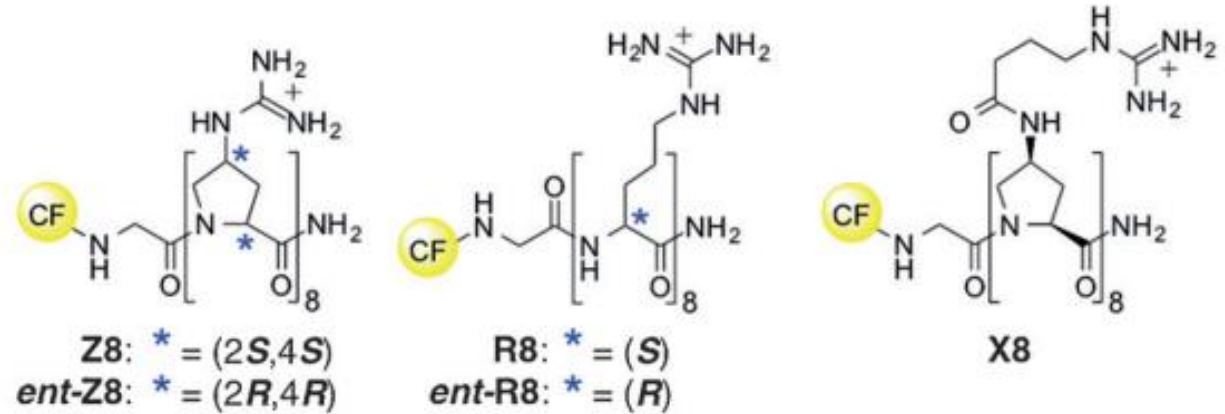
- Organic synthesis, SPPS, characterization & analysis
- Determination of binding constant (NMR, UV-Vis, ITC, Fluorescence...)
- Investigation of the binding mode
- Development of a sensor

Cell Penetrating Peptides

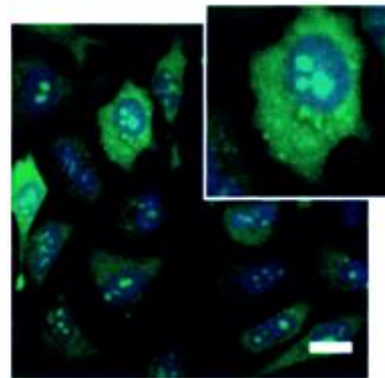


Projects

- Synthesis of new peptides by SPPS
- Analysis and characterization of the peptides
- Cell experiments and microscopy to determine localization in cells

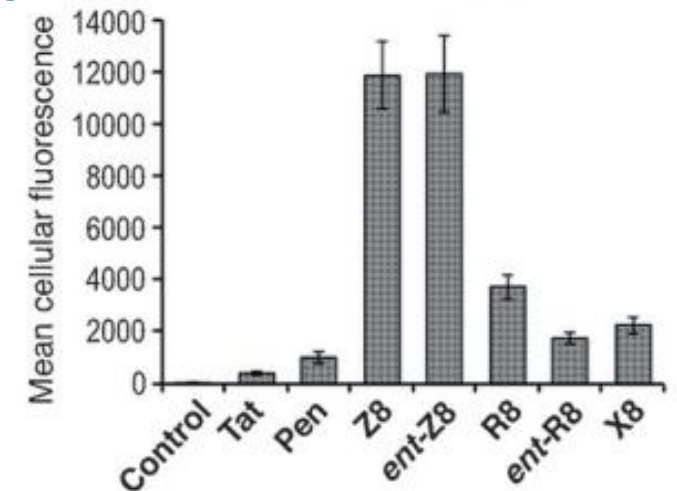


Confocal



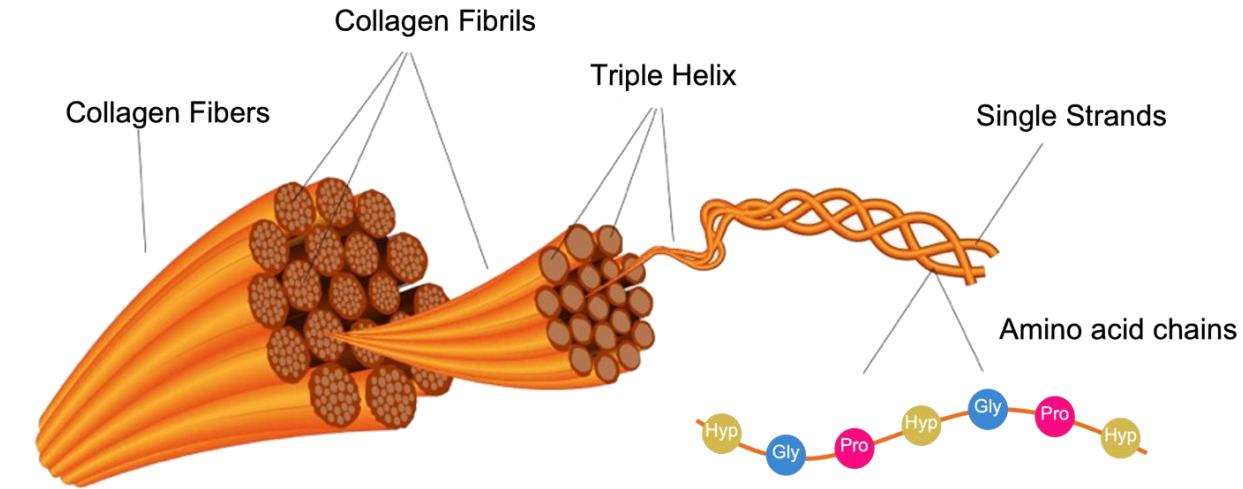
Hela, 10 μ M Z8 for
1 h at 37 °C

FACS



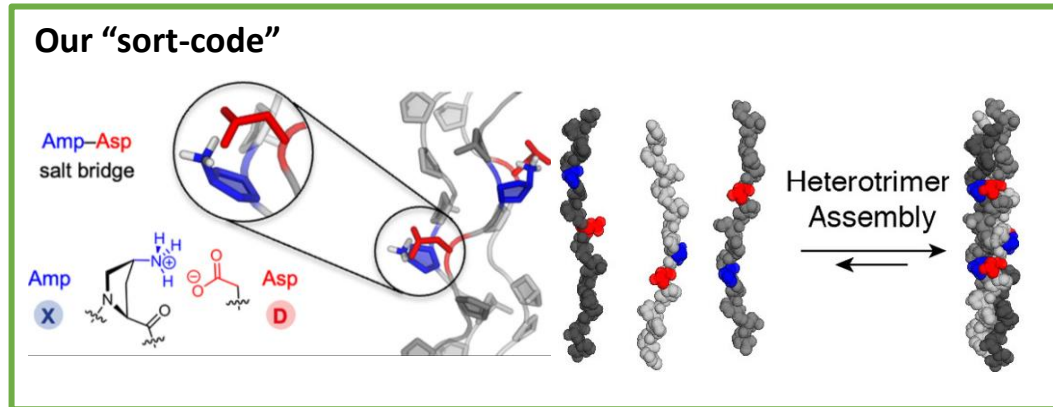
Hela, 10 μ M for 1 h at 37°C

Synthetic functionalized heterotrimeric collagen mimetic assemblies

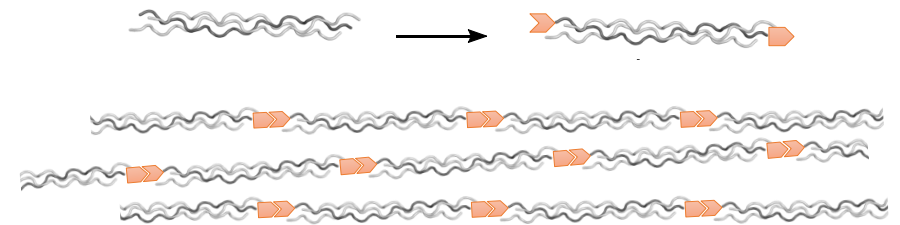


Going forward: Controlling the selective assembly of not only the triple helix, but also fibril formation!

So far: Successfully created a “self-sorting” code for selective synthetic collagen heterotrimer assembly!



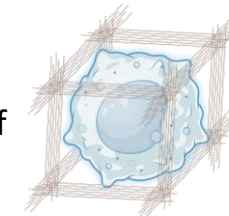
Ongoing project: incorporation of functional groups directing fibril propagation



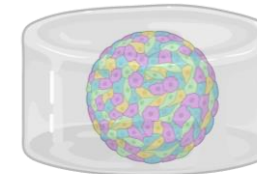
3

Ultimate challenge: Functionalized synthetic heterotrimeric collagen fibrils

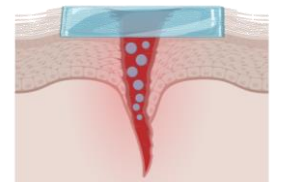
Incorporation of collagen functional sequences and testing recognition events in the presence of cells as a step towards development of wound-healing materials, 3D cell culture and others!



Cell encapsulation

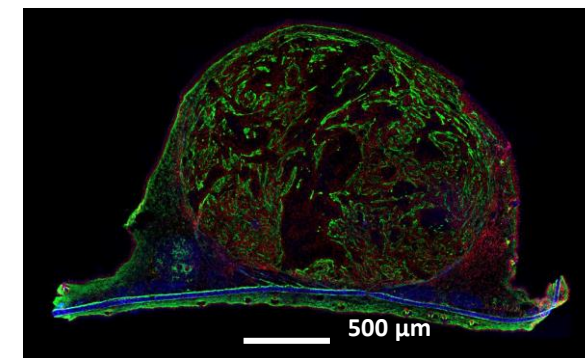
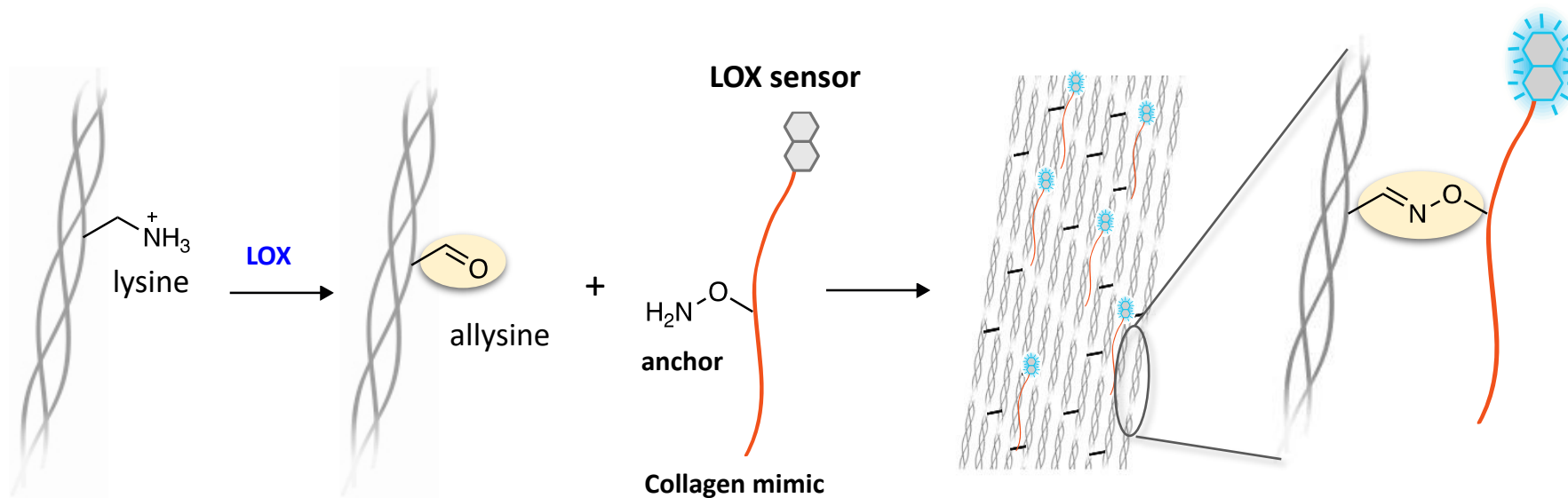


3D cell culture



Wound healing patches

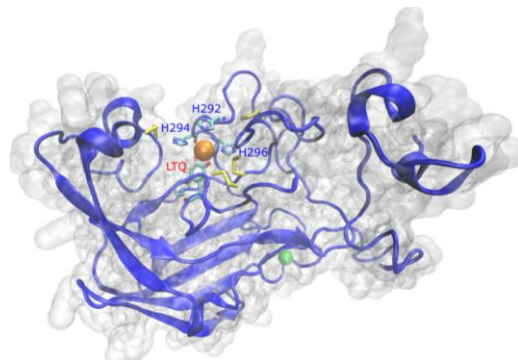
Monitoring and visualizing LOX activity



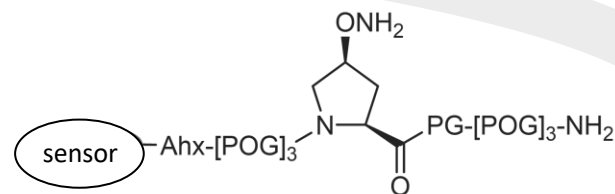
Projects

- Organic synthesis of new probes and dyes
- Investigation of new compounds for targeting proteins or as small molecule drugs against fibrosis
- Investigation of new fluorophores as sensors

LOX inhibitor/selectivity



Targeting moiety

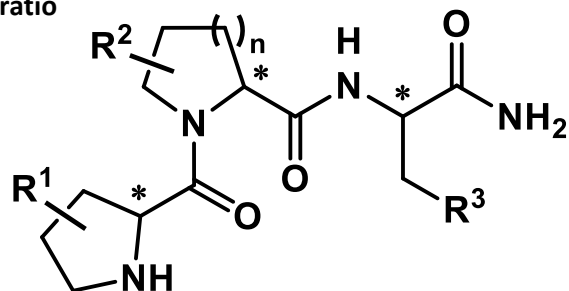


Diagnostic & therapeutic tools

under development

Asymmetric Organocatalysis with Peptides – the Pro-Pro-Xaa motif

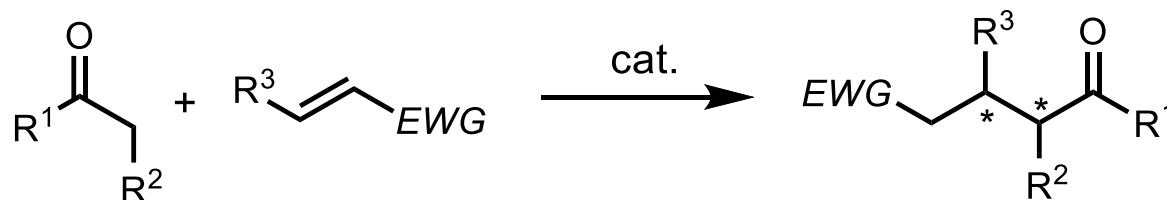
2nd amino acid
trans/cis ratio



3rd amino acid
Important for b-turn
side chain for
substrate coordination

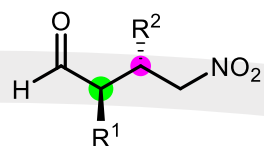
1st amino acid: Proline
reactive site: 2nd amine

Reactions catalyzed by Pro-Pro-Xaa catalysts:



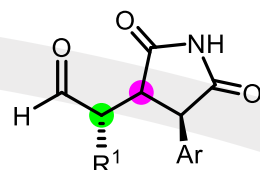
a) M. Wiesner, J. D. Revell, H. Wennemers, *Angew. Chem. Int. Ed.* **2008**, 120, 1897; **b)** J. Duschmalé, H. Wennemers, *Chem. Eur. J.* **2012**, 18, 1111; **c)** R. Kastl, H. Wennemers, *Angew. Chem. Int. Ed.* **2013**, 52, 7228; **d)** T. Schnitzer, H. Wennemers, *Synlett* **2017**, 28, 1282; **e)** T. Schnitzer, A. Budinská, H. Wennemers, *Nat. Catal.* **2020**, 3, 143; **f)** J. S. Moehler, T. Schnitzer, H. Wennemers, *Chem. Eur. J.* **2020**, 26, 15623; **g)** C. E. Grünenfelder, J. K. Kisunzu, H. Wennemers, *Angew. Chem. Int. Ed.* **2016**, 55, 8571; **h)** G. Vastakaite, C. E. Grünenfelder, H. Wennemers, *Chem. Eur. J.* **2022**, 28, e202200215; **i)** T. Schnitzer, J.W. Rackl, H. Wennemers, *Chem. Sci.*, **2022**, 13, 8963-8967. **j)** M. Schnurr, J. W. Rackl, H. Wennemers, *J. Am. Chem. Soc.* **2023**, 145, 23275–23280.; **k)** A. Budinská A., H. Wennemers, *Angew. Chem. Int. Ed.* **2023**, 62, e202300537.

H-Pro-Pro-Xaa Peptidic Catalysts –Applications



T. Schnitzer *et. al.*,
Nat. Catal. **2023**

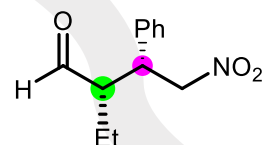
up to 98% yield
up to >20:1 *d.r.*
up to 98% ee



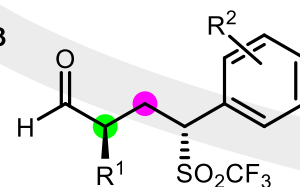
G. Vastakaite *et. al.*,
CEJ **2022**

up to 99% yield
up to >86:9:1:4 *d.r.*
up to 95% ee

reaction in
complex environments

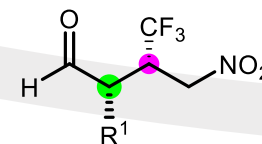


J. Rackl *et. al.*,
Chem. Sci. **2023**



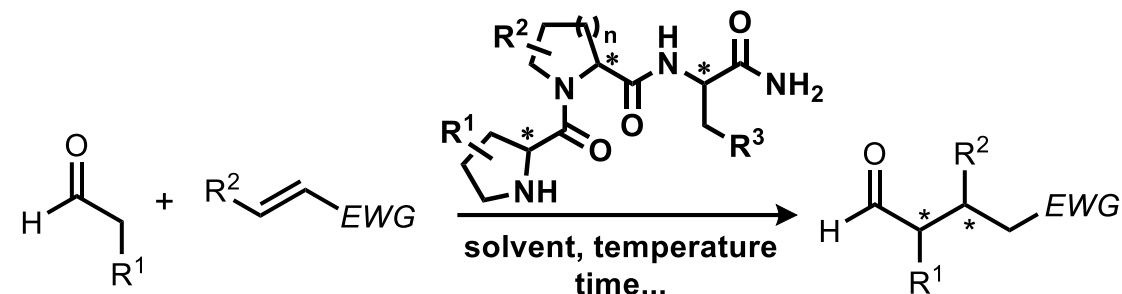
A. Budinská *et. al.*,
ACIE **2023**

56%-99% yield
3:1 to 13:1 *d.r.*
81-99% ee



M. Schnurr *et. al.*,
JACS **2023**

up to 99% yield
up to >20:1 *d.r.*
up to 99% ee



Projects

- Organic synthesis of starting materials
- Exploring new substrates and reactions for catalytic asymmetric transformations
- Optimization of catalyst and conditions
- Development of substrate scope

Complex environments: Whiskey, Coke, Honey, Limmat
water, fruit juice, cell lysate etc.
all > 95% ee





Questions?