Research Group Information Event

Discover the frontiers of chemical research!
Join us for insights into the various fields of chemistry at the Chemistry Research Group Event.

vseth Fachverein Verband der Studierenden an der ETH

50.942 V 23 12.011 C 6 32.065 S 16

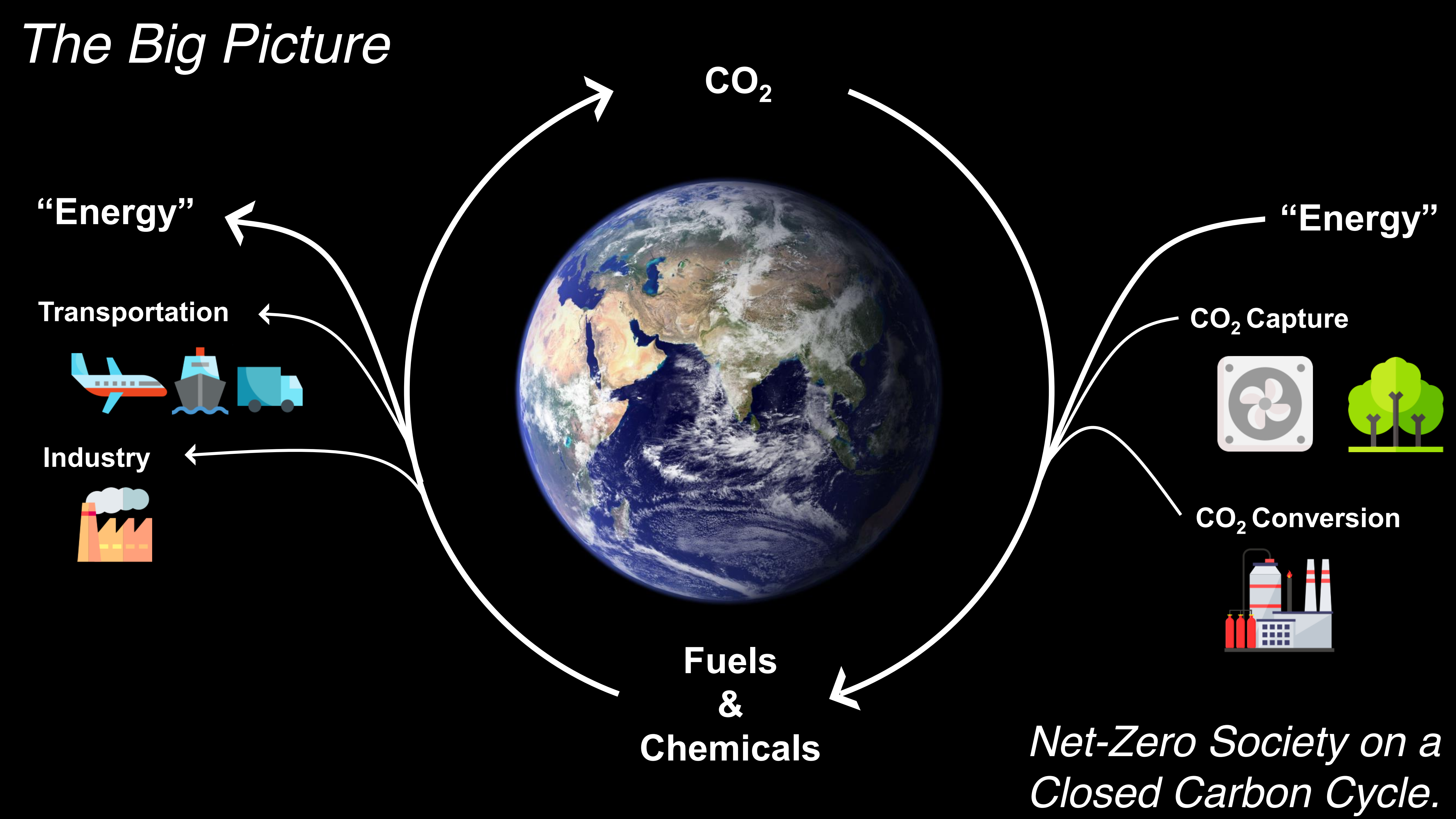
ETH zürich

Copéret Group

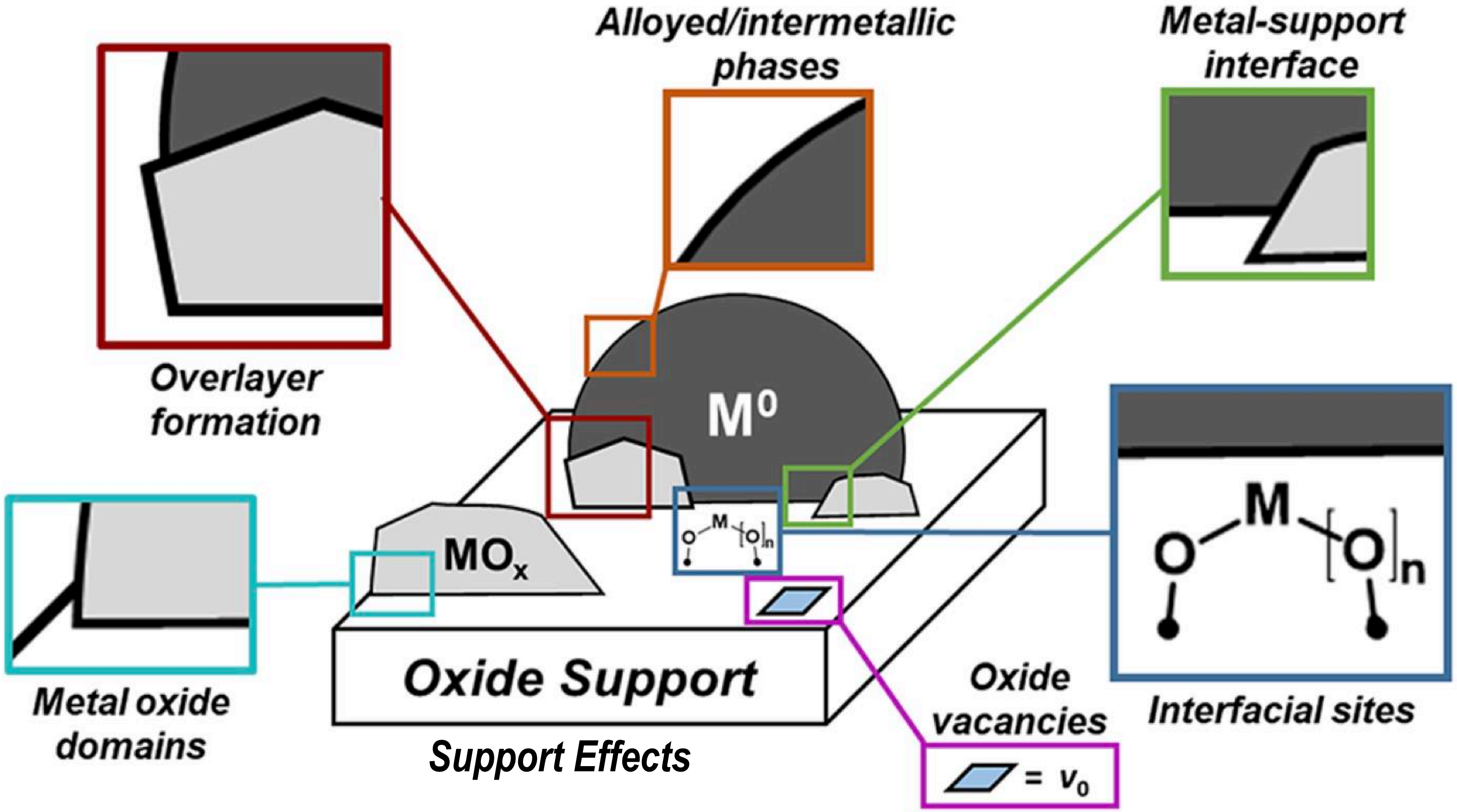
Research in the Copéret-Lab

Catalysis and Sustainable Chemistry from a Molecular Approach

Xiaoyu Zhou
VCS - Research Group Introduction
May 22nd, 2024, Zurich


The Big Picture
CO2
"Energy"
Transportation
Industry
"Energy"
CO2 Capture
CO2 Conversion
Fuels
&
Chemicals
Net-Zero Society on a
Closed Carbon Cycle.

Complexity of Catalyst Materials and Challenges for Atomistic Level Understanding



Which structural features matter most and drive reactivity?

J. Am. Chem. Soc. **2021**, 143, 6767–6780, *JACS Au* **2023**, 3, 2314−2322.

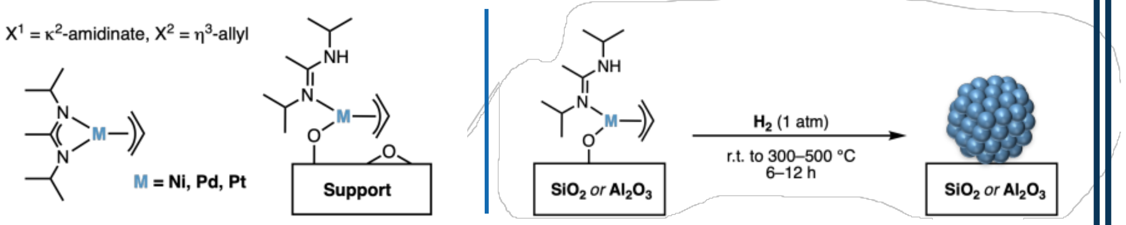
Core-Aspects of Copéret Group to Extract Guiding Principles for Homogeneous and Heterogeneous Catalysts

Copéret Group

Tailored Precursors

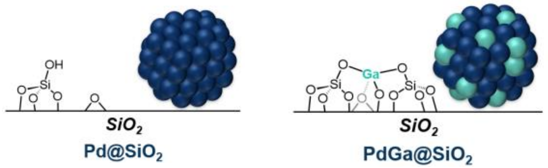
Group 10 Precursors:

- Facile grafting
- Clean nanoparticles



JACS Au, **2023**, 3, 8, 2314–2322.

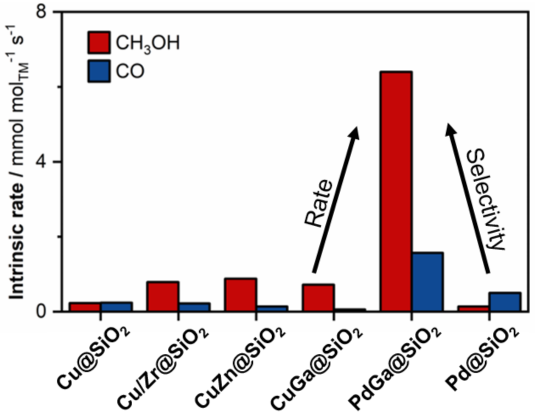
Catalysis



$$CO_2 + 3\,H_2 \rightleftharpoons CH_3OH + H_2O$$

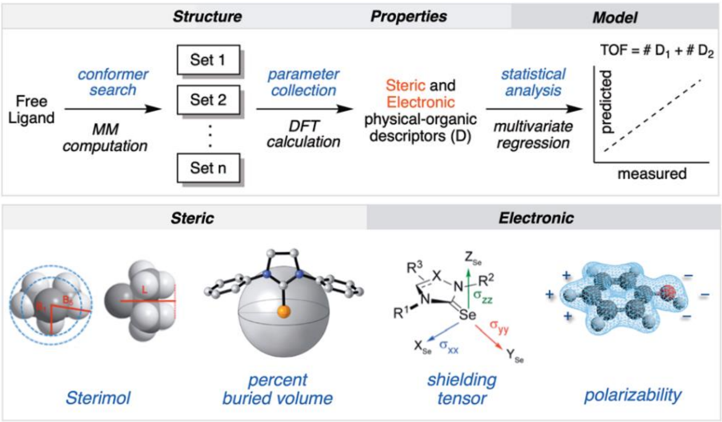
$$CO_2 + H_2 \rightleftharpoons CO + H_2O$$

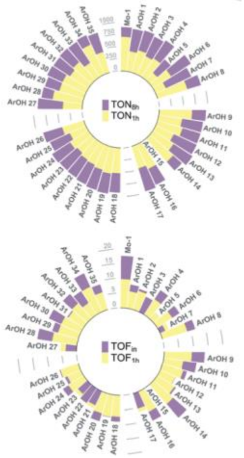
- Multi metallics
- Alloying / De-Alloying
- Reactivity



JACS Au, **2021**, *1*, 450-458 (10.1021/jacsau.1c00021)

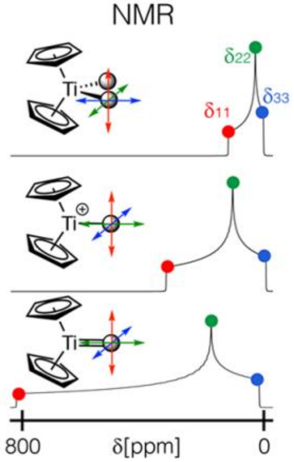
Computation and (HTE) Data Analysis

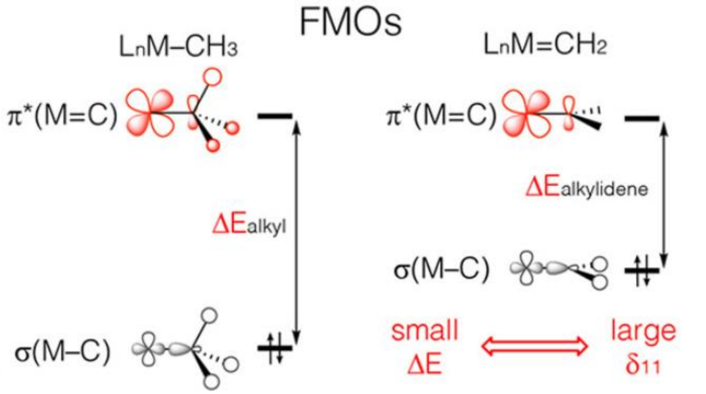




Chem. Sci., **2020**, *11*, *6717-6723* (10.1039/D0SC02594A)

Spectroscopy & Microscopy

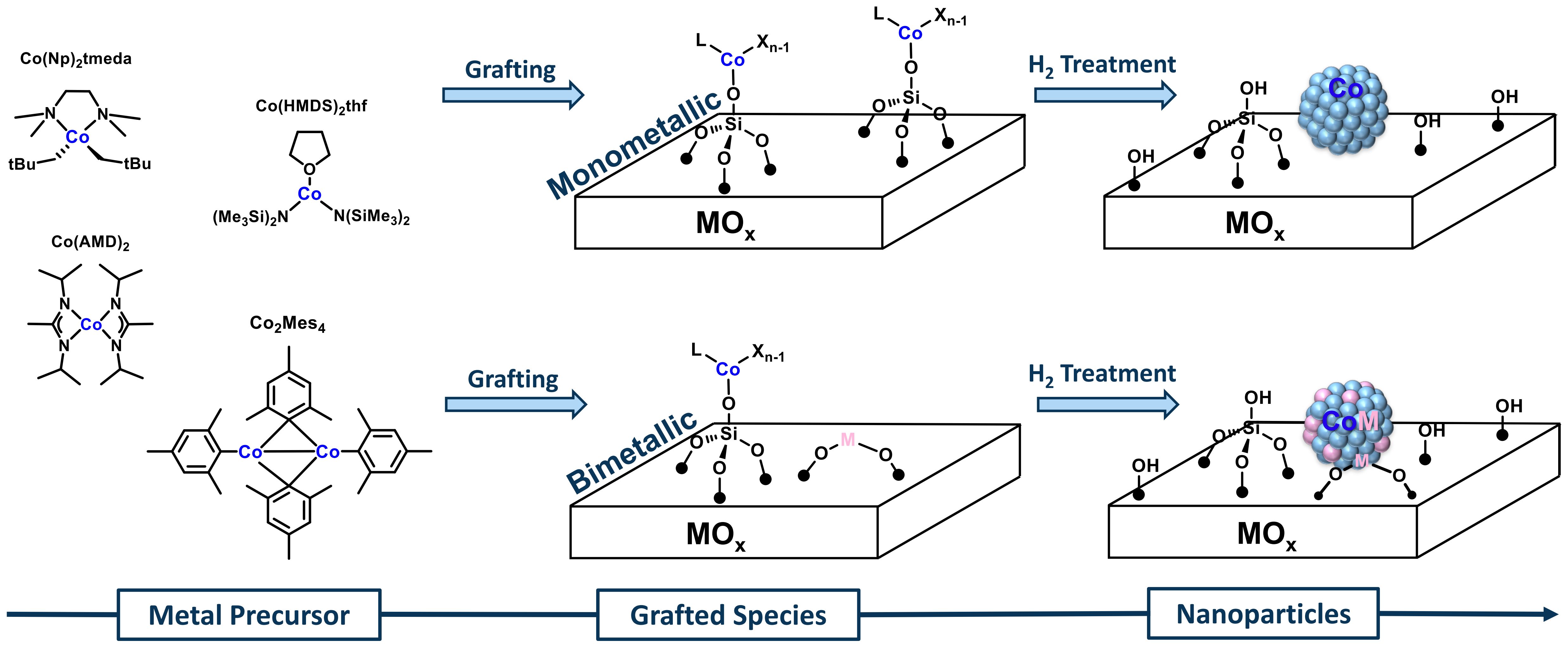




Acc. Chem. Res., **2019**, *52*, *2278-2289* (10.1021/acs.accounts.9b00225)

Surface Organometallic Chemistry (SOMC)

➡ Example – Mono- and Bimetallic Cobalt Catalysts

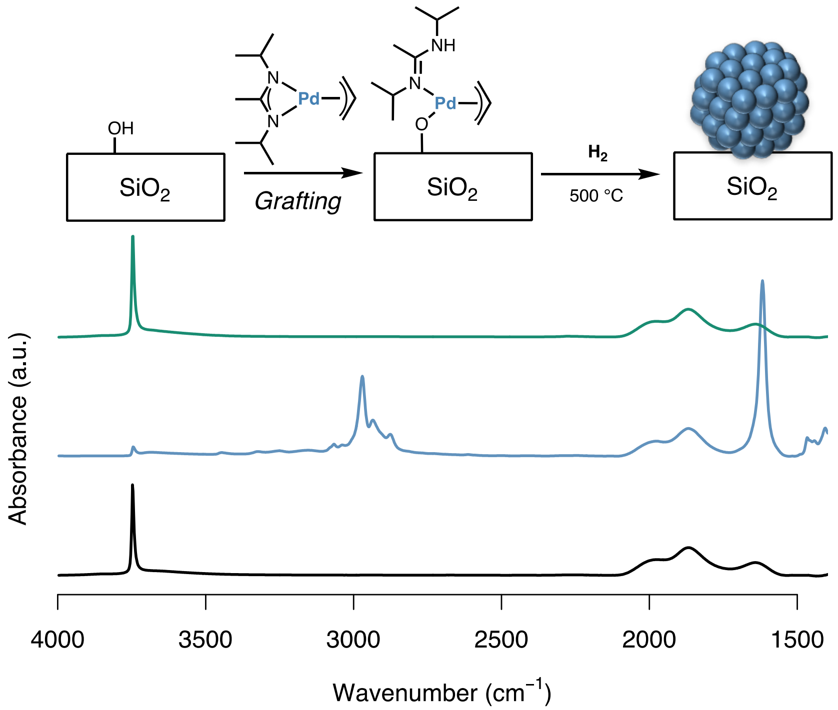


From molecules to surfaces and nanoparticles

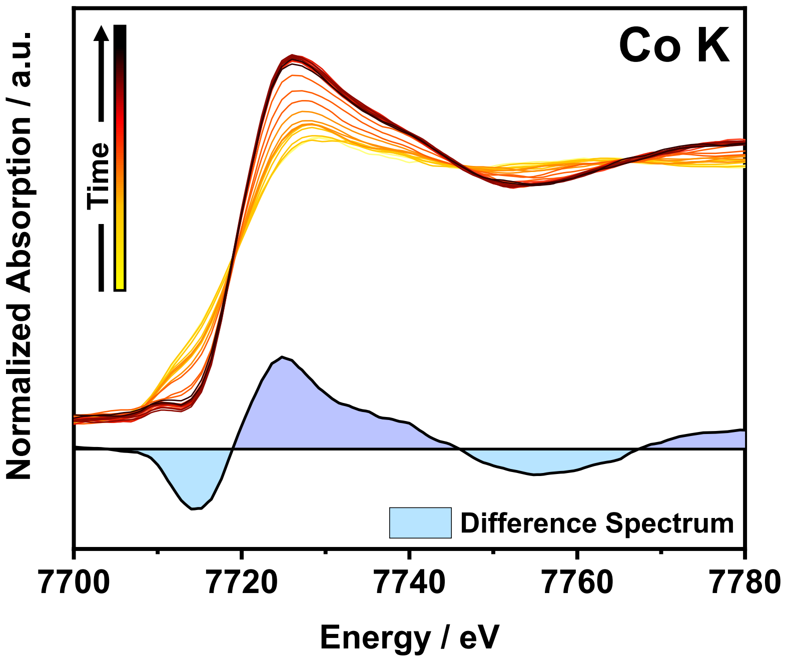
Angew. Chem. Int. Ed., **2023**, 62, e202314274.

Spectroscopy and Microscopy

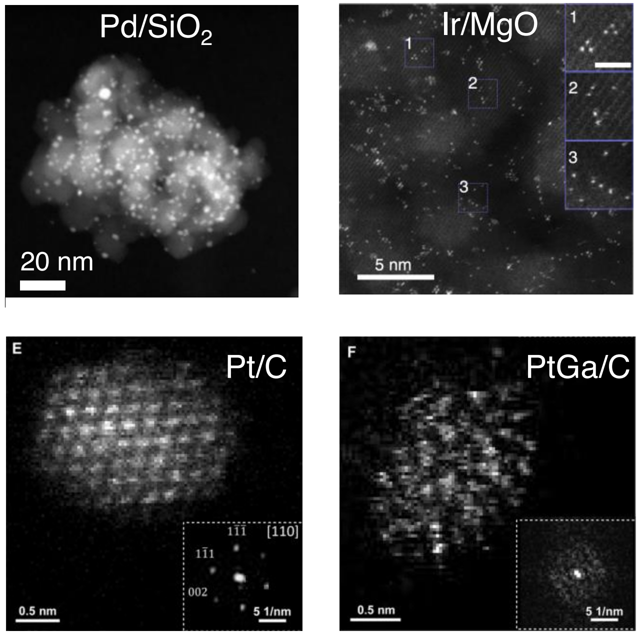
IR Spectroscopy



X-Ray Absorption Spectroscopy



Electron Microscopy



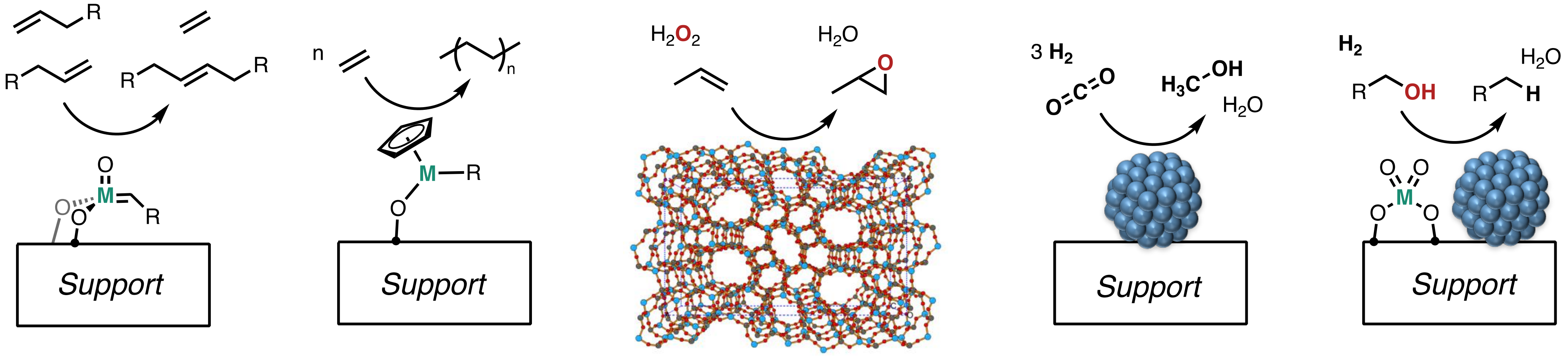
… and Solid-State NMR spectroscopy, probe molecules, chemisorption, physisorption, X-Ray diffraction, cyclic voltammetry …

A broad array of characterization techniques are required to understand surfaces

JACS Au **2023**, 3, 2314–2322, *Chem. Sci.* **2023**, 14, 12739–12746., *Angew. Chem. Int. Ed.*, **2023**, 62, e202314274.

Heterogeneous Catalysis

Reactions with an impact on society and a more sustainable future



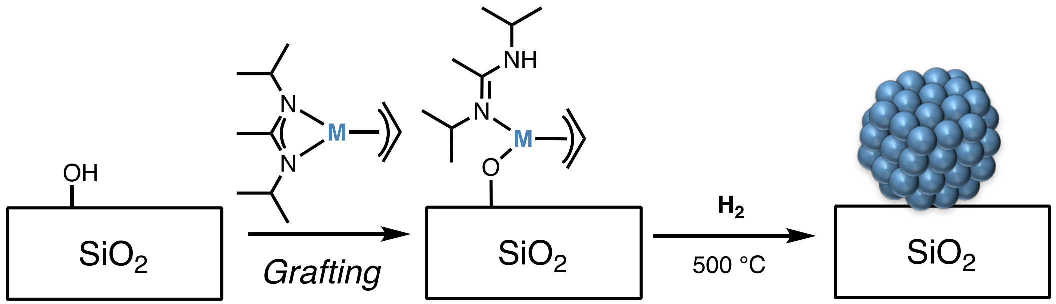
Surface Sites ***Zeolite Catalysts*** ***Supported TM Nanoparticles***

What makes a good catalyst – which structural features determine reactivity?

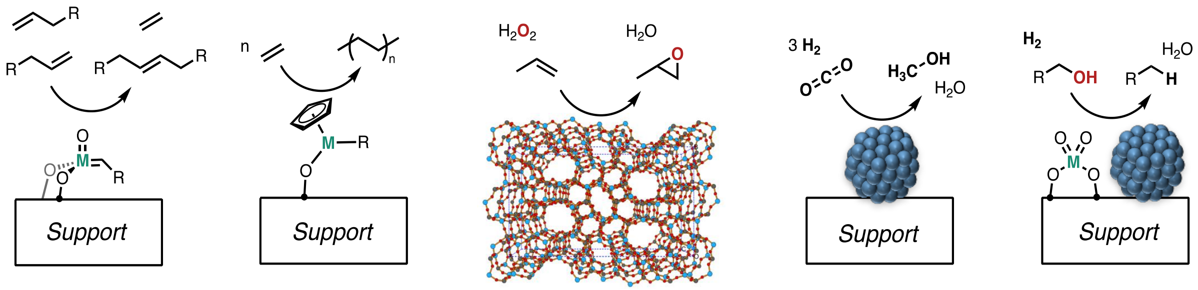
➡ **Linking spectroscopic / microscopic data with catalytic data**

Research in the Copéret Group

From Molecular to Tailored Material Synthesis



Understanding Heterogenous Catalysts



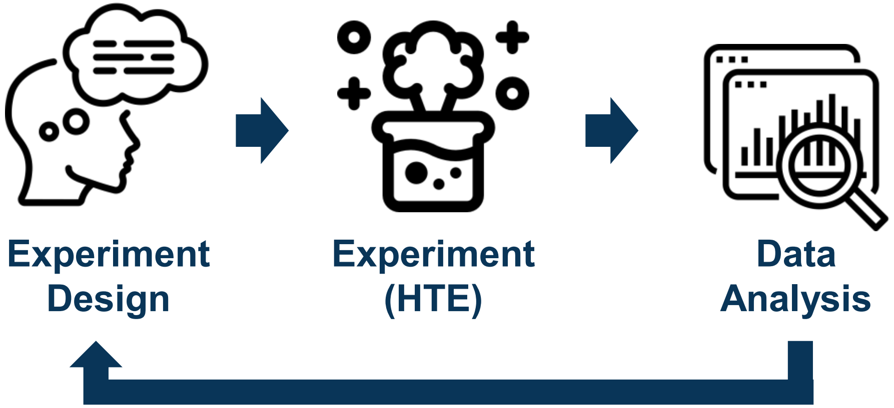
State-of-the-Art Characterization

NMR
DNP & High-Fields

Synchrotrons
PSI & SNBL

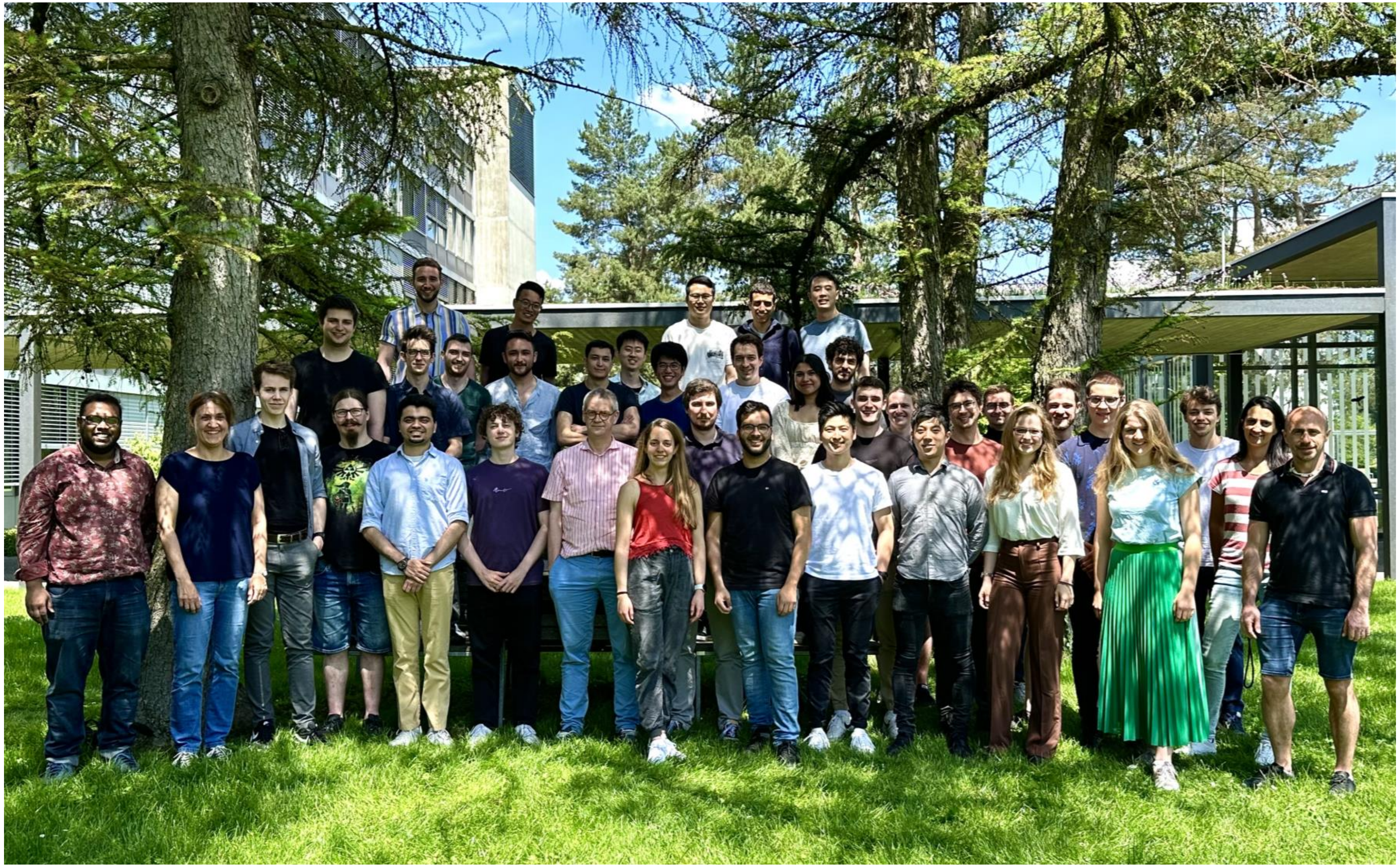
ScopeM
Environmental EM

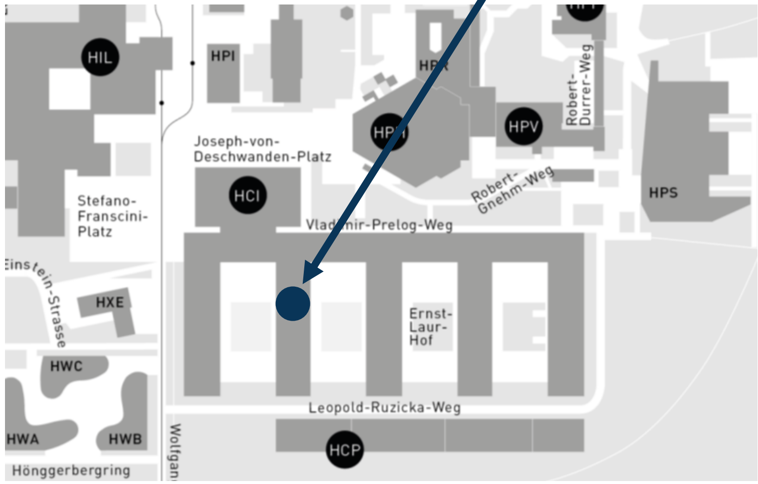
Computation and HTE



➡ **Structure-activity relationship**

The Copéret-Lab





- Prof. Christophe Copéret
- Dr. Alexander Yakimov
- Dr. Millivoj Plodinec
- 6 Postdocs
- 18 PhD Students
- 5-15 Semester students/year
- 1-2 Master students/year
- 2 Visitors

Copéret Group

90	11	19	39	8	92
Th	Na	K	Y	O	U
Thorium	Sodium	Potassium	Yttrium	Oxygen	Uranium
232.038	22.990	39.098	88.906	15.999	238.029

For further questions:

Xiaoyu Zhou

xiazhou@ethz.ch

Interested? Reach out directly to:

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ccoperet@ethz.ch

coperetgroup.ethz.ch

Many thanks to our collaborators and industrial partners

NCCR Catalysis

CAT+

BASF We create chemistry

bp

CLARIANT

ifp Energies nouvelles

ETH AI CENTER

Trace Element and Micro Analysis @ D-CHAB

Detlef Günther

Laboratory of Inorganic Chemistry, Department of Chemistry and Applied Biosciences, ETH Zurich

www.guenther.ethz.ch

Trace Element- and Microanalysis

Trace Element and Micro Analysis @ D-CHAB

Trace Element- and Microanalysis

ETH zürich

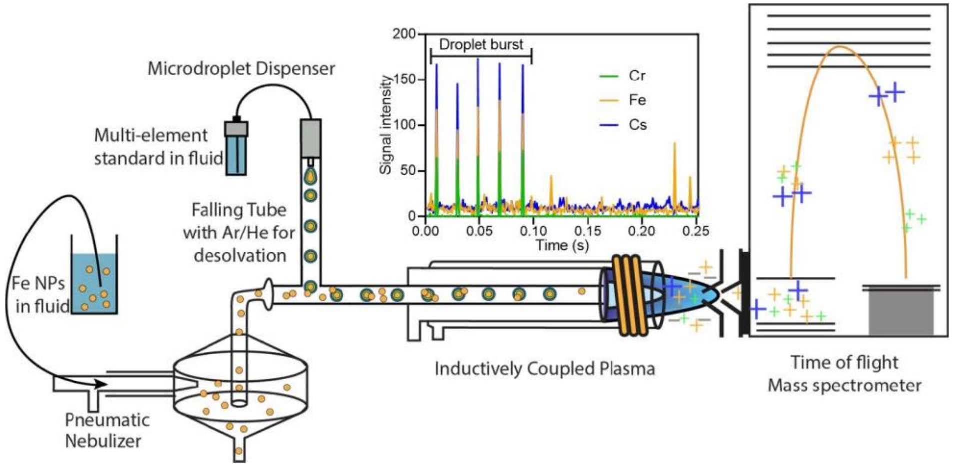
eawag aquatic research

FNSNF

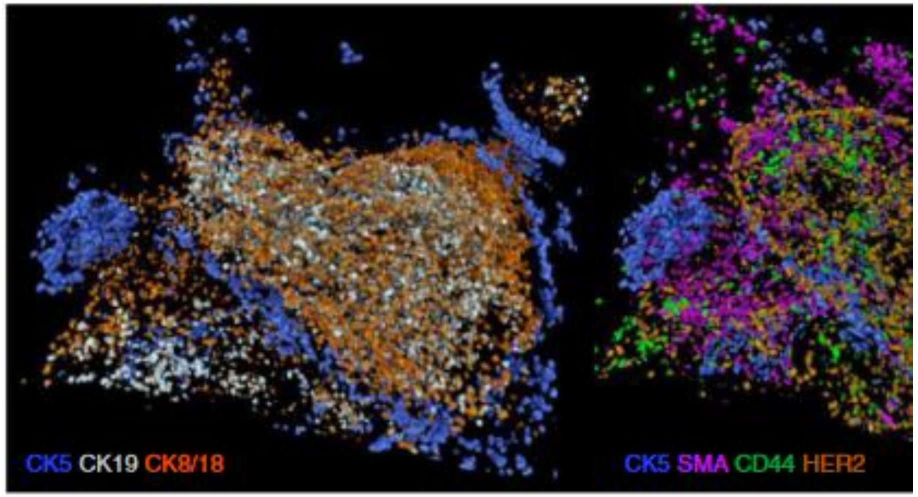
Main Fields of Application for Analytical Science

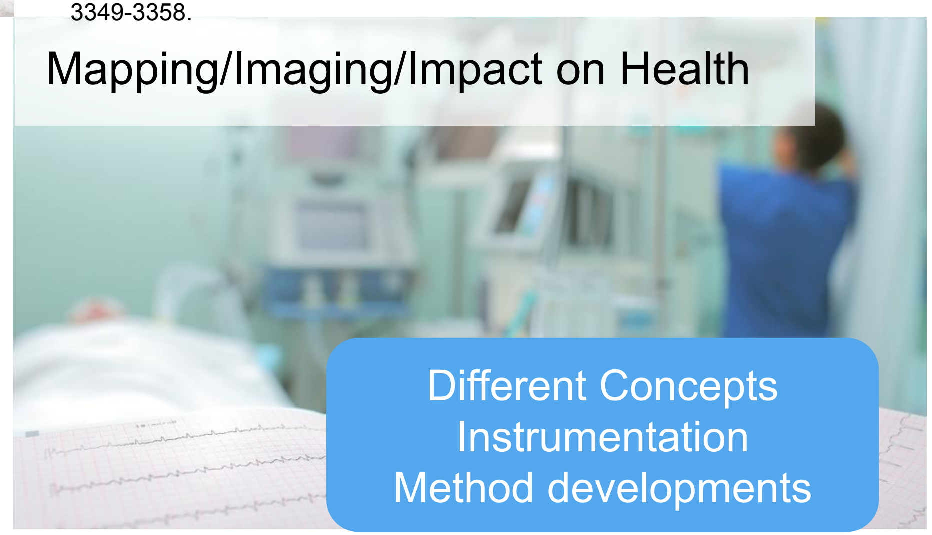
Quantification of pollutants
Monitoring
Quality control

Climate Change, Energy & Environment



B. Ramkorun-Schmidt, et. al., Anal. Chem., 2015, 87, 8687. L. Hendriks, et. al., J. Anal. At. Spectrom., 2019, 34, 716-728. K. Mehrabi, et. al., Environ. Sci.: Nano, 2019, 6, 3349-3358.

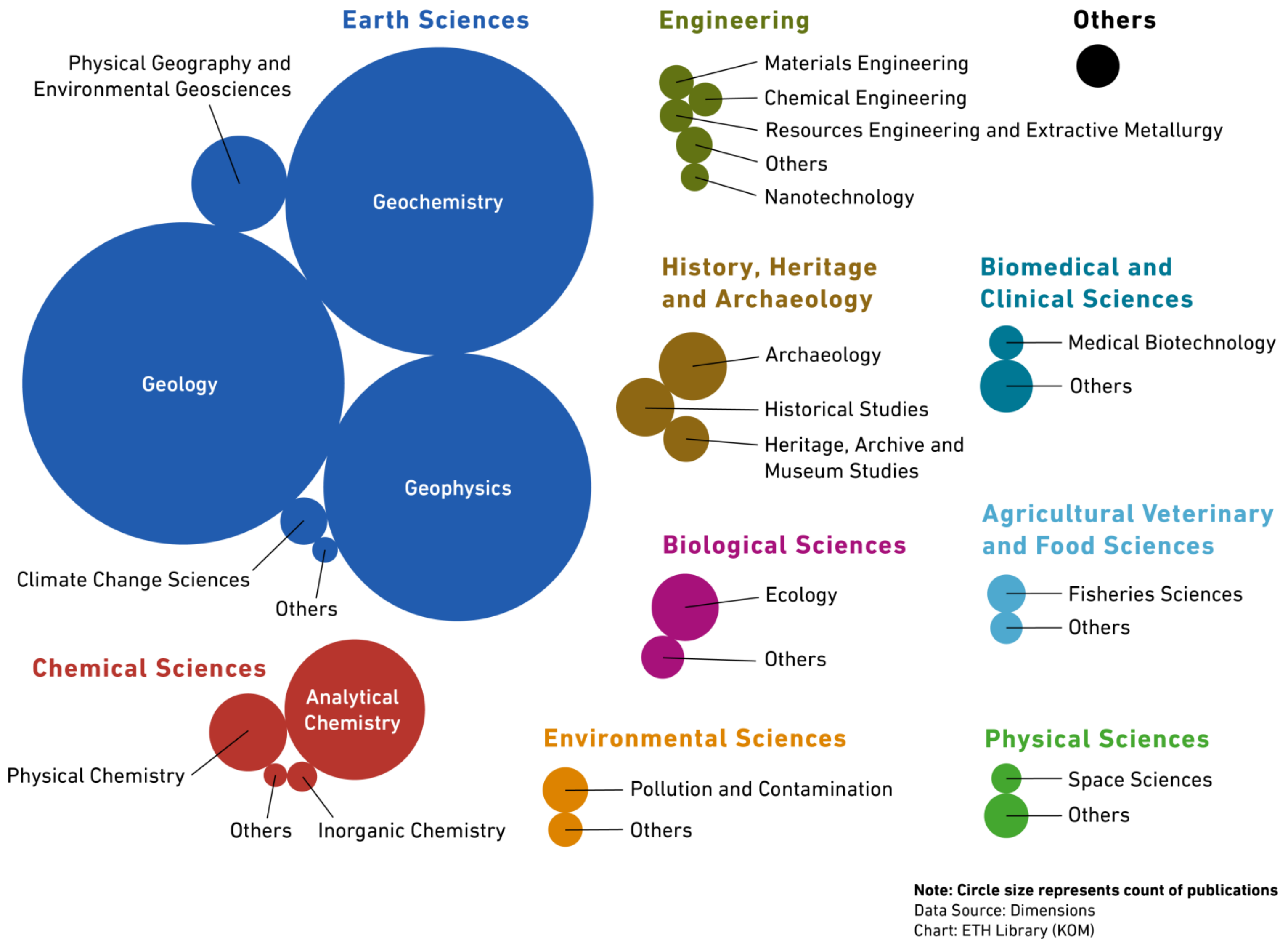




Mapping/Imaging/Impact on Health

Different Concepts
Instrumentation
Method developments

Major Fields of LA-ICP-MS



Laser Ablation-Inductively Coupled Plasma Mass Spectrometry

References

1. Thompson, M., Goulter, J. E., and Sieper, F., *Analyst*, 1981, **106**, 32.
2. Carr, J. W., and Horlick, G., *Spectrochim. Acta, Part B*, 1982, **37**, 1.
3. Ishizuka, T., and Uwamino, Y., *Spectrochim. Acta, Part B*, 1983, **38**, 519.
4. Date, A. R., and Gray, A. L., *Analyst*, 1983, **108**, 159.
5. Gray, A. L., and Date, A. R., *Analyst*, 1983, **108**, 1033.
6. Gray, A. L., "Proceedings of the Symposium on Instrumental Multi-Element Analysis, Julich 1984," Verlag Chemie, Weinheim, in the press.
7. Scott, R. H., and Strasheim, A., *Spectrochim. Acta, Part B*, 1970, **25**, 311.
8. Chow, T. J., Snyder, C. B., and Earl, J. L., IAEA-SM-191/4, "Proceedings of the Symposium on Isotope Ratios as Pollutant Source and Behaviour Indicators, Vienna, 1974," IAEA, Vienna.

Paper A4/308
Received September 3rd, 1984
Accepted October 25th, 1984

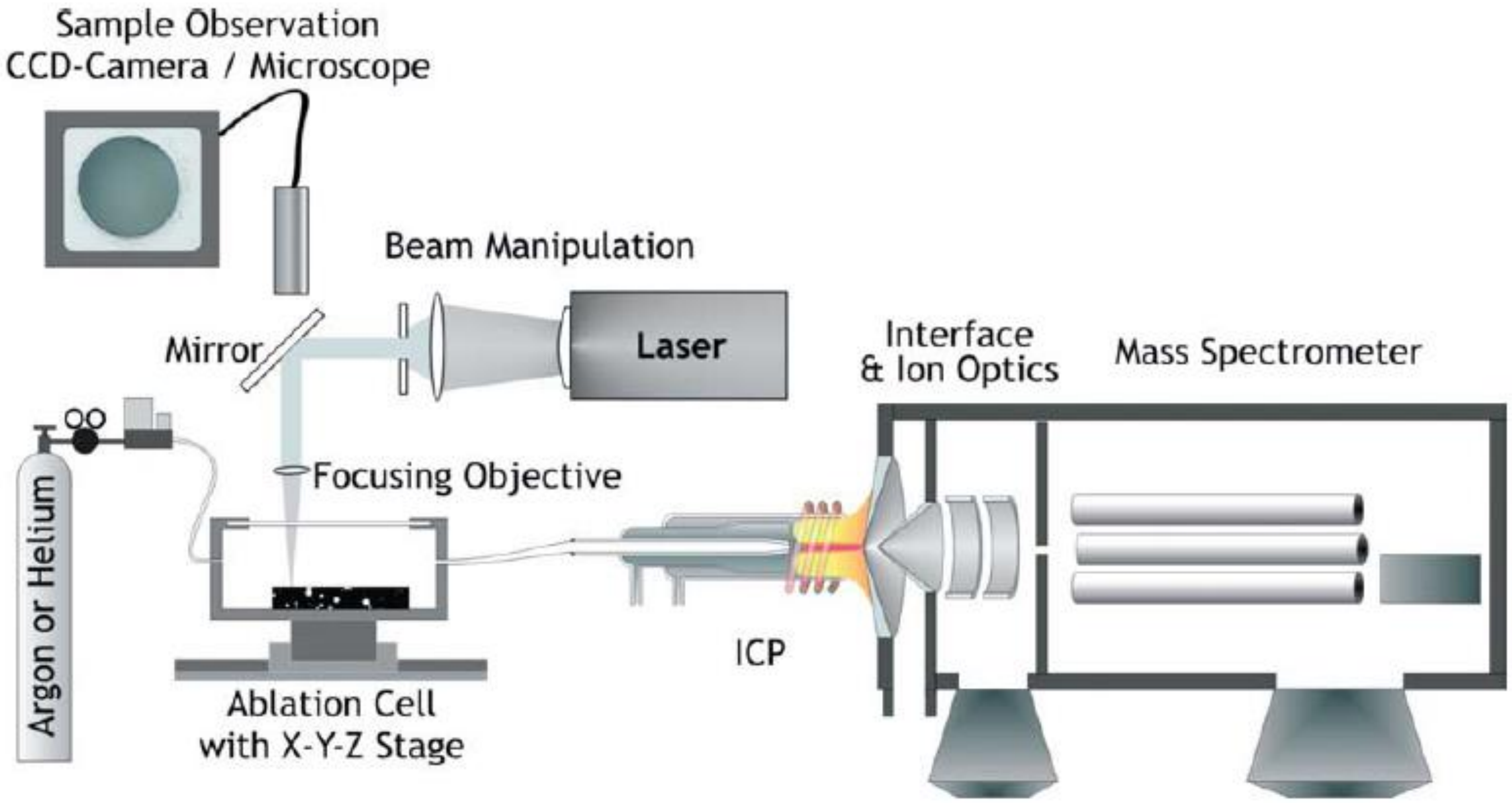
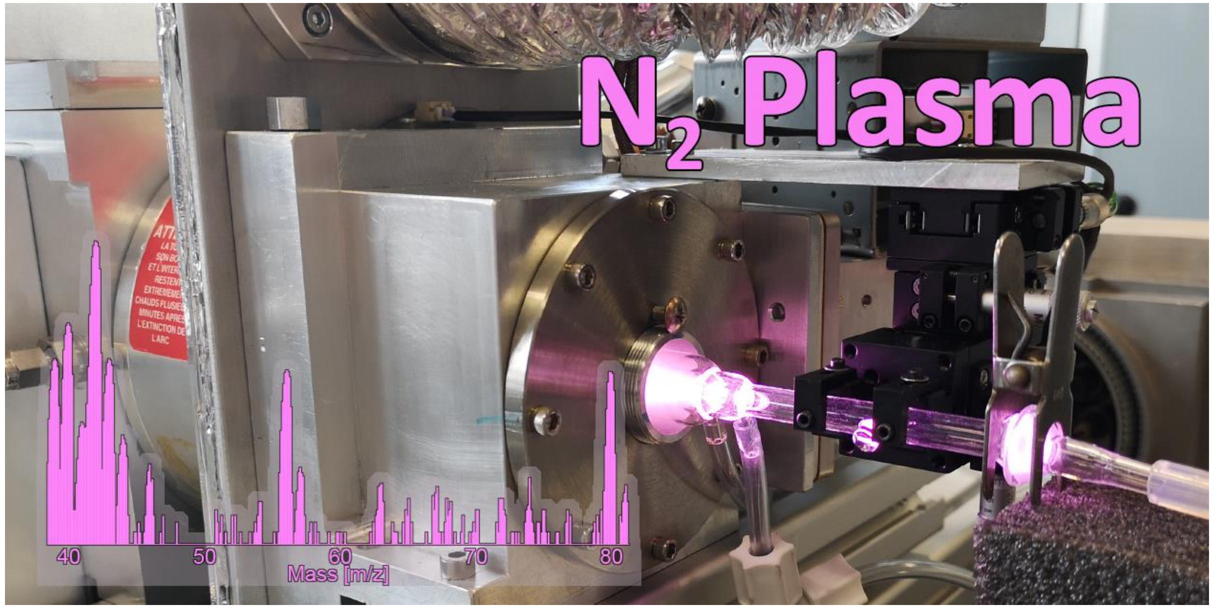


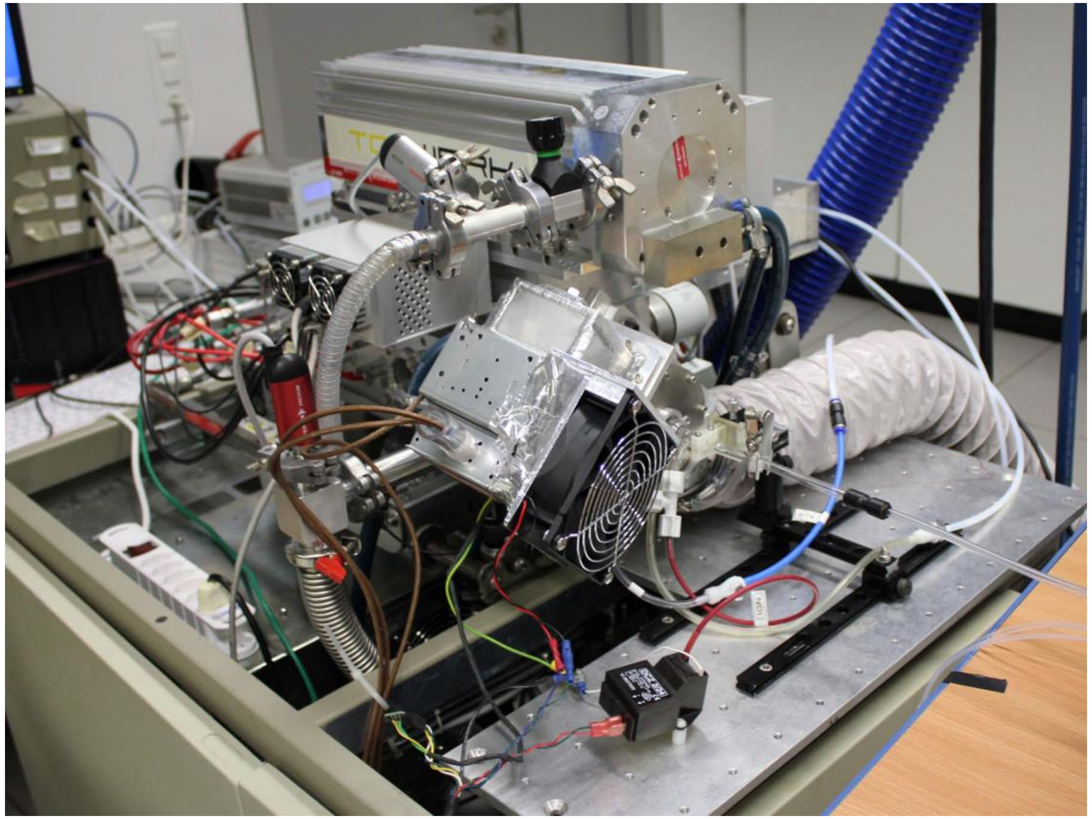
Figure 1. Schematic set-up of LA inductively coupled plasma Lmass spectrometry (LA-ICP-MS).

Gray AL. Solid sample introduction by laser ablation for inductively coupled plasma source mass spectrometry. Analyst. 1985;110(5):551–6.

Capabilities of a Nitrogen Plasma for Solid Analysis

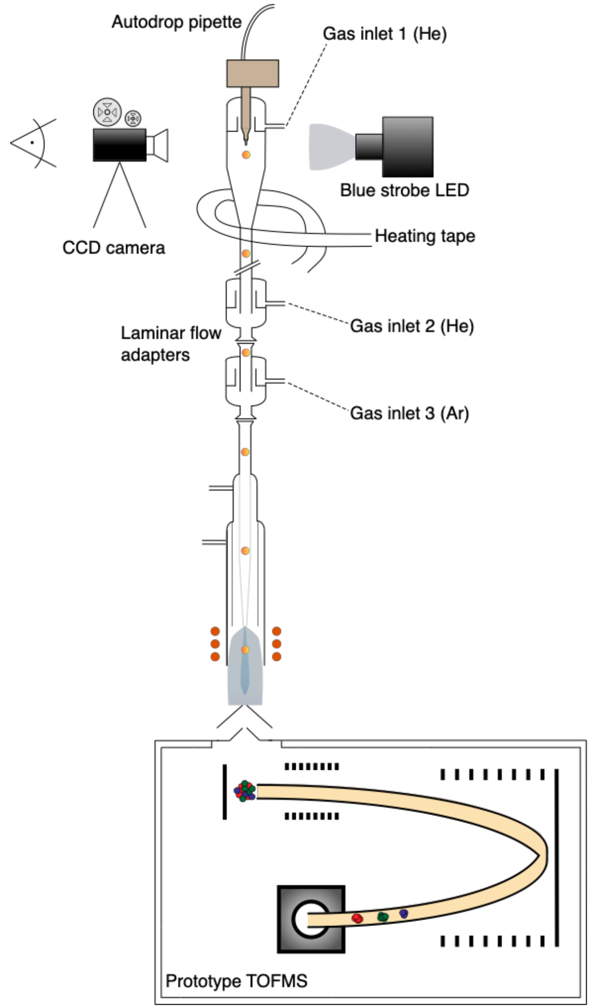


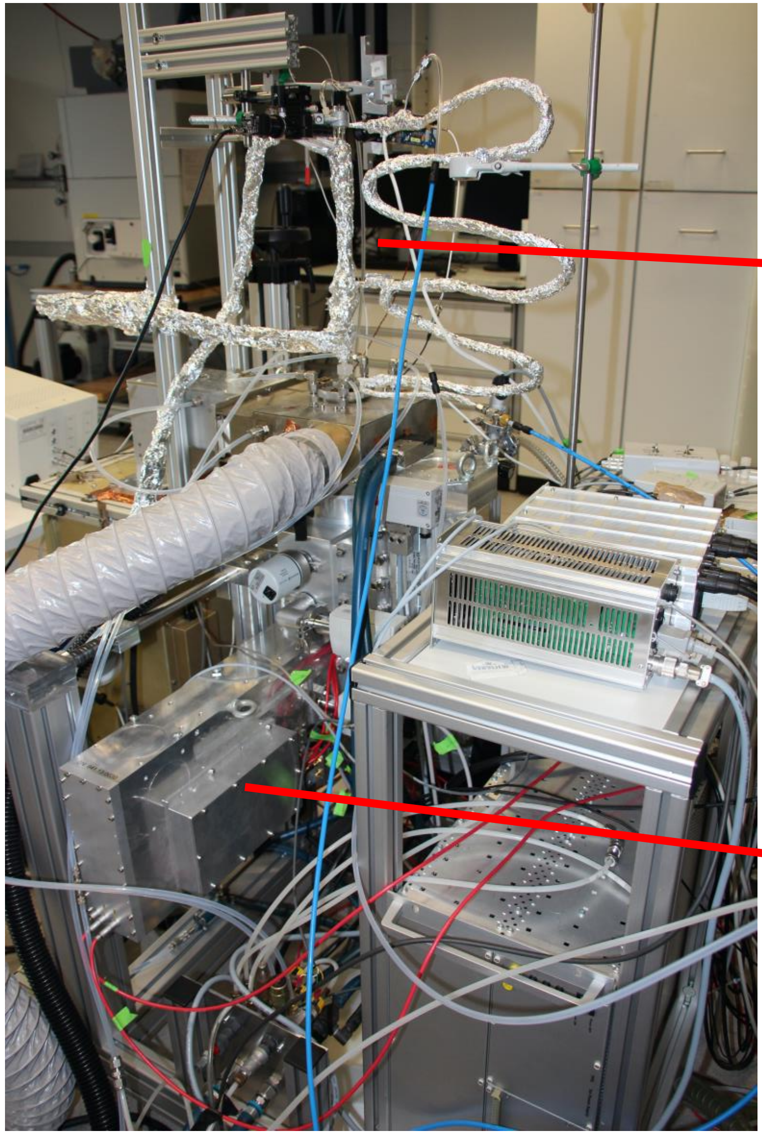
Ch. Neff et al., *J. Anal. At. Spectrom.*, 2021, **36,** 1750-1757



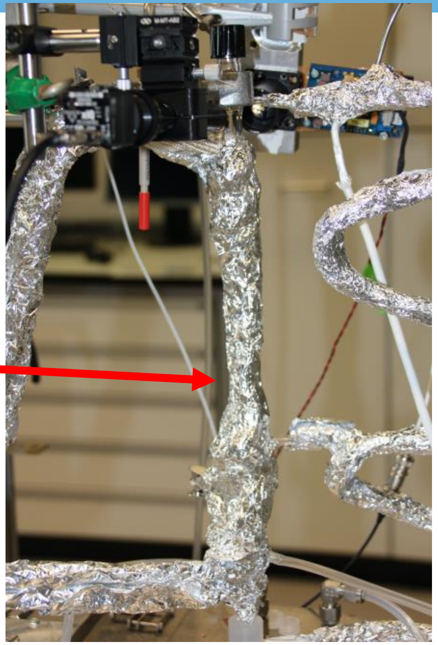
M. Schild et al, 2018, *Anal. Chem. 2018, 90, 13443−13450*

Rethinking Inductively Coupled Plasma Mass Spectrometry

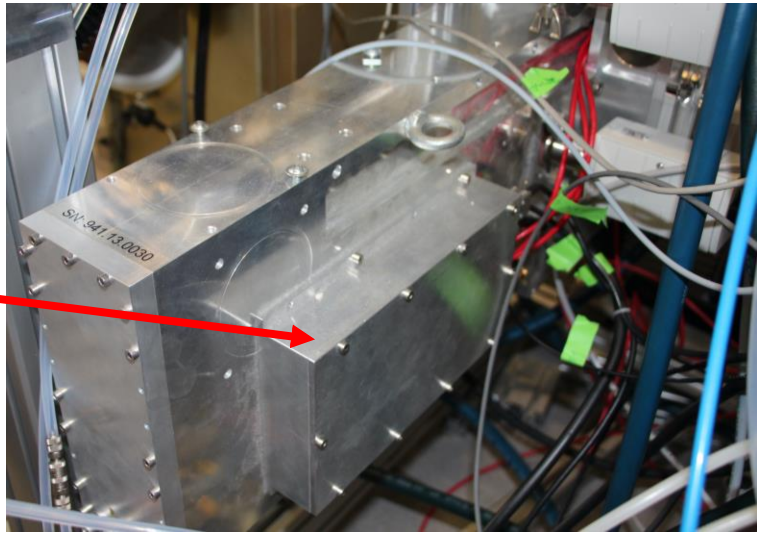




Heated falling tube

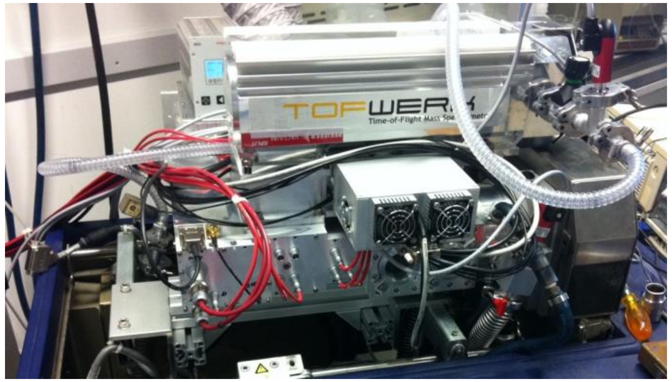


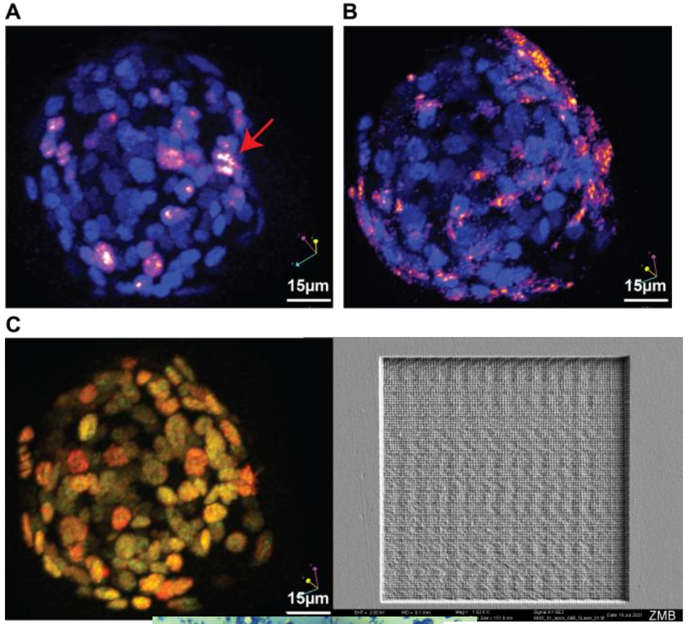
Flight tube

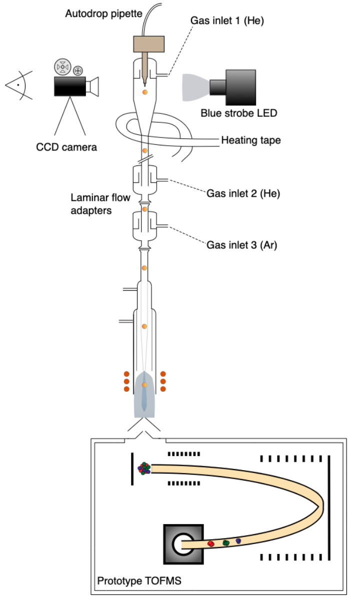


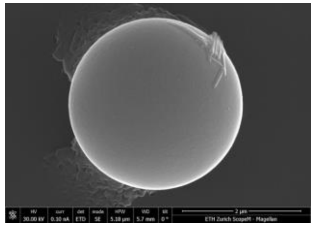
Vonderach, Hattendorf and Günther, *Anal. Chem.* **2021**, 93, 1001−1008

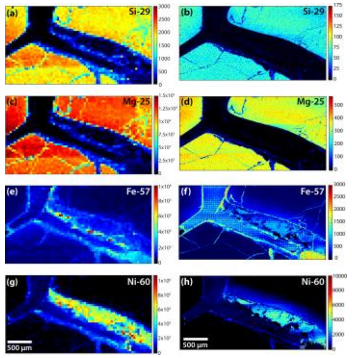
Fundamental and Applied Research

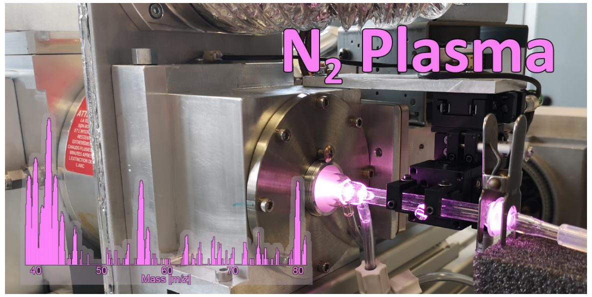


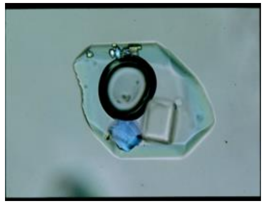


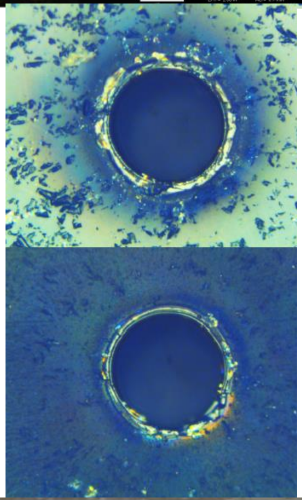


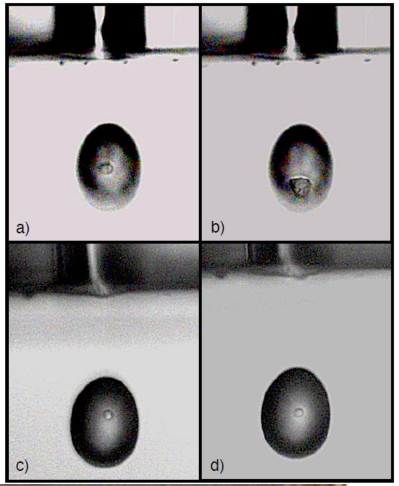


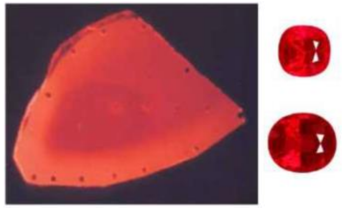












THE CHALLENGE OF THE IDENTIFICATION OF A NEW GEMSTONE

CHEMISTRY AND CRYSTALLOGRAPHY (NEW BERYL-GROUP MINERAL)

MINERAL NAME: PEZZOTTAITE

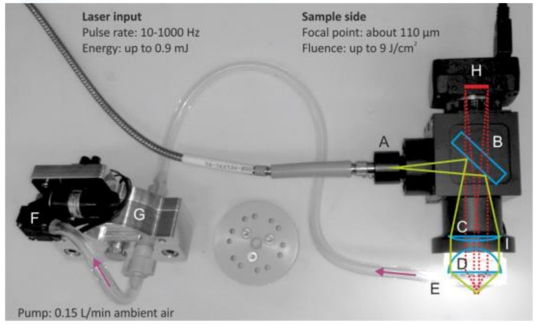
CHEMICAL FORMULA:

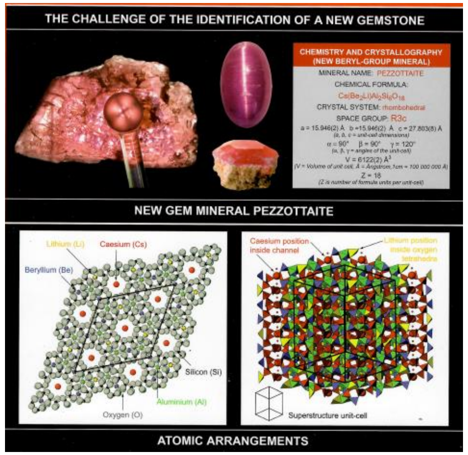
CRYSTAL SYSTEM: rhombohedral

SPACE GROUP: R3c

NEW GEM MINERAL PEZZOTTAITE

ATOMIC ARRANGEMENTS





Trace Element- and Microanalysis

Options for Students

Semester projects

- mainly applied research

Master projects

- fundamendal and applied research

Doctoral studies (last generation)

- fundamental and applied research

PAUL SCHERRER INSTITUT PSI

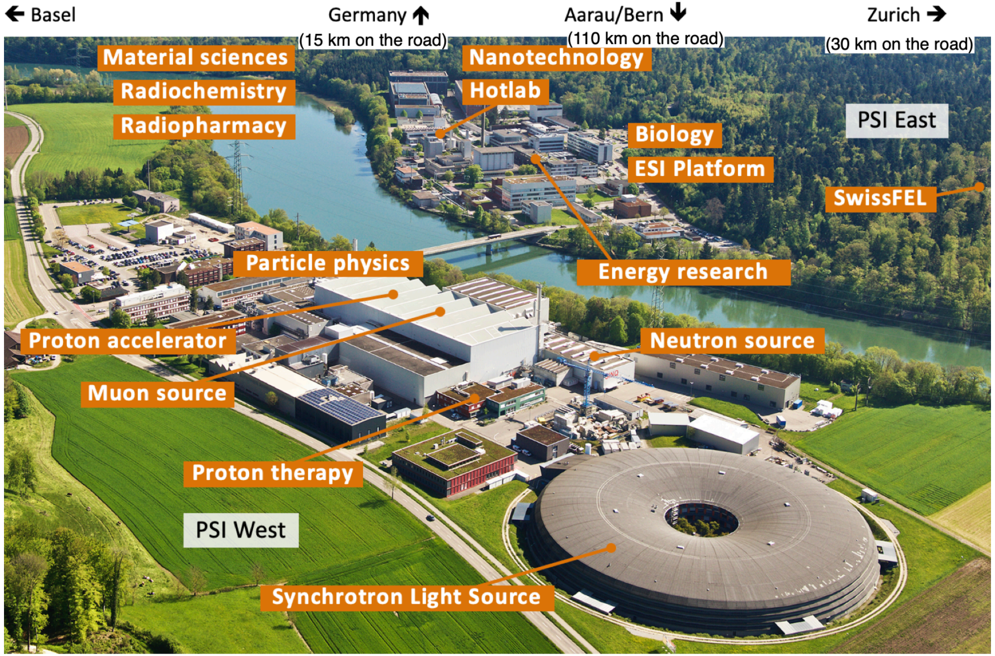
ETH zürich

Nick Shepelin :: Scientist :: Paul Scherrer Institute

Thin Films and Interfaces Group
https://psi.ch/materials

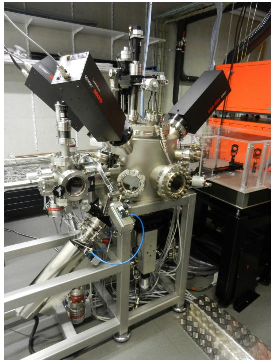
Laboratory of Inorganic Chemistry, Department of Chemistry and Applied Biosciences, ETH Zürich

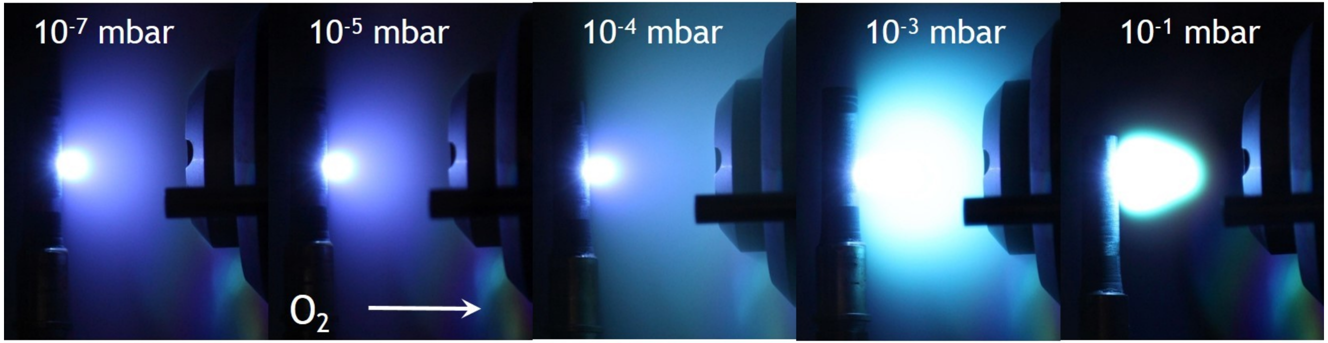
Thin Films and Interfaces group

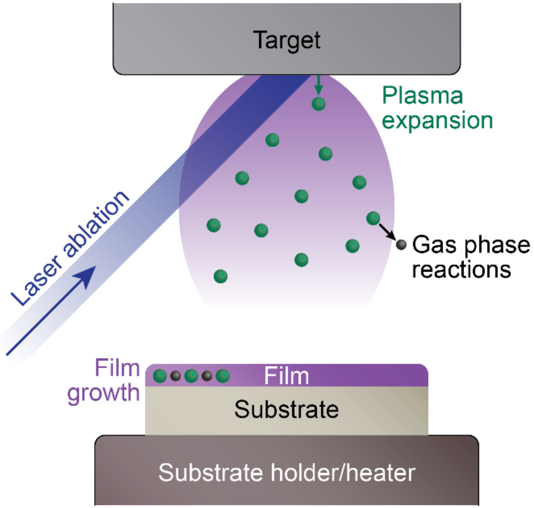


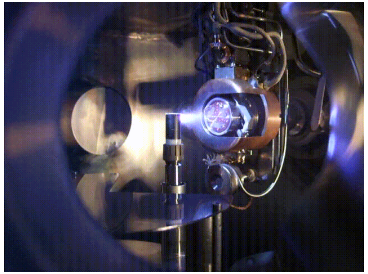
Prof. Dr. Thomas Lippert
Head of Group

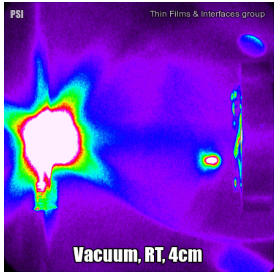
Thin Films and Interfaces group - Methods





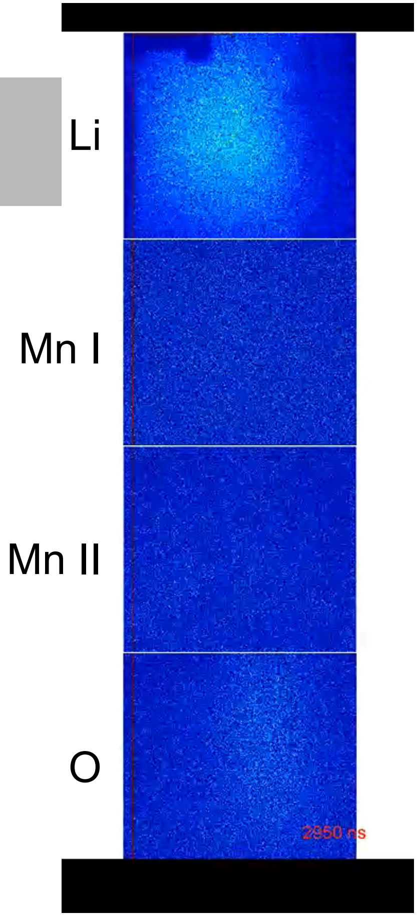


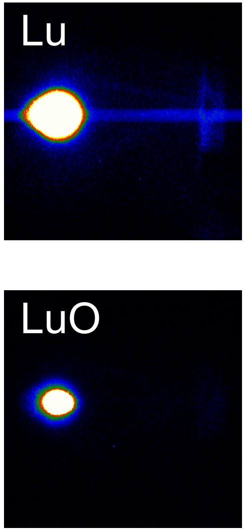




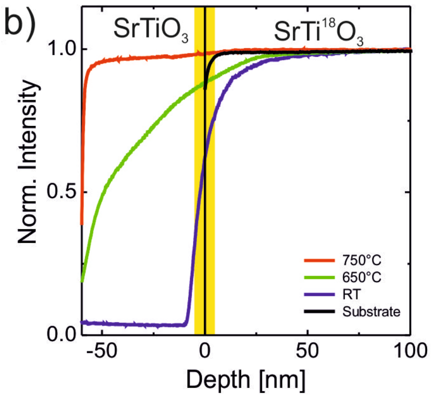
Pulsed laser deposition – Technique for making advanced materials atom-by-atom. High powered lasers create a plasma from a target material, which travels to a substrate and self-assembles into the desired chemical and crystalline phase.

Understanding pulsed laser deposition





Observe chemistry in the plasma plume



Understand diffusion kinetics in materials

Probe the composition in multilayered thin films

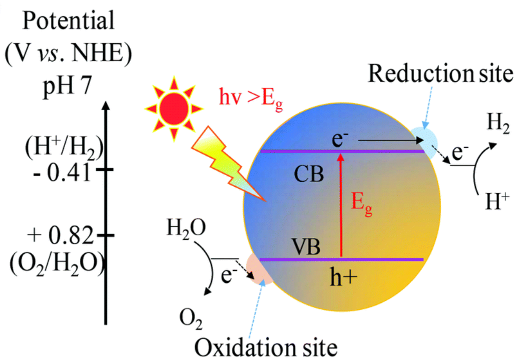
(La0.66Ca0.33MnO3-YBa2Cu3O7 shown here)

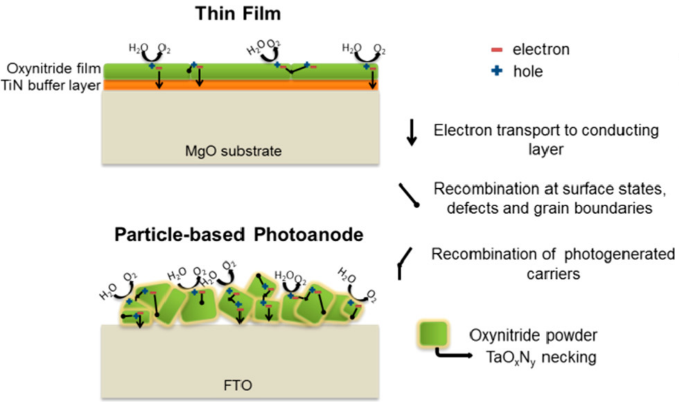
Understanding the pulsed laser deposition process enables us to engineer the chemistry, structure and functionality in the thin films

Photoelectrochemical water splitting

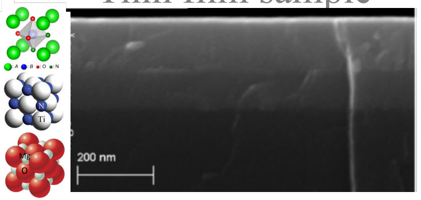
H2 generation by solar water splitting

Using thin films to engineer material heterostructures with suitable optical, conductive and catalytic properties to split water molecules into H2 and O2 using sunlight

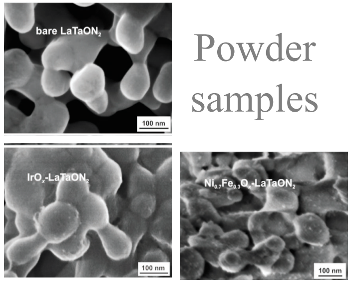




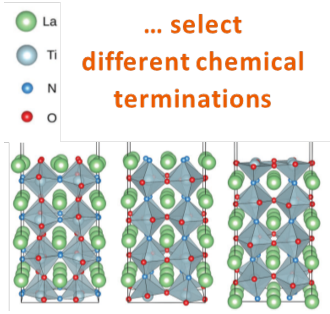
Thin film sample

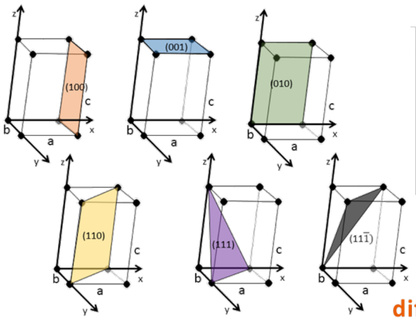


Powder samples



... select different chemical terminations

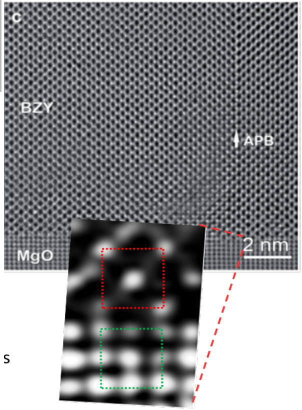


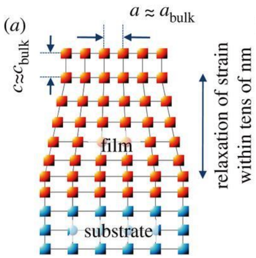


... face the electrolyte with different crystal planes

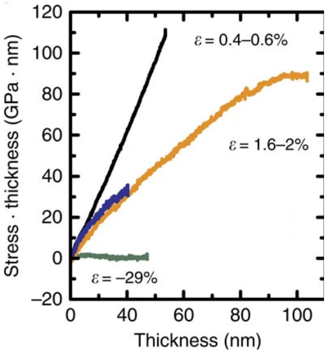
Strain engineering in thin films

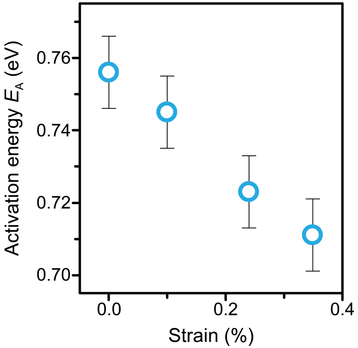
Oxygen ion and proton conduction in solids for energy conversion systems (solid oxide fuel and electrolyzer cells)



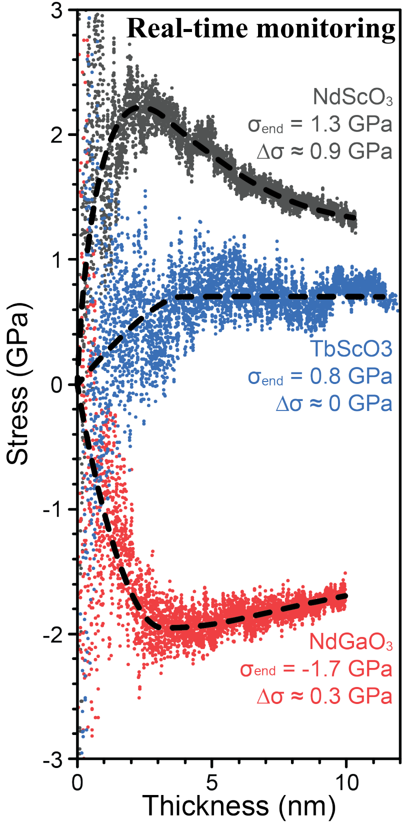


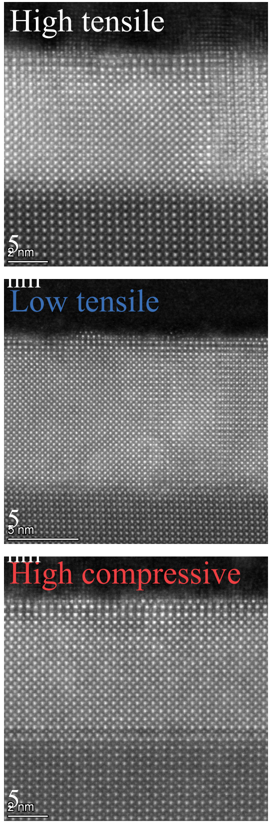
$$\sigma(T) = A\exp\left(\frac{-E_a}{RT}\right)$$

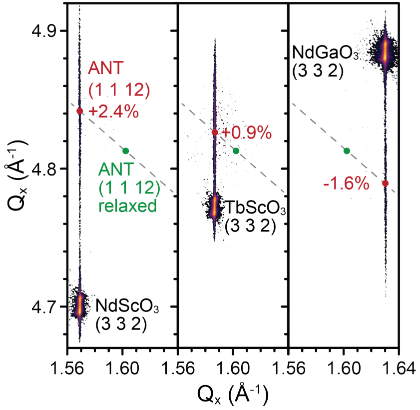


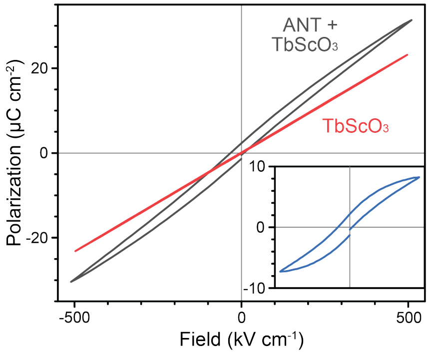


Polar materials for engineering energy storage systems with high energy density (ferroelectricity for use in capacitors)

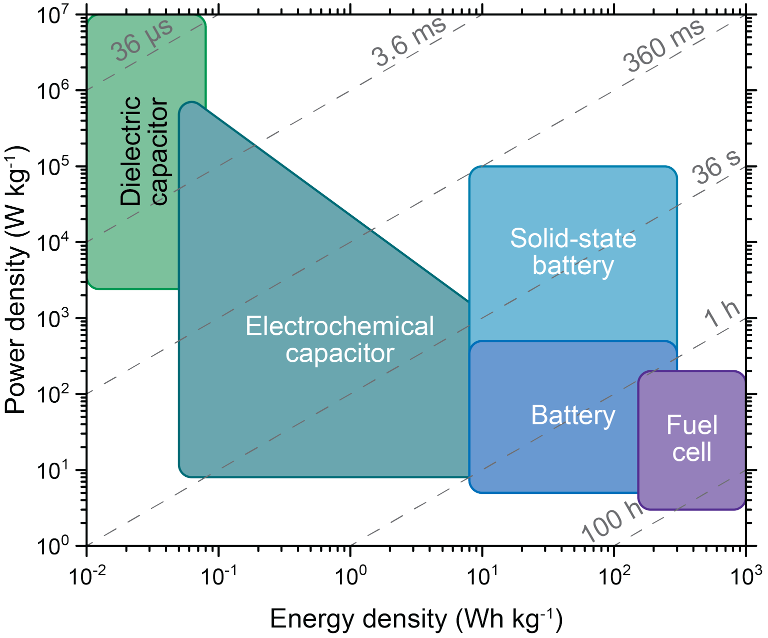


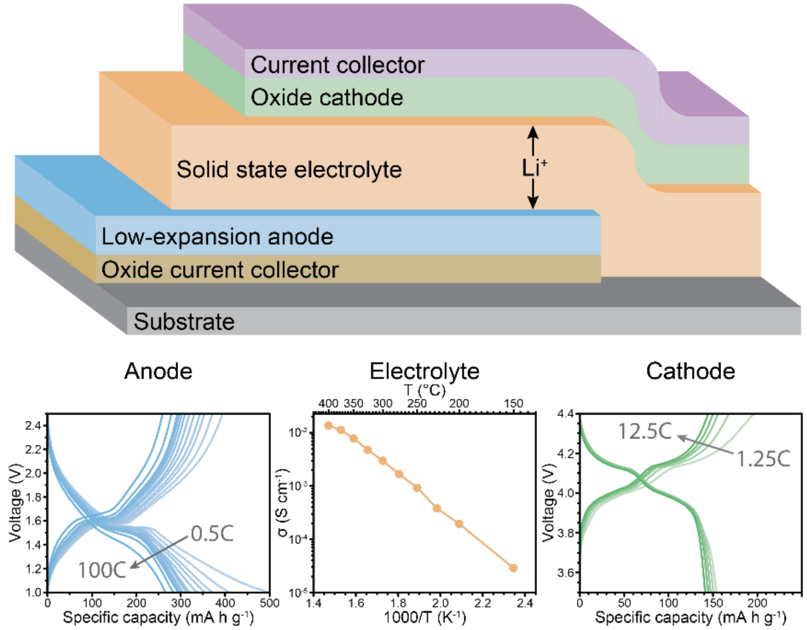






Solid state thin film batteries



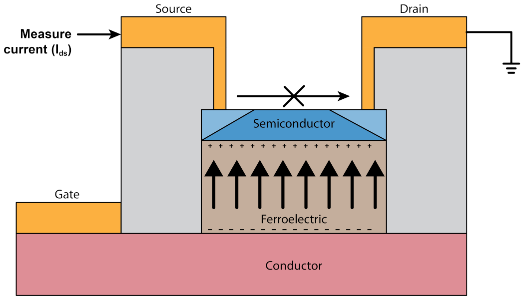


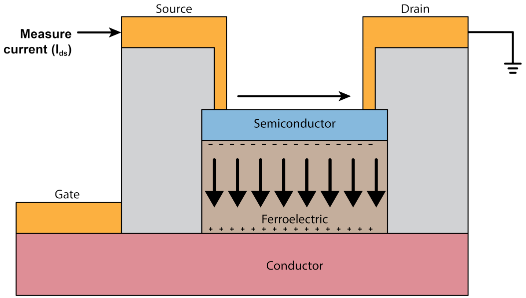
Investigating new materials for thin film solid state batteries: potential for significantly faster charge/discharge

Understanding the behavior of thin film anode, cathode and electrolyte

PAUL SCHERRER INSTITUT

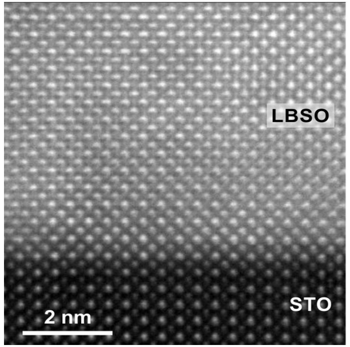
Next generation computing devices

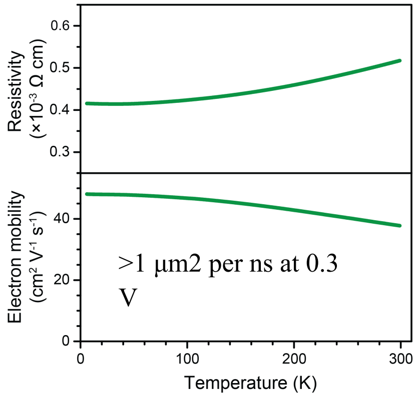




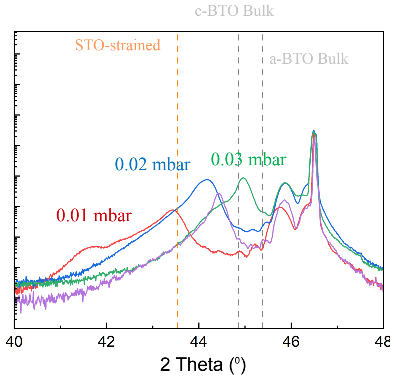
Growth and investigation of all-oxide transistors with extremely low energy use for beyond-CMOS memory-in-computing applications

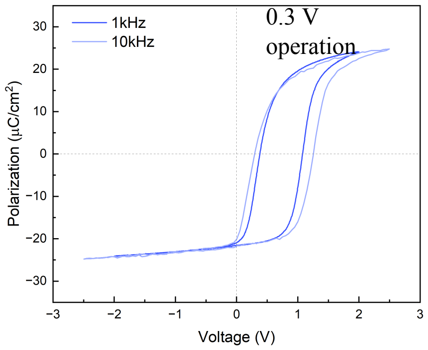
1. Growth of optimal semiconductor(La0.07Ba0.93SnO3) layer
- Film growth, structural and physical property characterization





2. Low voltage switching ferroelectric (BaTiO3) layer
- Film growth and ferroelectric property characterization





Shuttle Catalysis & Skeletal Editing

Recent Adventures in the Morandi Group

Yannick Brägger

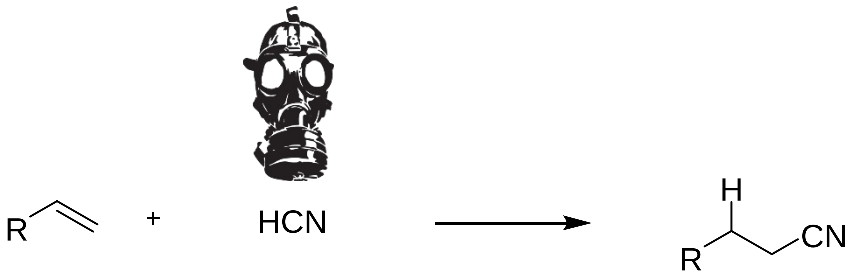
Our Group

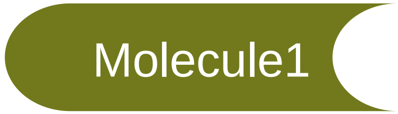
Shuttle Catalysis - Concept

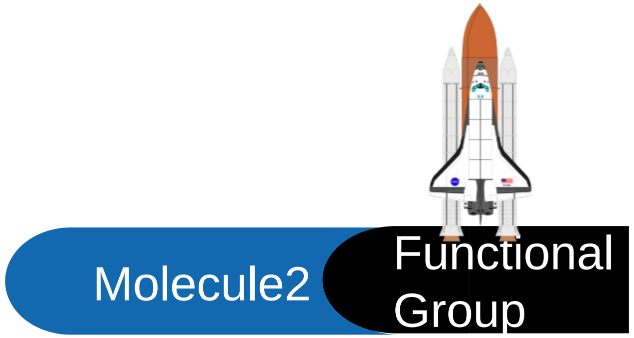
Pictures from https://publicdomainvectors.org

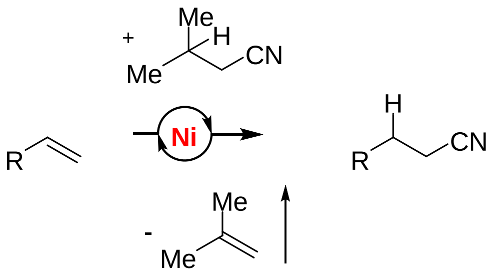
Fang et al. *Science*, **351**, 832-836 (2016).

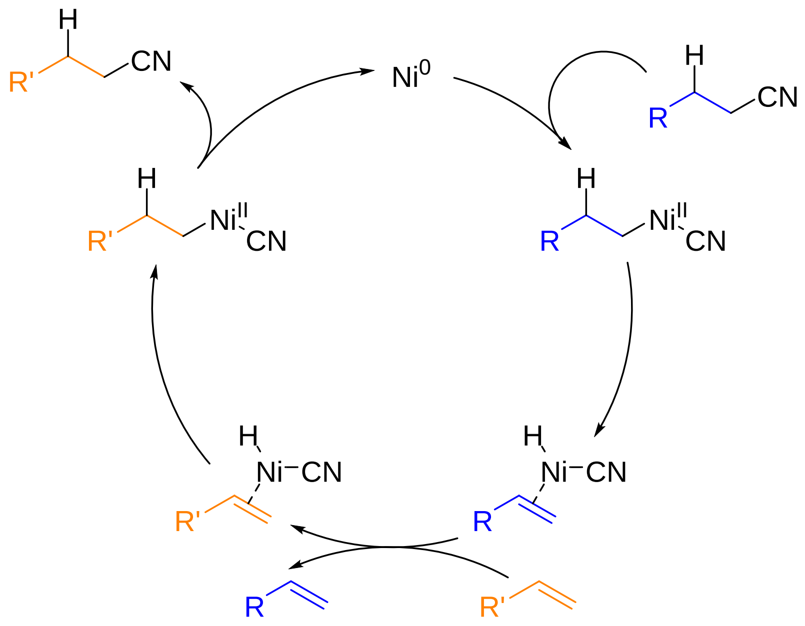
Shuttle Catalysis - Concept

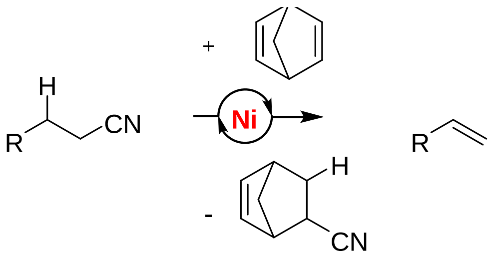












Pictures from https://publicdomainvectors.org

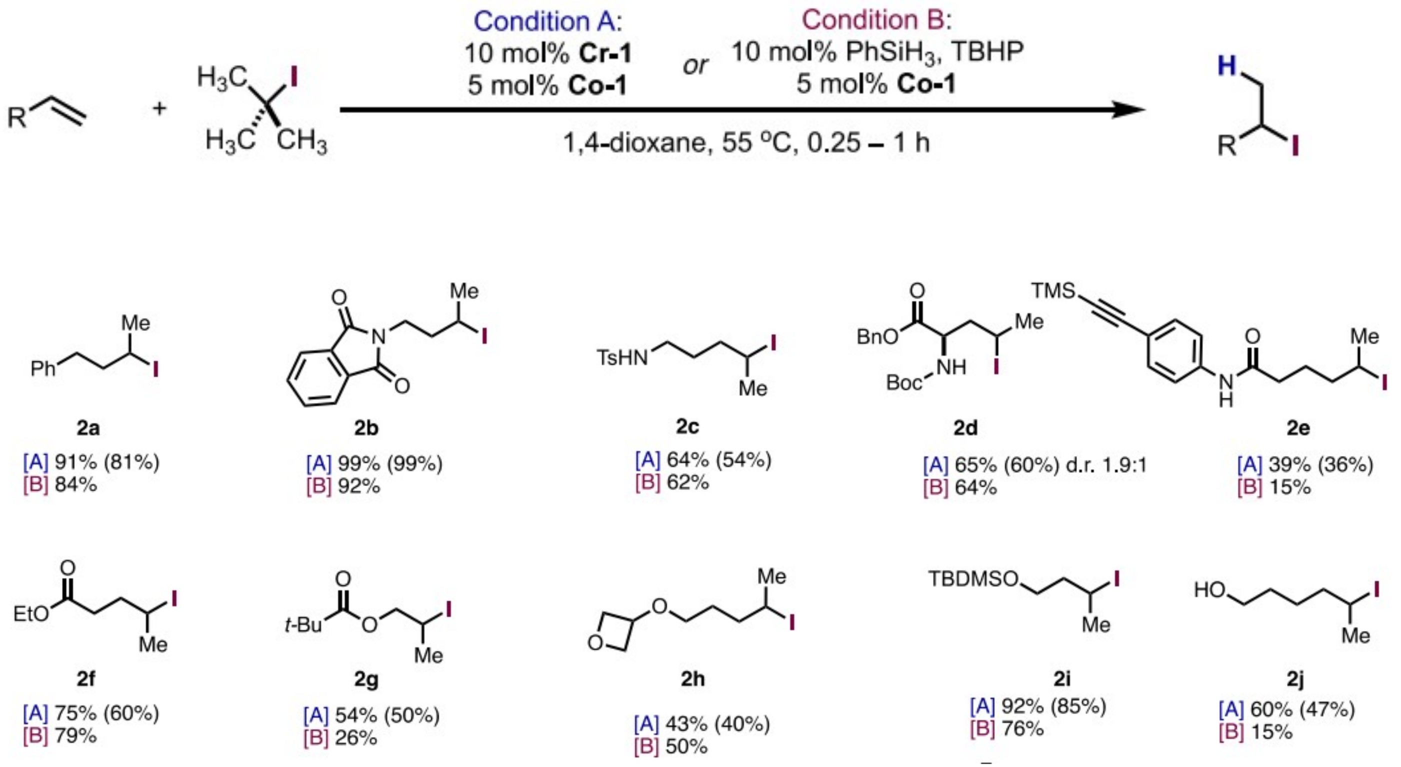
Fang et al. *Science*, **351**, 832-836 (2016).

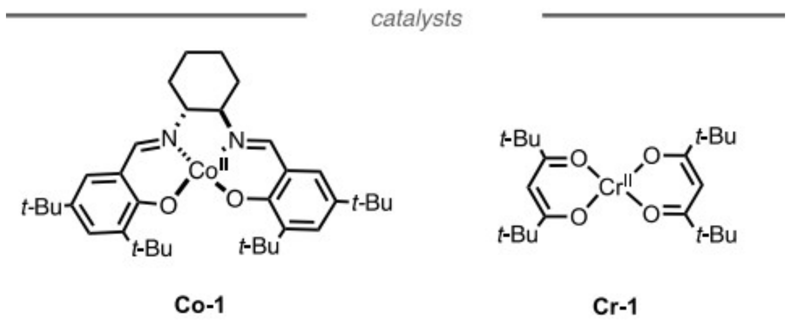
Shuttle Catalysis – Recent Developments

How to overcome limitations of classical approach?

Use 1 e^- logic instead!

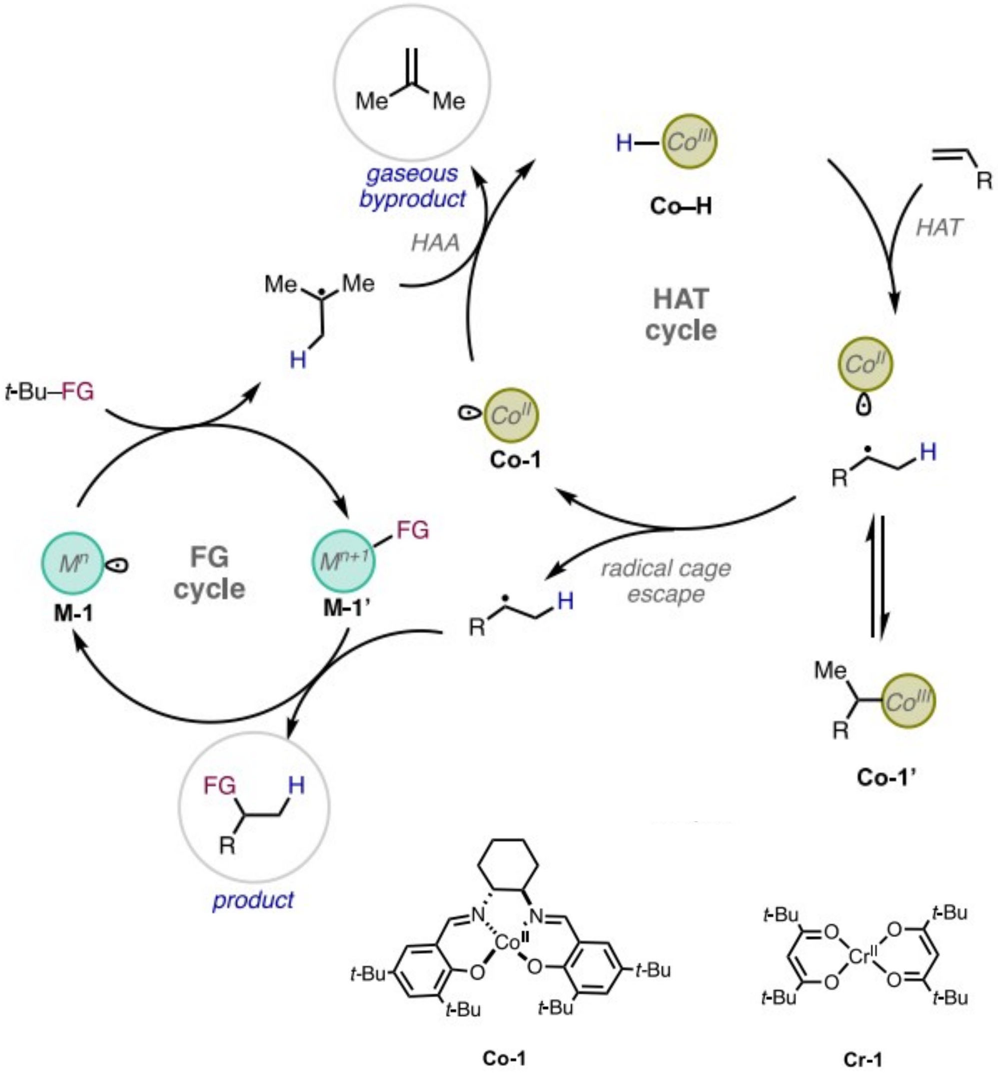
Dr. Tanner Jankins





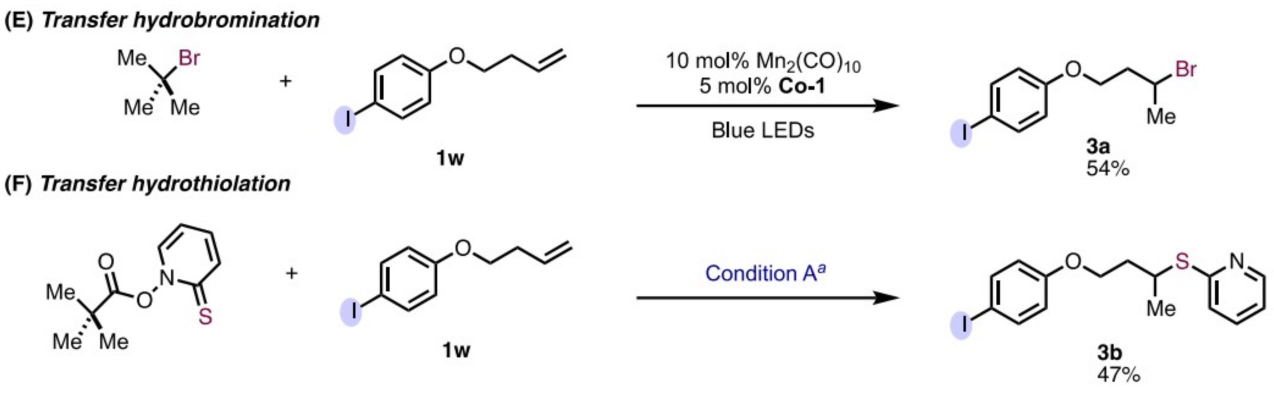
Jankins et al. *ChemRxiv* (2024).

Shuttle Catalysis – Recent Developments



Dr. Tanner Jankins

Many different groups transferable!

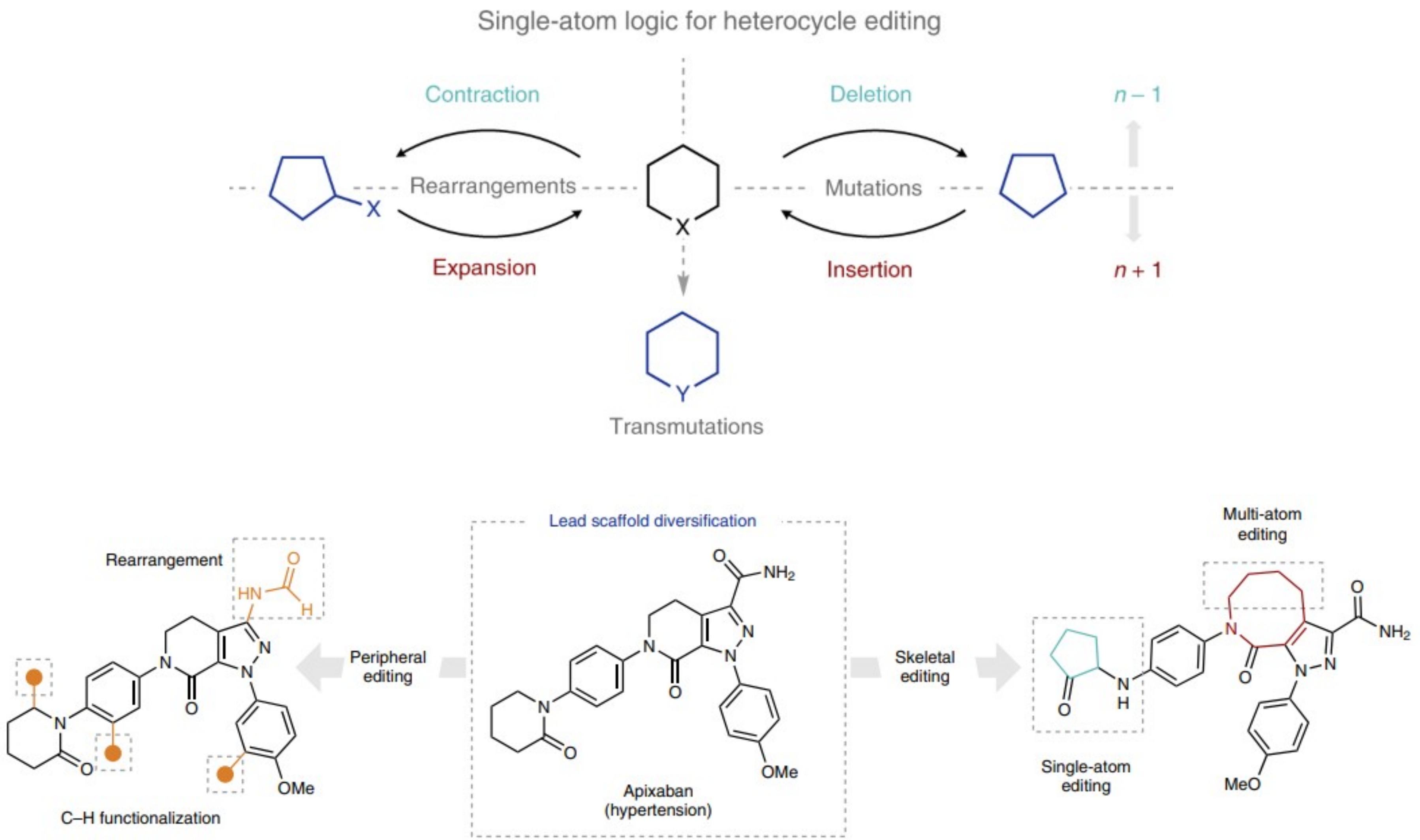


+ …

Many ongoing projects in our group

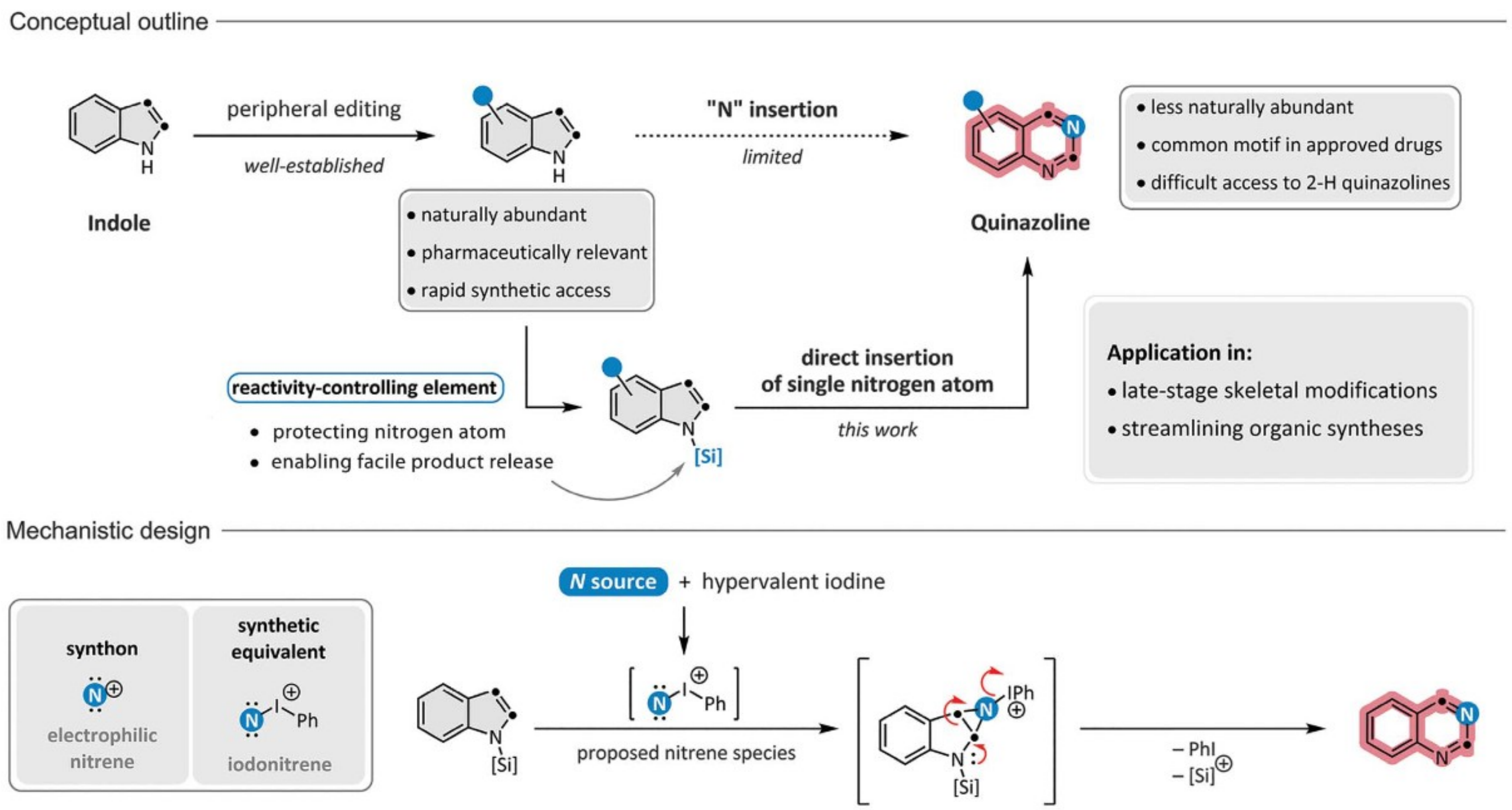
Jankins et al. *ChemRxiv*, (2024).

Skeletal Editing



Jurczyk et al. *Nature Synthesis*, **1**, 352-364 (2022).

Skeletal Editing – Recent Developments

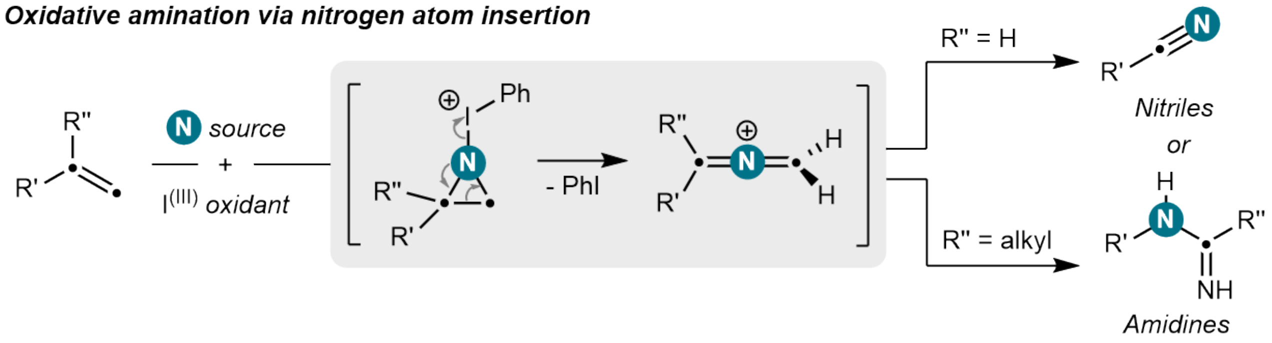


Dr. Julia Reisenbauer

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

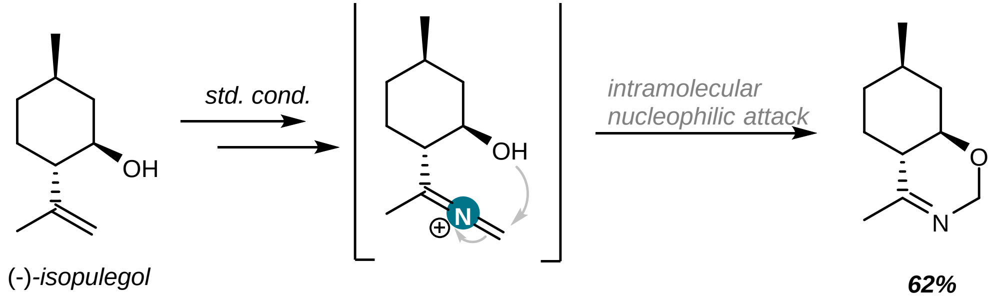
Reisenbauer et al. *Science*, **377**, 1104-1109 (2022).

Skeletal Editing – Recent Developments



Ann-Sophie Paschke

Yannick Brägger



Can aza-allenium salts be leveraged for modular amination strategies?

Many follow-ups possible!

Brägger et al. *ChemRxiv* (2024)

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
- Try to be early (one semester in advance)

Morandi Group Website

Thanks for your attention!

Exploring New Catalyst Designs for Sustainable Organic Synthesis

Josep Mas-Roselló
Group Leader

Research group information event @ETHZ
May 22nd 2024

ETH zürich
Swiss National Science Foundation

My Chemistry Career

2008 – 2013
B.Sc.
University of València

2013 – 2017
Ph.D.
University of Bristol

Synthesis of unnatural α-amino acids

Advisor: J. Clayden

2017 – 2021
Postdoc
EPFL Lausanne

Iridium catalysts for asymmetric hydrogenation

Advisor: N. Cramer

2021 – 2022
Postdoc
University of Zurich

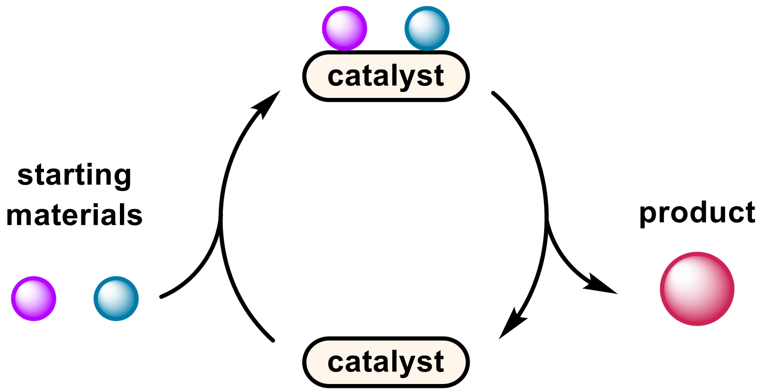
Inhibitors for bacterial pathogens

Advisor: K. Gademann

2022 – 2026
Group Leader
ETH Zurich

Sustainable catalysis

Green chemistry needs catalysis



- ✓ Mild conditions
- ✓ High atom-economy
- ✓ High product selectivity
- ✓ High industrial impact

R. A. Sheldon, *J. R. Soc. Interface* **13**: 20160087.

Project 1

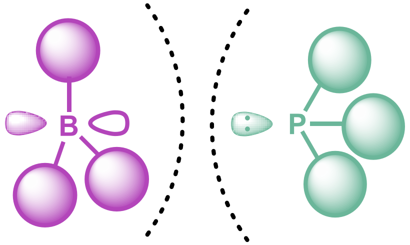
Organic catalysts for asymmetric hydrogenations


N. Shcherbakov
(2nd year PhD)

L. Schefer
(BSc project)

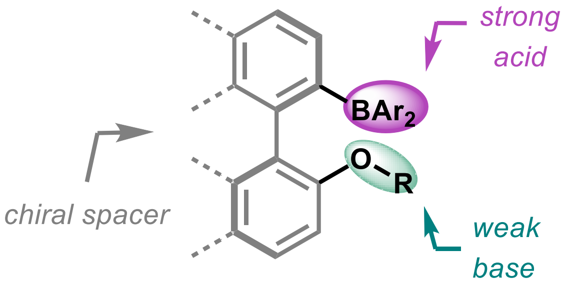
Design

Based on Frustrated Lewis Pairs (FLPs)



Chem. Soc. Rev. **2019**, *48*, 3592

Our design - next generation FLPs



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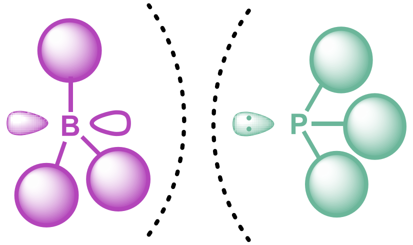

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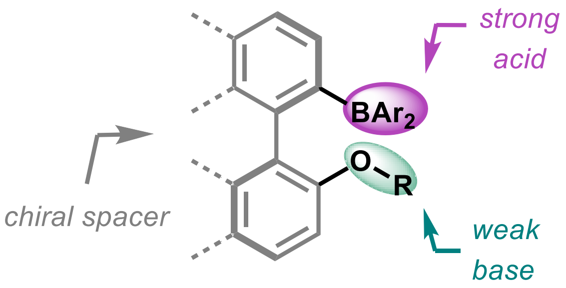
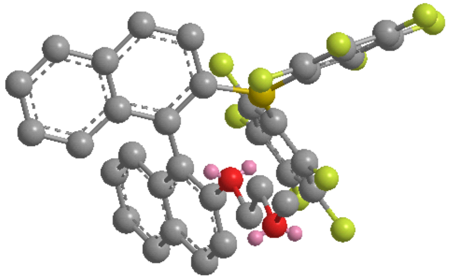
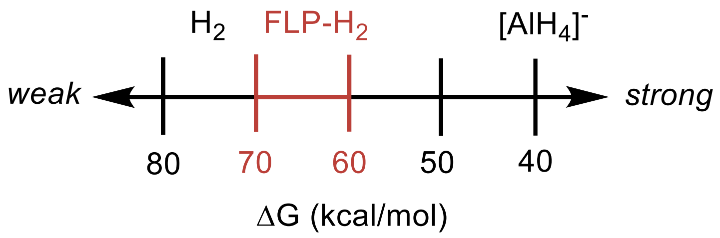


Understand

Molecular shape: X-Ray



Hydride-donor capacity: DFT



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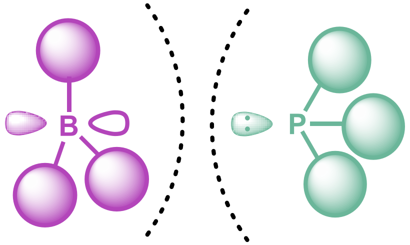

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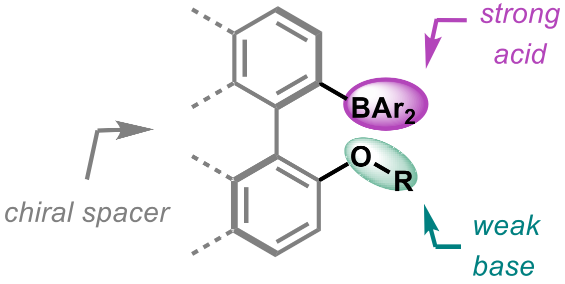

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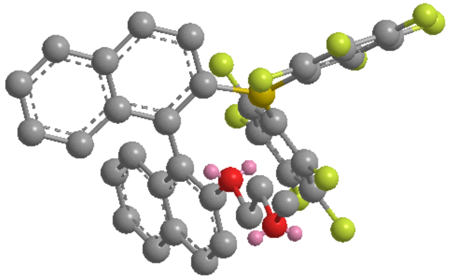

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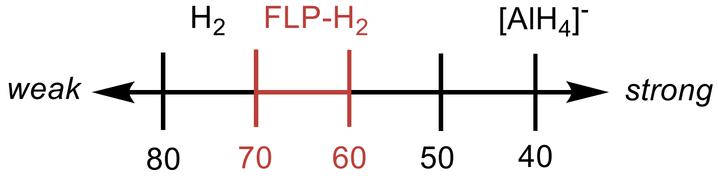
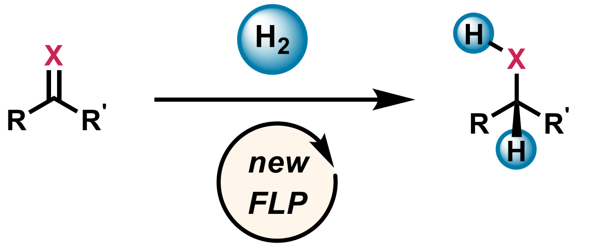
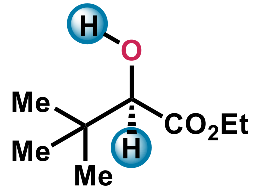


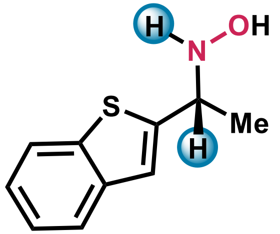
Apply



Selected relevant examples:



Thrombine inhibitor



Zileuton
Antiasthma

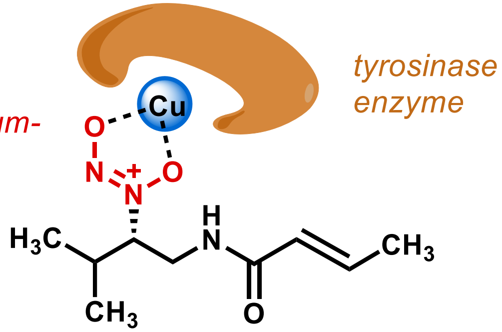
Project 2

Bioinspired ligands for copper catalysis

N. Liedtke
(BSc project)

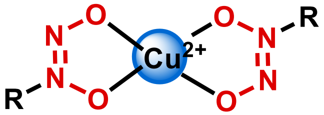
Design

Based on 'rare' bacterial metallophores
(e.g. Dopastin)**:**



Bioorg. Med. Chem. **2001**, *9, 1233*

Our synthetic mimics:



R = alkyl, aryl...

♦ highly-stable ✓ ♦ reactive ✓

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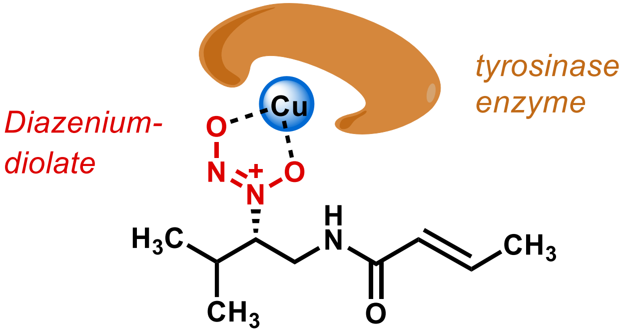

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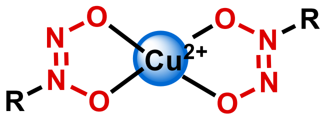

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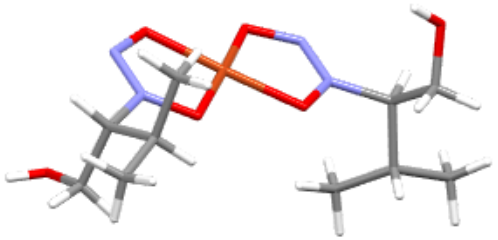
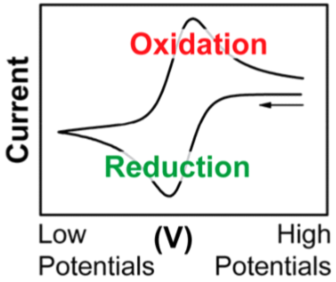
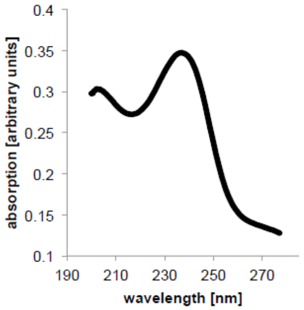


Electronic & redox properties:

Cyclic Voltammetry



UV spectroscopy



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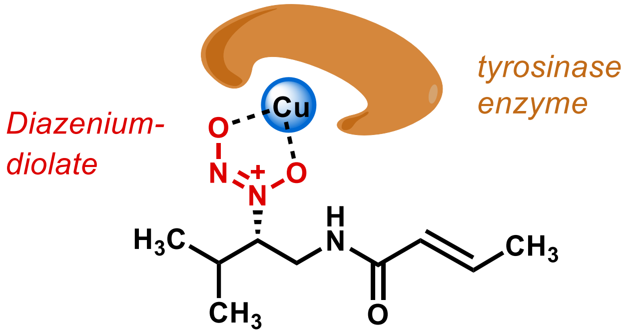

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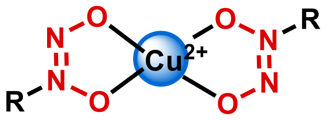

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- ♦reactive ✓

Understand

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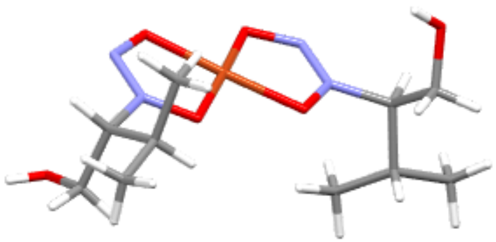

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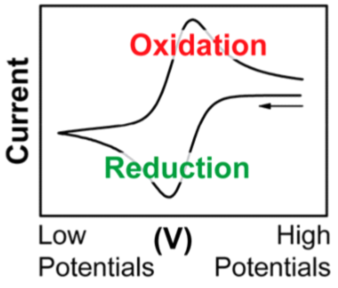

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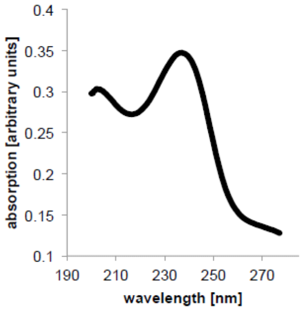

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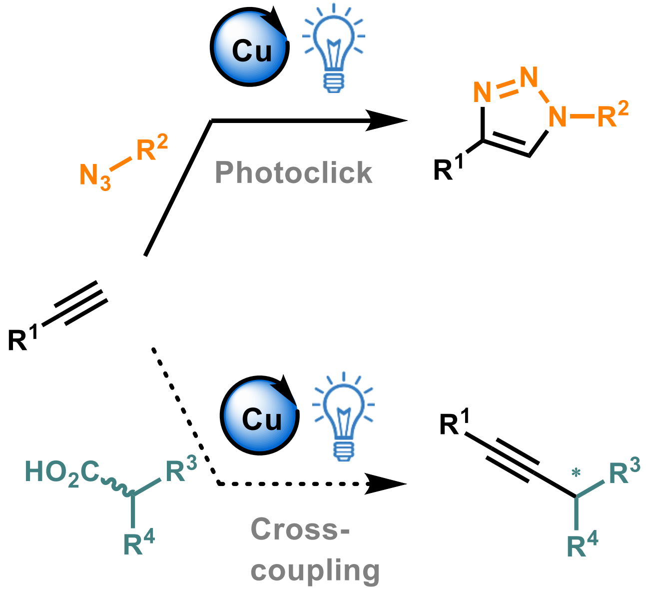


Big thanks to:

N. Shcherbakov
(2^{nd} year PhD)

S. Sutter
(BSc project)

L. Schefer
(BSc project)

N. Liedtke
(BSc project)

The Wennemers Group (our colleagues and hosts)

ETH zürich

SNF

Interested in joining us? Reach out!

Email:
jmasrosello@ethz.ch

Group website:
https://masrosello-group.org

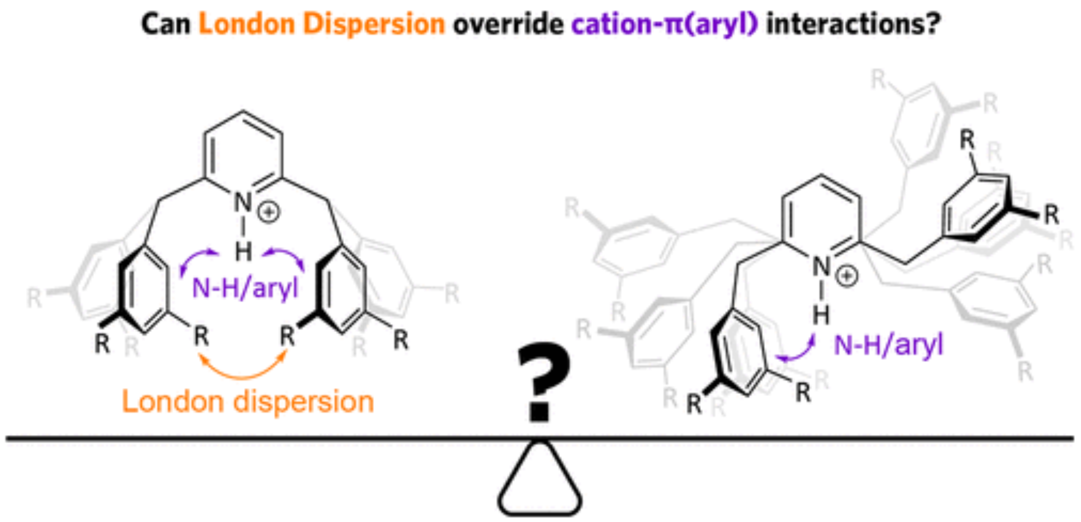
Lab H314

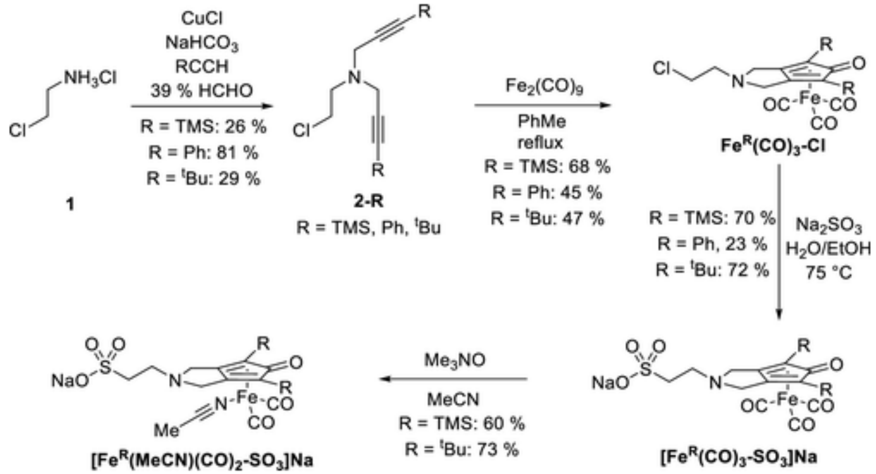
Chen Group

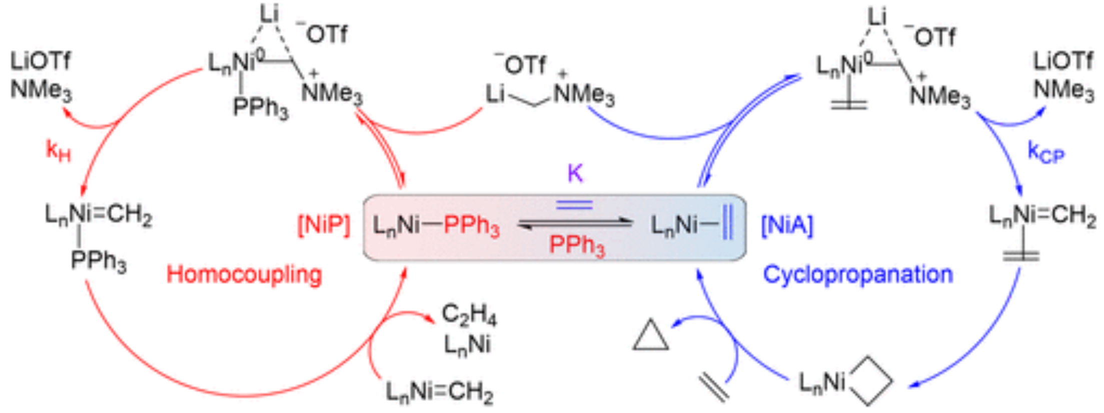
Fundamentals of Transition Metal Catalysis

Overview

- Organometallic Chemistry
- Physical Organic Chemistry
- Reaction Mechanisms
- Computational Studies

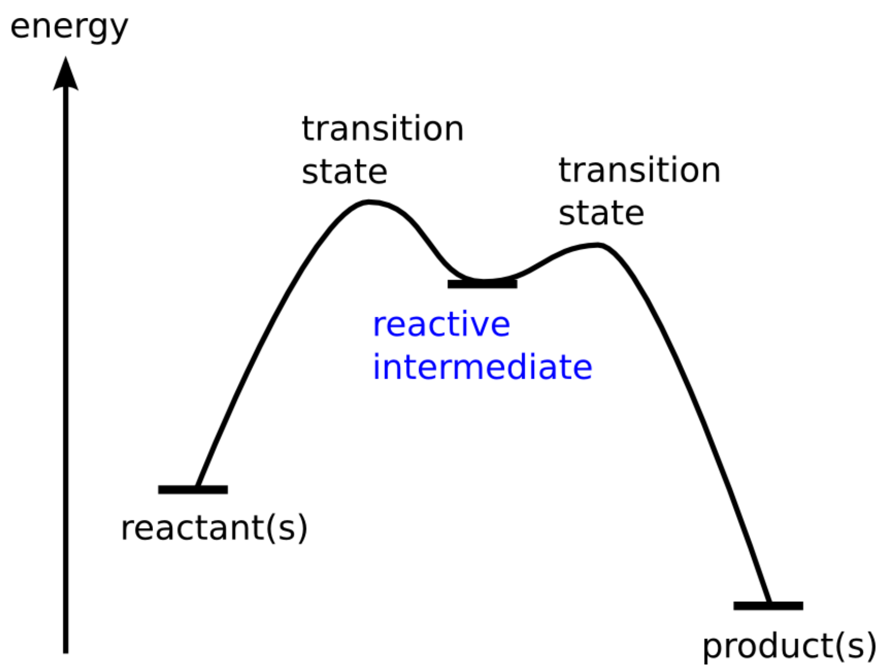






Current Projects

- Gold catalyzed hydroamination
- Rhenium catalyzed alkene metathesis
- Iron catalyzed hydrogenation
- Iridium catalyzed carboxylation
- Nickel catalyzed cyclopropanation
- Iron catalyzed oxidation reactions
- Dispersion studies in bipyridines
- …



Possible Student Projects

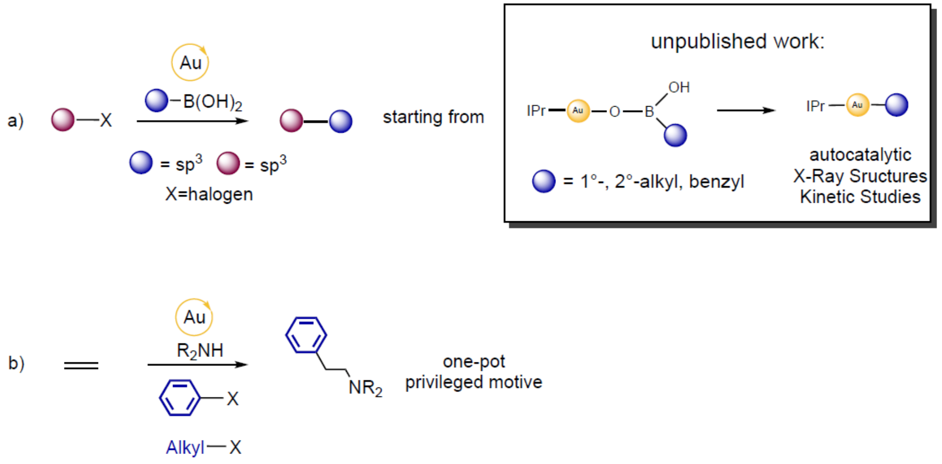
- Semester Projects (7 weeks full time) can be accomodate for sure
- For Masters Theses, we would need to discuss
- Experimental, theoretical or combined projects are possible

Gold Catalyzed sp3-sp3 Coupling Reactions/ Low Cohesion Energy Scaffolds

Your tasks:
- Organic Synthesis
- Organometallic Gold Synthesis
- Stoichiometric Studies

Alternative, non-fluorinated structures to fluorocarbons, since they are being phased out.

(prior experience in organic synthesis desired)



Contact:
Mitar Radić
HCI G204
mradic@org.chem.ethz.ch

Rhenium Catalyzed Alkene Metathesis

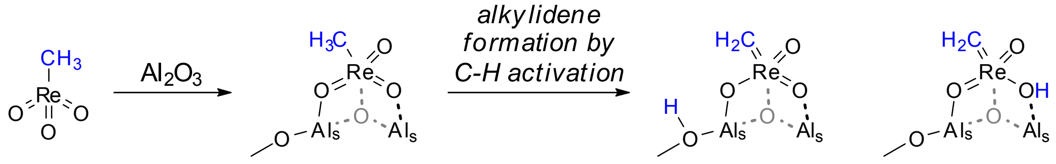
Your tasks:
- Organometallics Synthesis
- Catalytic Experiments
- Mechanistic Studies by ESI-MS, kinetics, NMR, etc.

Contact:
Péter Kalapos
HCI G214
peter.kalapos@org.chem.ethz.ch

Re(VII)-oxo compounds (MTO) on alumina (Al2O3) supports are highly active **heterogenous alkene metathesis catalysts.**

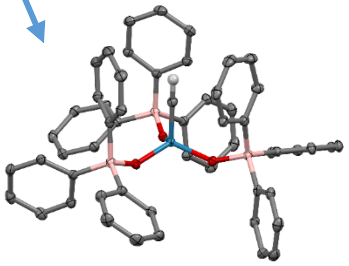
□ Mechanistic studies are impeded by a wide distribution of surface species, and very small number of active sites

□ **Structure and nature of active sites is poorly understood**



MTO 1 2a 2b

Our approach: **Homogenous model systems** for the heterogenous catalyst



Intramolecular frustrated Lewis-pairs to mimic both Lewis-acidic and basic sites

Re-activation and reactivity of an isolated off-cycle species

Gold Catalyzed Hydroamination

Your tasks:
- Synthesize bidentade ligands
- Make the Au(I)-complexes
- Test them for hydroamination

Contact:
Serena Schilling
HCI G218
serena.schilling@org.chem.ethz.ch

What you can learn

- Organic and organometallic Synthesis (Schlenk line, Glovebox, pressurized gases, …)
- Working with a wide variety of analytical techniques (NMR, ESI-MS, UV-VIS, XRD, IR, …)
- Tools for investigating reaction mechanisms (real-time MS, kinetics, KIEs, …)
- DFT calculations and/or MD simulations

Thank you for listening!

For general questions: andre.buetikofer@org.chem.ethz.ch / maurice.andrey@org.chem.ethz.ch
To apply (CV, short motivation letter, transcripts of record): peter.chen@org.chem.ethz.ch

PAUL SCHERRER INSTITUT PSI

ETH zürich

Noemi Cerboni :: Laboratory of Radiochemistry :: Paul Scherrer Institut | ETH Zürich

The Laboratory of Radiochemistry at PSI (at ETHZ: Steinegger group)

VCS Research Group Introduction 2024, May 22nd, 2024

PAUL SCHERRER INSTITUT PSI

The Laboratory of Radiochemistry at PSI

Postdoctoral researchers

PhD students

Prof. Dr. Robert Eichler

UNIVERSITÄT BERN

Sandha Keller (Admin, 80%)
TBD (deputy lab head)

ETH zürich

HEAVY ELEMENTS
Prof. Dr. Patrick Steinegger

Dr. Rugard Dressler
Alexander Vögele
Dominik Herrmann

Jennifer Wilson (SNF)
Georg Tiebel (SNF)
Paul Dutheil (ENSI, LOG)
Michael Hofstetter (BABS)

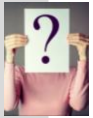
ISOTOPE & TARGET CHEMISTRY
Dr. Zeynep Talip

Dr. Jörg Neuhausen
Dr. Emilio Maugeri
Dr. Djordje Cvjetinovic

Ivan Zivadinovic (EU, PATRICIA)
Noemi Cerboni (PSI)
Vladislav Zobnin (EU, PASCAL)
Xuandong Kou (Uni Bern)

RADIONUCLIDE DEVELOPMENT
Dr. Nick van der Meulen

Dr. Who (CRS, BIO)
Dr. Pascal Grundler (CRS, BIO)
Colin Hillhouse (ITM)
Dr. Anzhelika Moiseeva
Dr. Maryam Mostamand

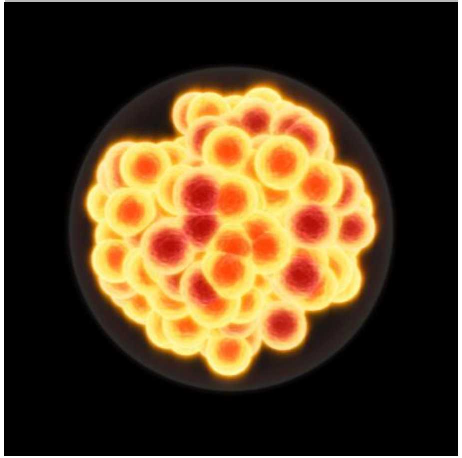


Edoardo Renaldin (Uni Bern)

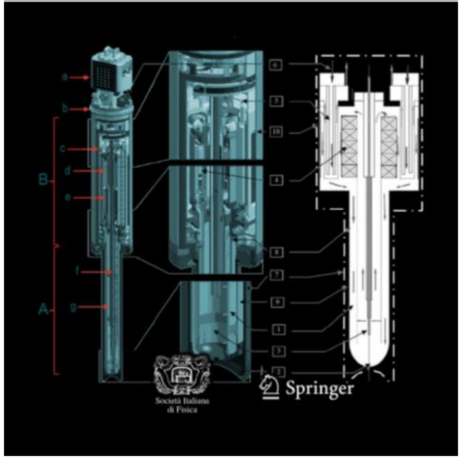
+ 2 to 3 Master- / Bachelor- / semester students

The Laboratory of Radiochemistry at PSI

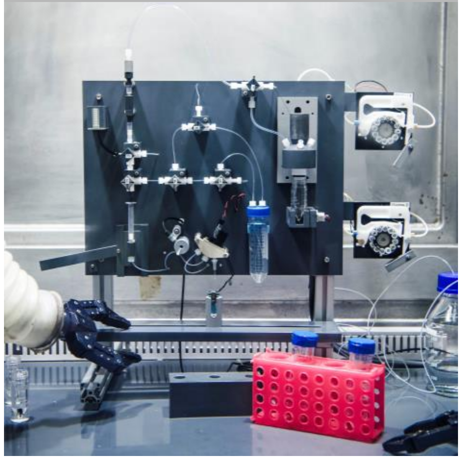
Heavy Elements



Isotope and Target Chemistry



Radionuclide Development

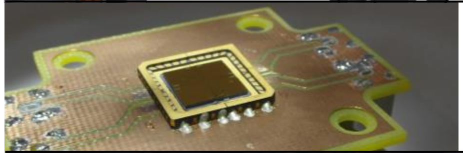


Pictures from: https://www.llnl.gov/; title page of the *European Physical Journal Plus* (vol. 131, no. 7, 2016) with a picture showing the MEGAPIE-target

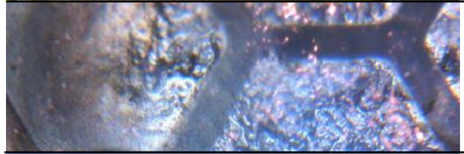
The Laboratory of Radiochemistry at PSI

Heavy Elements | Isotope and Target Chemistry | Radionuclide Development

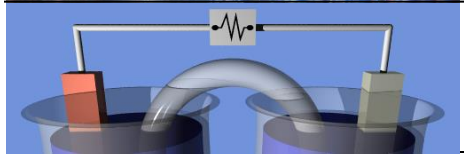
Gas adsorption chromatography with transactinide elements



Detector development for extreme conditions



Targets for heavy ion beam irradiations



Electrochemistry with transactinide elements

Daniell cell adapted from http://en.wikipedia.org

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The Laboratory of Radiochemistry at PSI

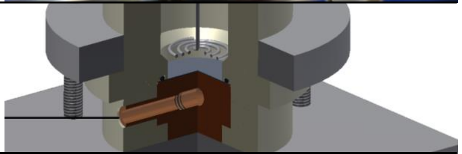
Heavy Elements

Isotope and Target Chemistry

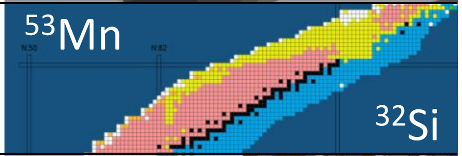
Radionuclide Development

Liquid metal chemistry

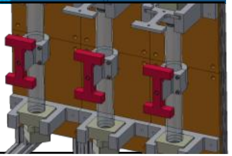
Isotope extraction and target manufacturing



Improvement of nuclear physics data



Waste treatment and isotope reclamation



The Laboratory of Radiochemistry at PSI

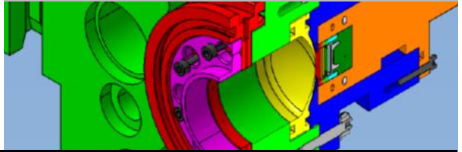
Heavy Elements

Isotope and Target Chemistry

Radionuclide Development

LRC + CRS

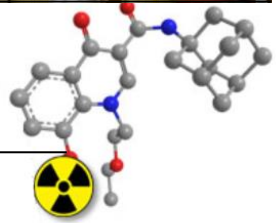
Target Development



Production of new radionuclides

Chemical separation and processing

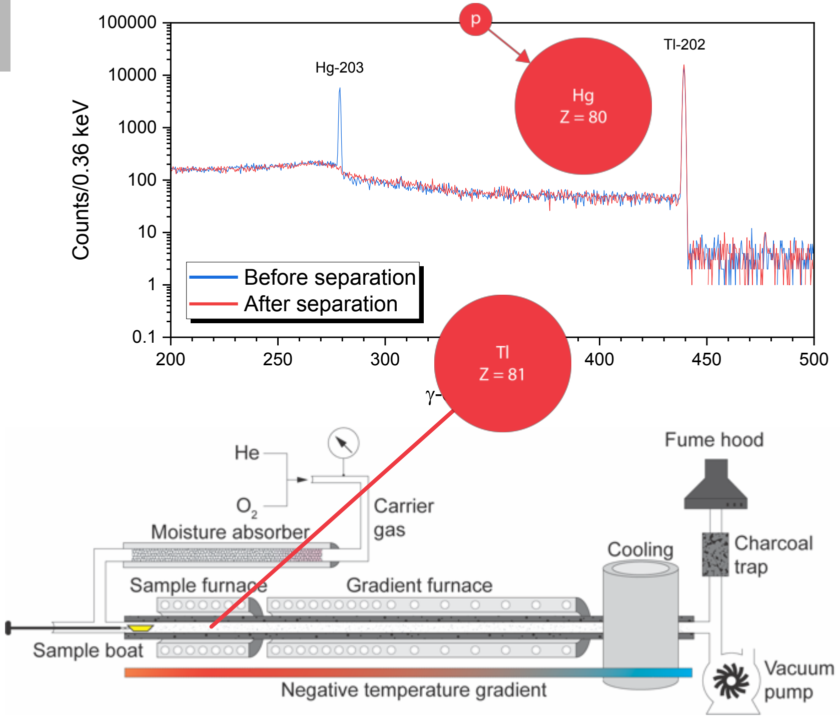
Theragnostics

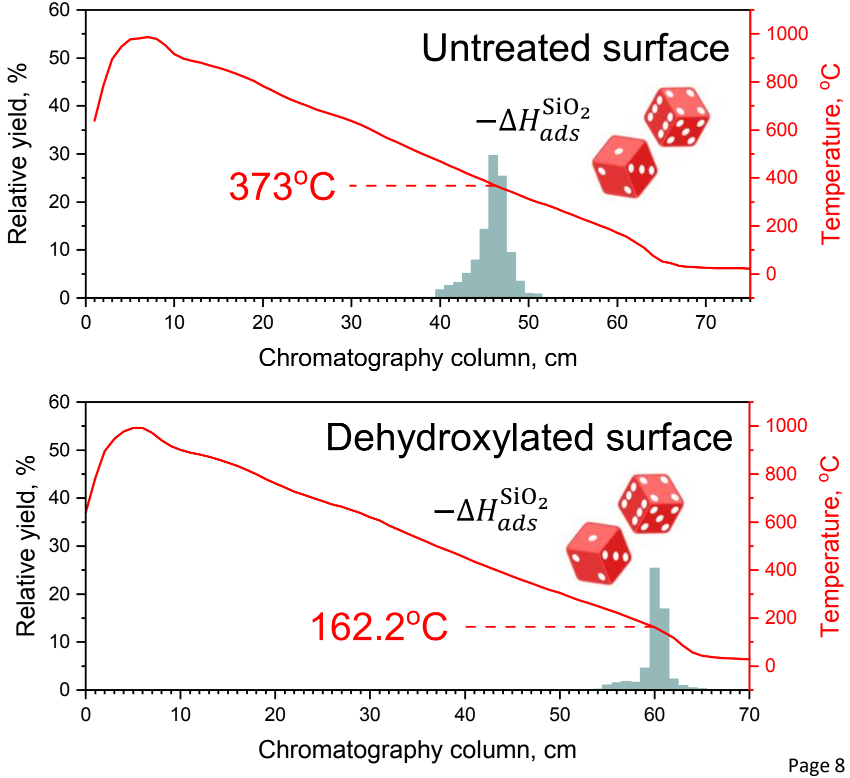


https://www.radiopharmaceutical-science.ethz.ch und https://www.psi.ch/

Project examples

Example (final project upon discussion)

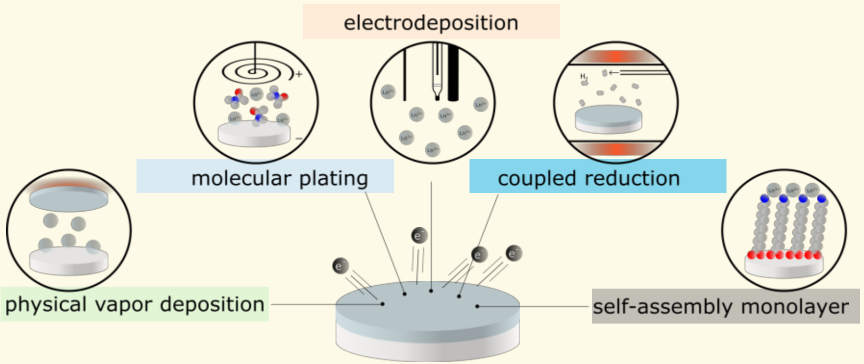




Isotope and Target Chemistry

Uniform and radioactive thin films

Preparation



Characterization

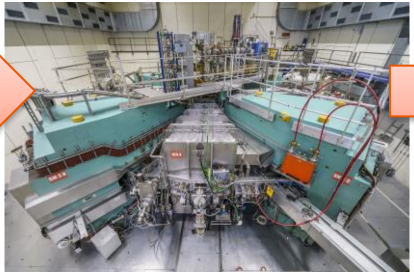
- Gamma and alpha spectroscopy
- Radiography
- SEM, EDX,
- XPS, XRD,
- RAMAN, IR,
- SIMS, AFM/STM
- Profilometry

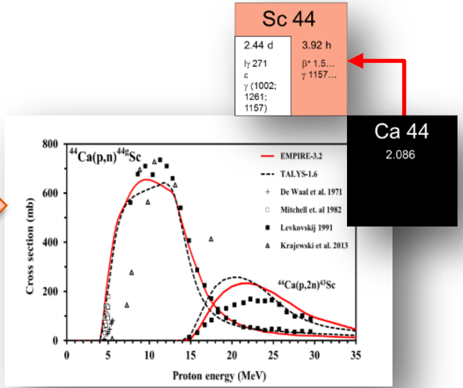
Courtesy: N. Cerboni

Radionuclide Development

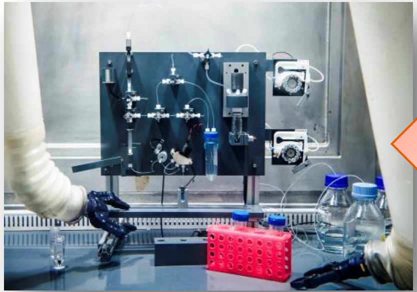
Target preparation

Proton irradiation of target material

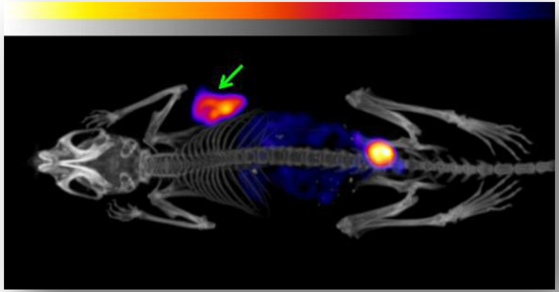




Chemical separation and processing



Preclinical radiolabelling and imaging



Grundler *et al.*, Chimia (2020); van der Meulen *et al.*, Proc. Cyclotrons2019 (2019)

Thank you very much!

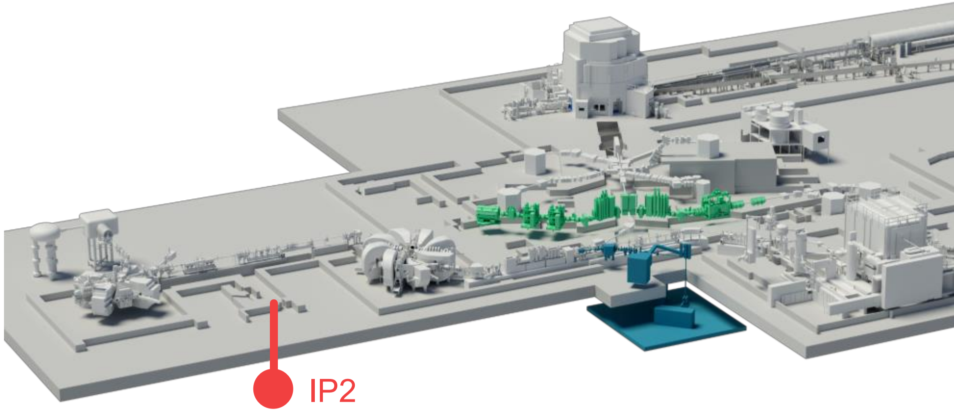
PSI

ETH zürich

The large-scale research facilities of PSI for the production of radionuclides

PAUL SCHERRER INSTITUT

Nuclear reactions (p)

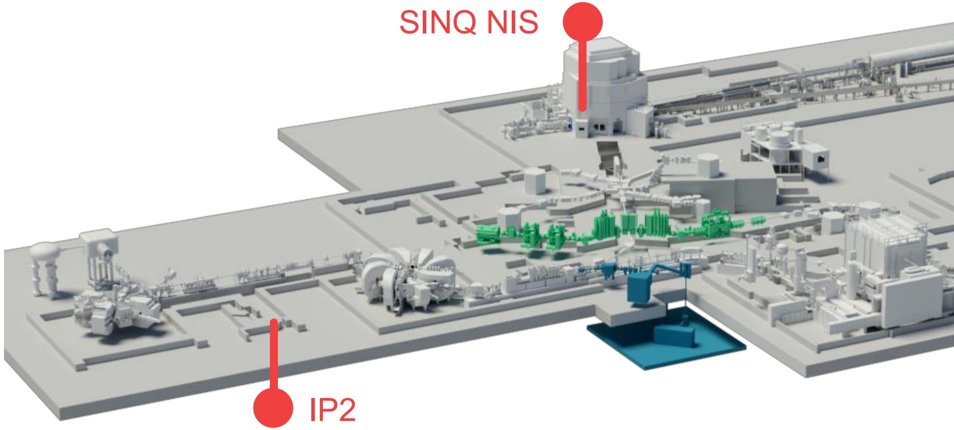


Bilder: PSI

PAUL SCHERRER INSTITUT

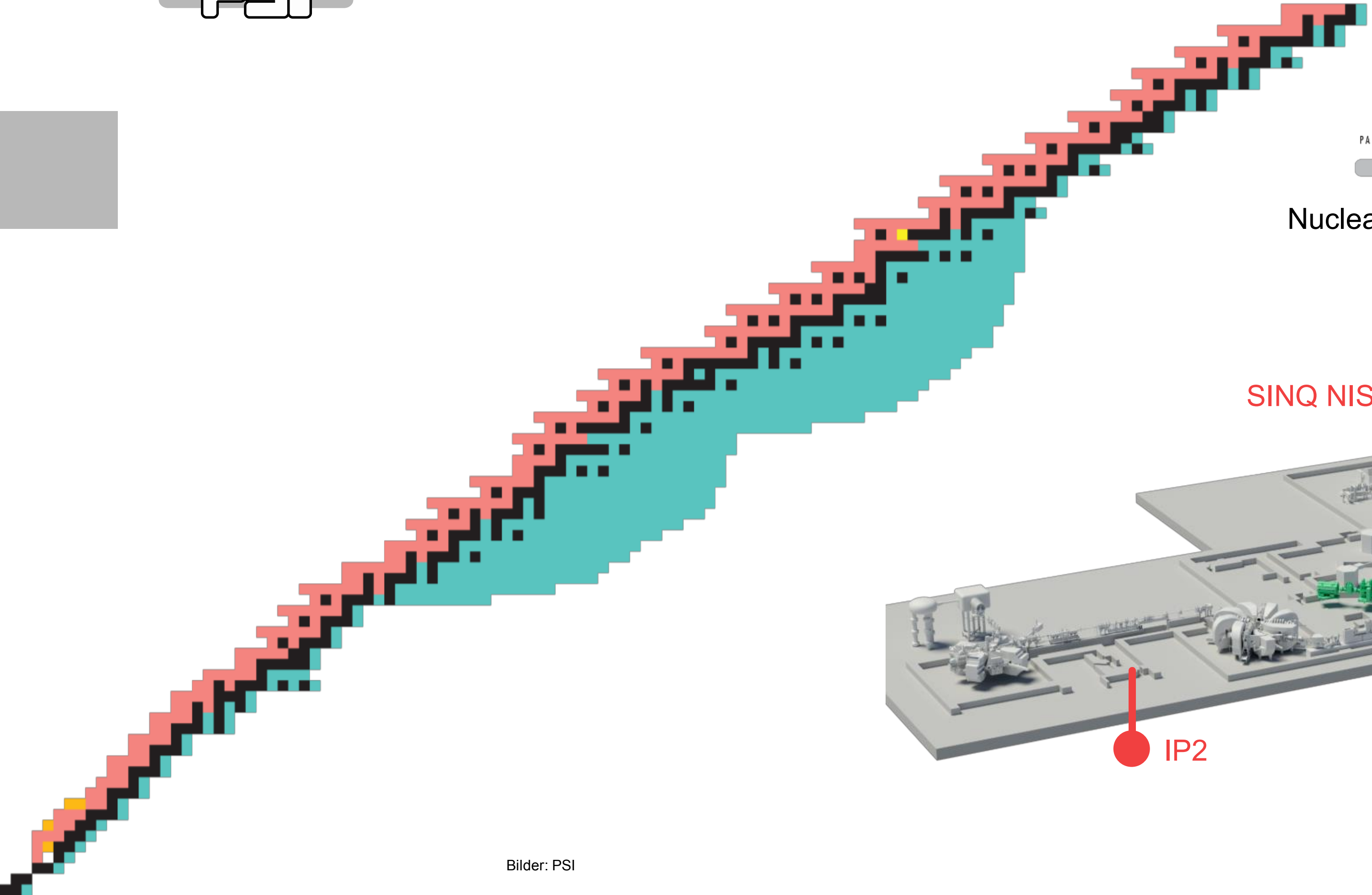
PSI

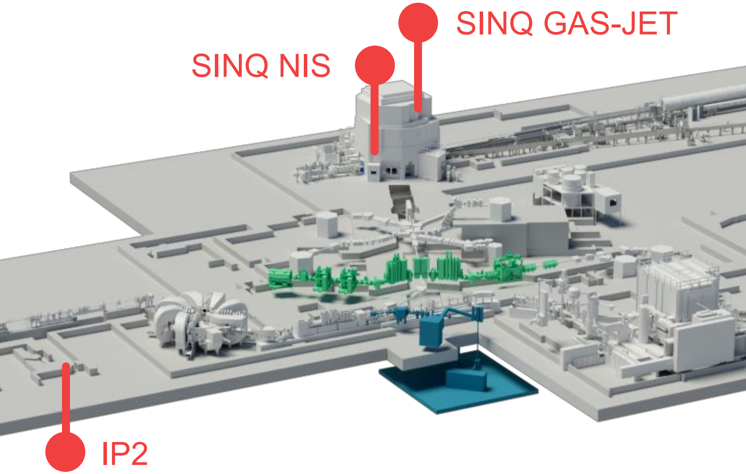
Nuclear reactions (n)



Bilder: PSI

Nuclear reactions (f)

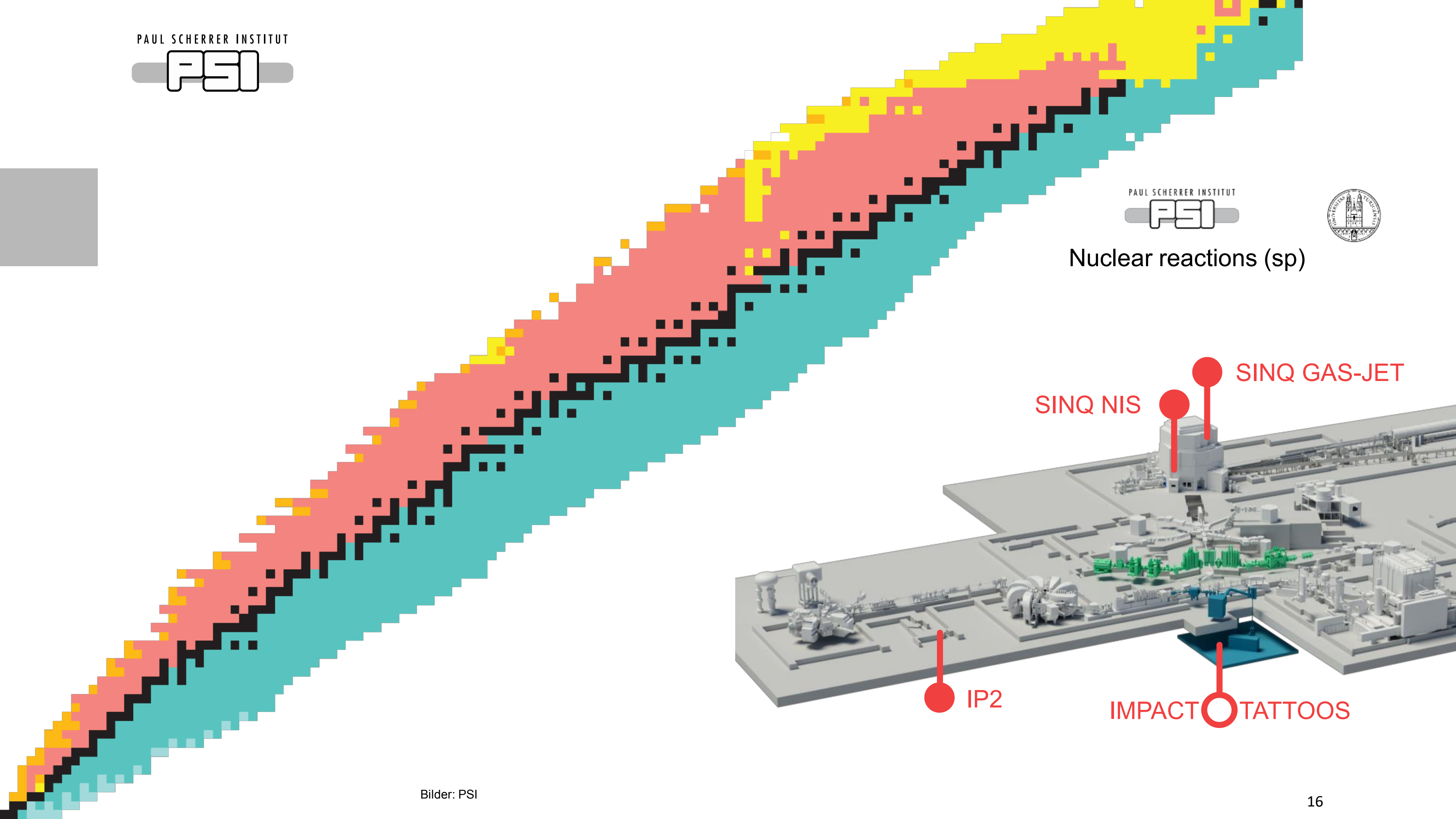




Bilder: PSI

PAUL SCHERRER INSTITUT PSI

Nuclear reactions (sp)



Bilder: PSI

ETH zürich

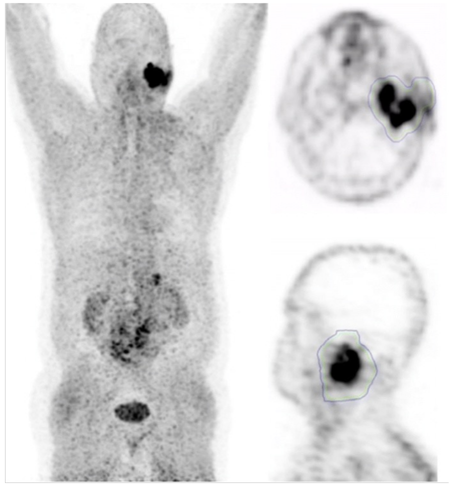
DEL Technology

at the Scheuermann-Lab

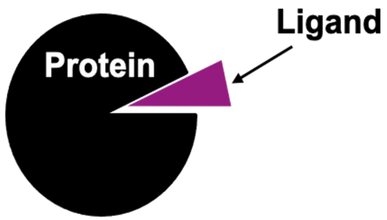
www.del-technology.ethz.ch

Targeted Therapy

Targeted therapy[1]

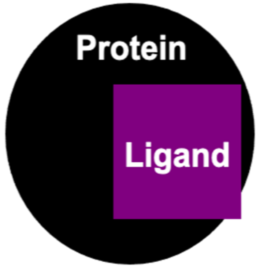


Easy to target



- Proteins with small pockets
- e.g. kinases

Difficult to target

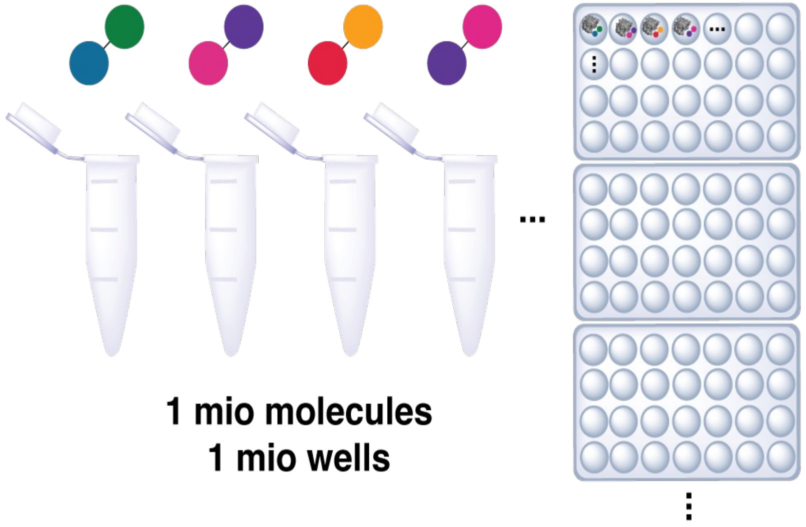


- Proteins with flat surfaces
- Protein-protein interactions
- e.g. RAS GTPases in cancer

1) Syed, M., Flechsig, P., Liermann, J. et al. Fibroblast activation protein inhibitor (FAPI) PET for diagnostics and advanced targeted radiotherapy in head and neck cancers. *Eur J Nucl Med Mol Imaging* 47, 2836–2845 (2020).

Small-molecule drug discovery

High-Throughput Screening Library



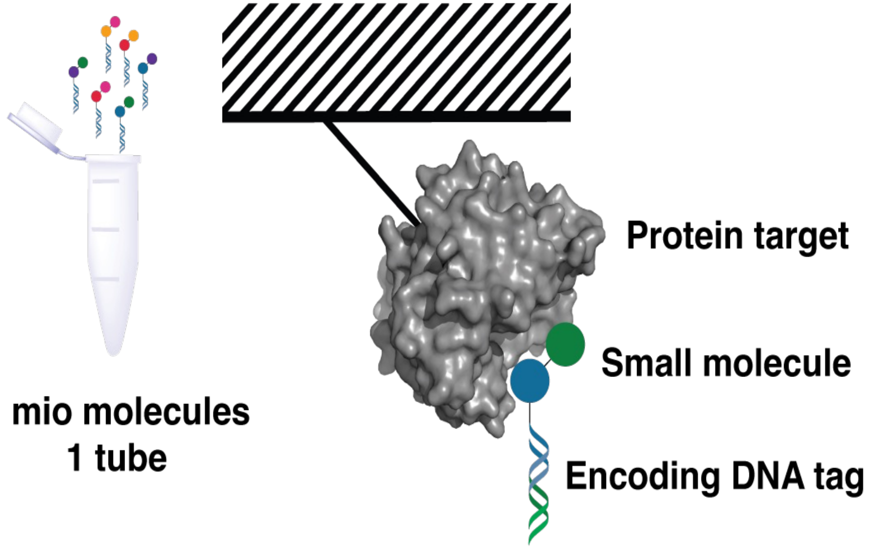
1 mio molecules
1 mio wells

Collection of max. 5 mio molecules
Time for screening: weeks

$ 2 b / 1 mio molecules

vs

DNA-Encoded Library (DEL)

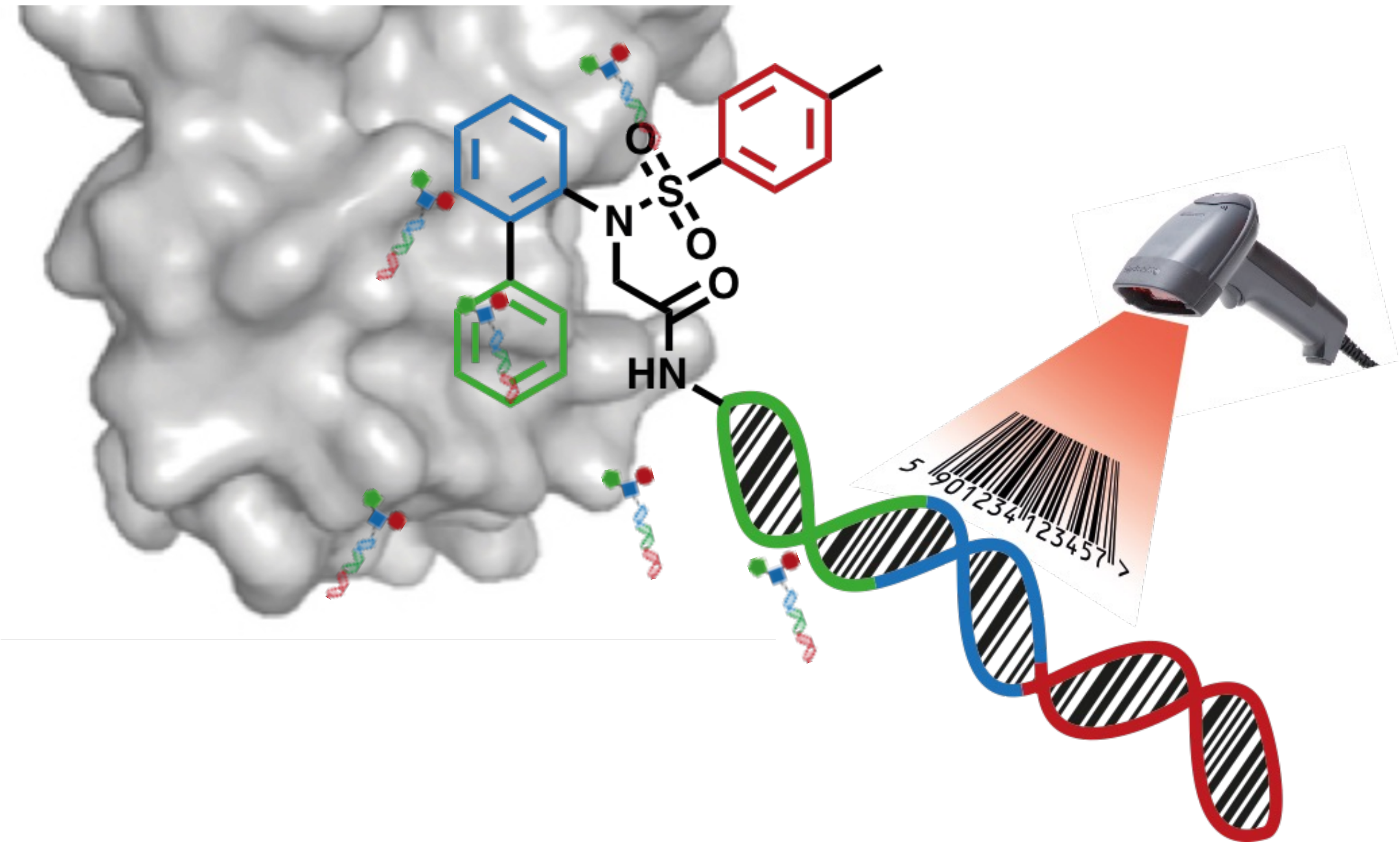


1 mio molecules
1 tube

Up to billions of molecules & fast synthesis of new libraries
Time for screening: days

$ 0.001 b / 1 mio molecules

DNA-encoded Chemical Libraries (DELs or DECLs)



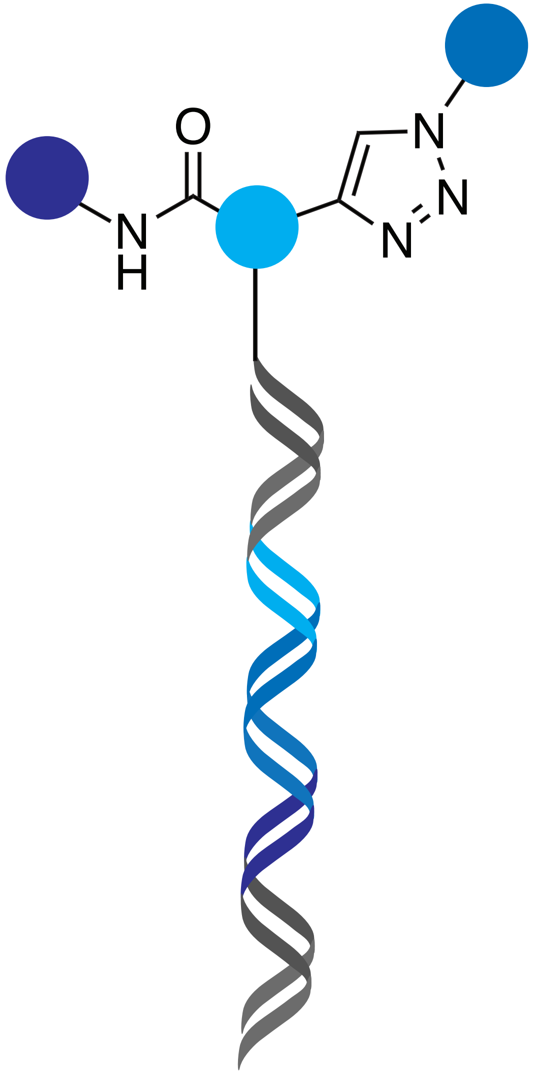
The DNA-tag („barcode“) unambiguously identifies each molecule in the library

DNA is chemically stable and compatible with a wide range of synthetic reactions

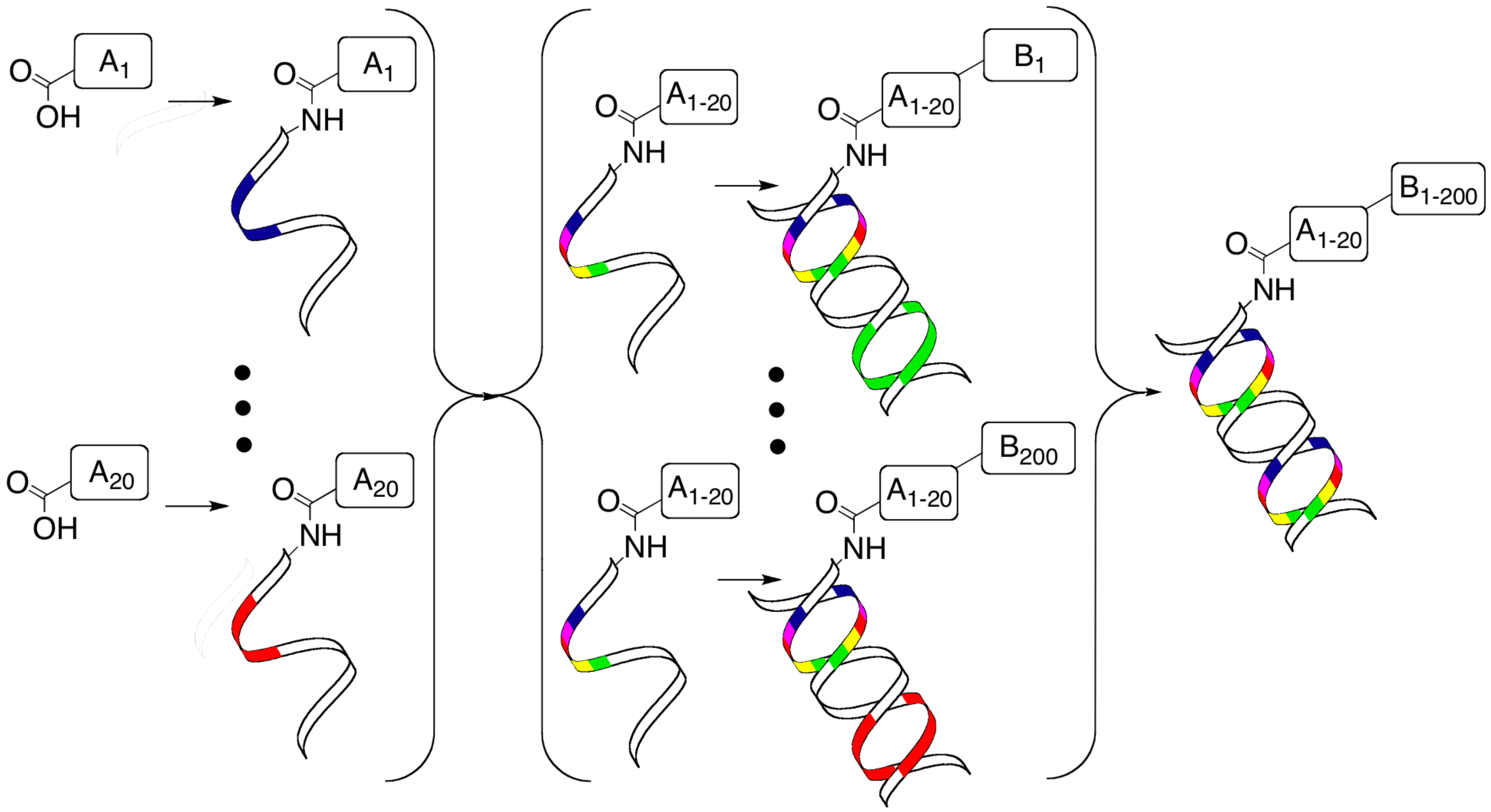
PCR and **high-throughput DNA sequencing** enable the efficient identification of binders to protein targets of interest

DNA-encoded Chemical Libraries (DELs or DECLs)

- **Collections of Millions of Compounds**
- **Generated by Split-and-Pool Synthesis**
- **Unique Identifiers: DNA-“Barcodes”**
- **Used in Affinity based Selections**
- **Widely used in Industry and Academia**



Split-and-Pool Synthesis of DNA-encoded Chemical Libraries

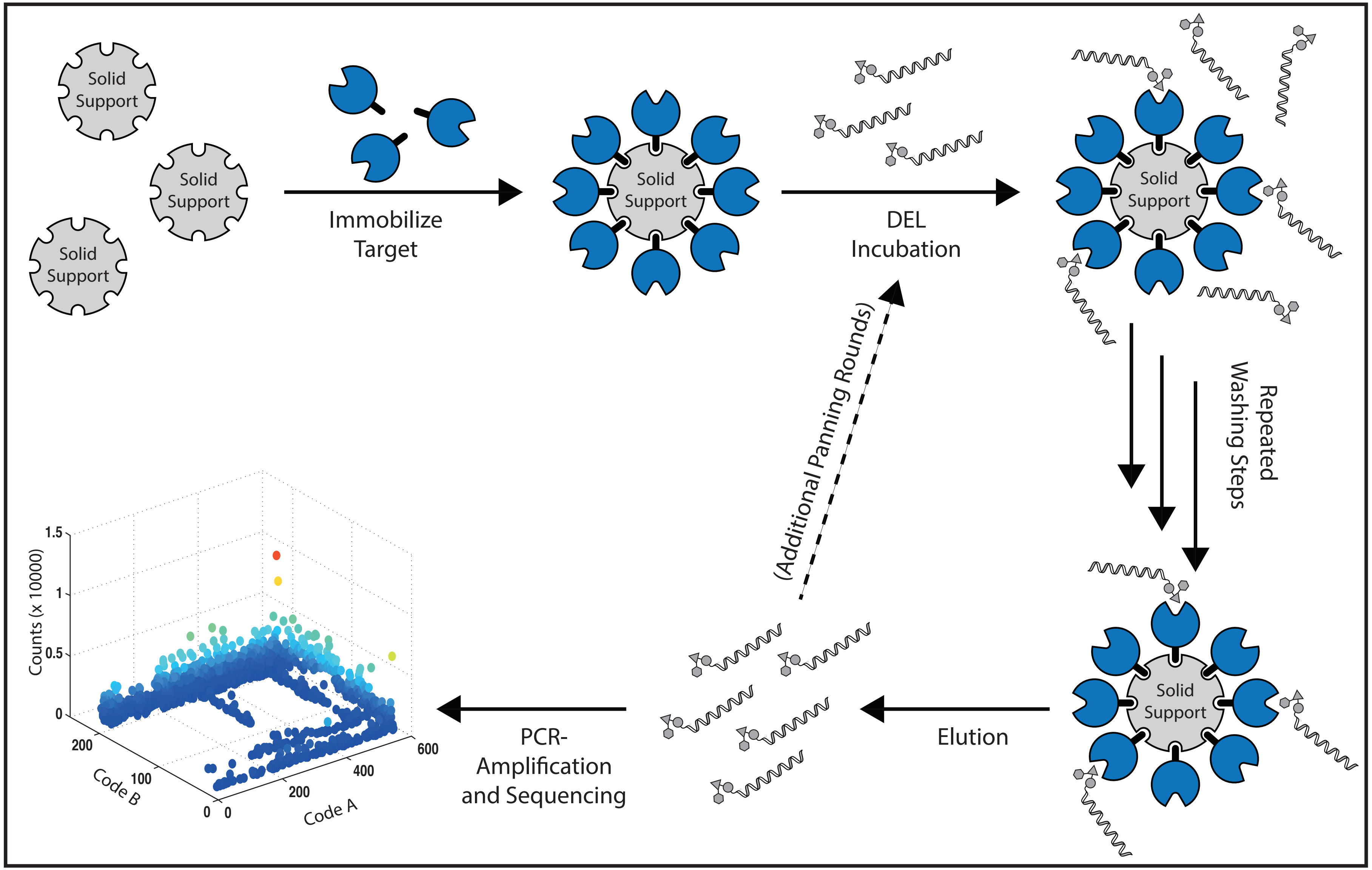


Buller et al. (2008) *Bioorg Med Chem Lett*, **18**, 5926

Mannocci et al. (2008), *PNAS*, **105**,17670-5

Clark, M. A. et al. (2009) Nature Chemical Biology 5, 647–654

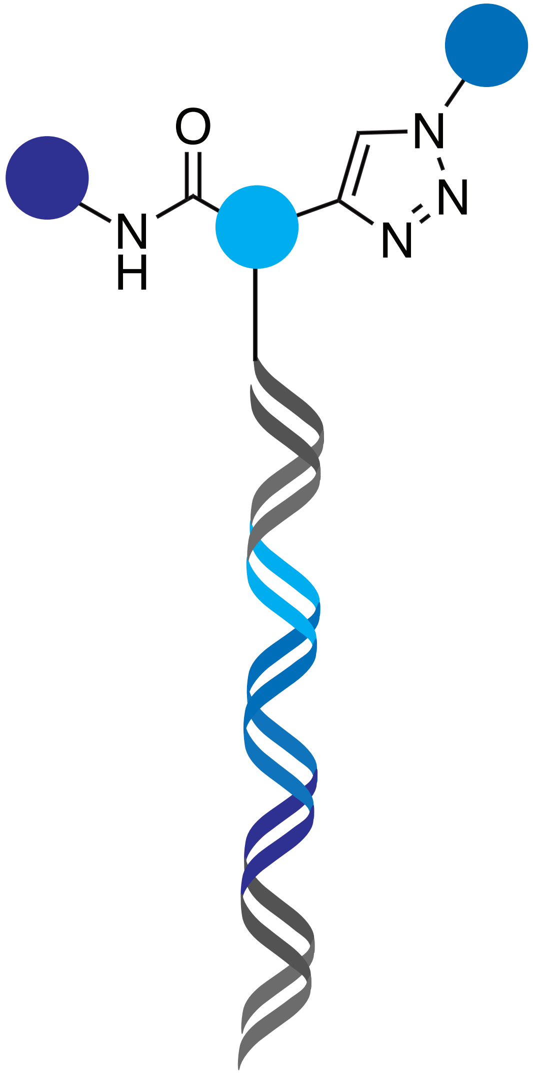
Use of DNA-encoded Chemical Libraries / selection on targets



Decurtins, W., Wichert, M., Franzini, R.M., Buller, F., Stravs, M.S., Zhang, Y., Neri, D. & Scheuermann, J. (2016) *Nature Protocols* 11, 764–780

DNA-encoded Chemical Libraries @ ETH Zurich

- **Design and Construction of DELs**
- Screening for Internal Targets & Collaborators
- Development of new, DNA compatible Reactions
- Hit Validation Strategies
- Enzymatic Reactions on DNA



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Roche

St. Jude Children's Research Hospital

Finding cures. Saving children.

ETH zürich

药明康德

WuXi AppTec

Paul-Ehrlich-Institut

DNA-encoded Chemical Libraries @ ETH Zurich

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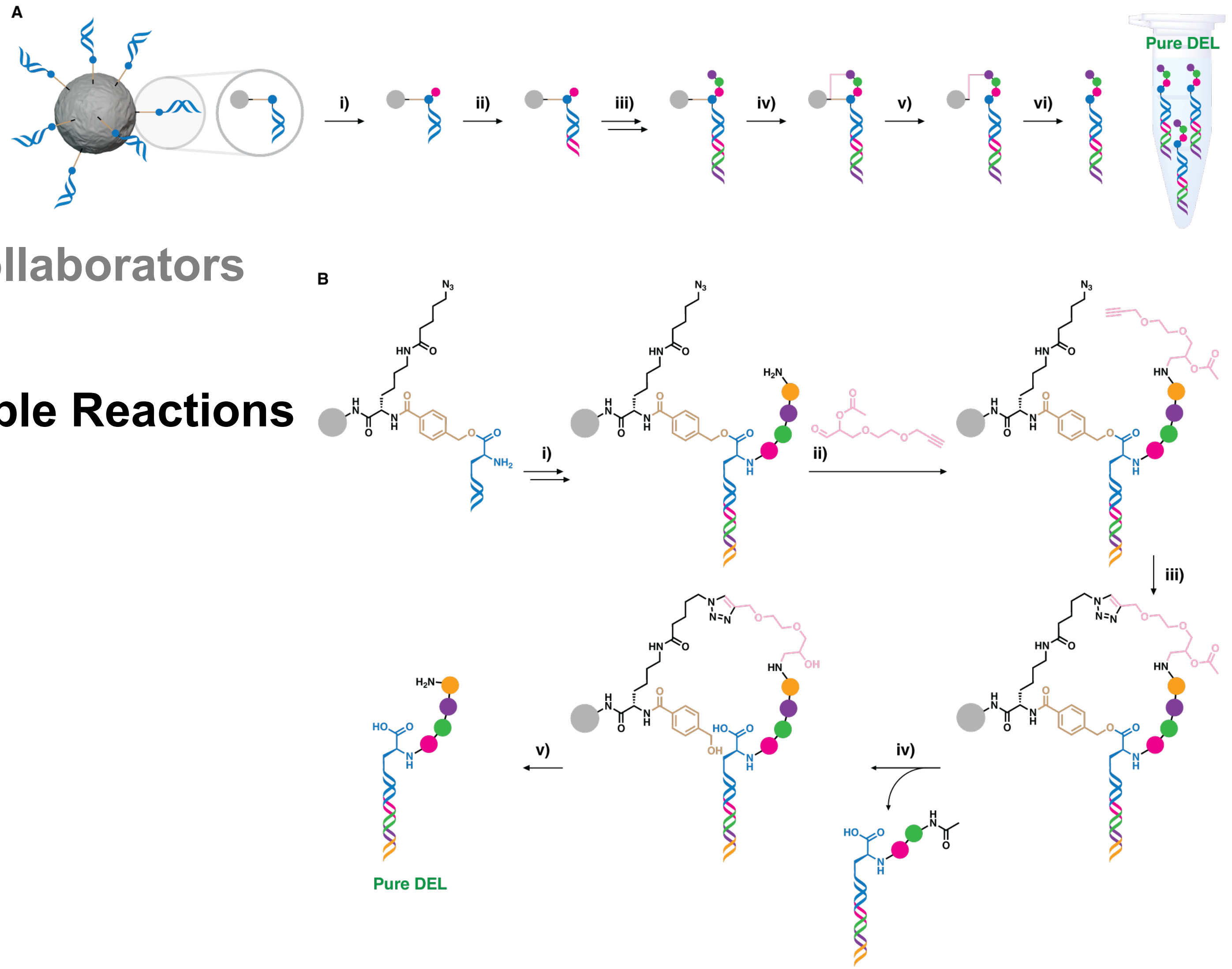

Keller, Petrov et al. (2024) *Science*, in press

DNA-encoded Chemical Libraries @ ETH Zurich

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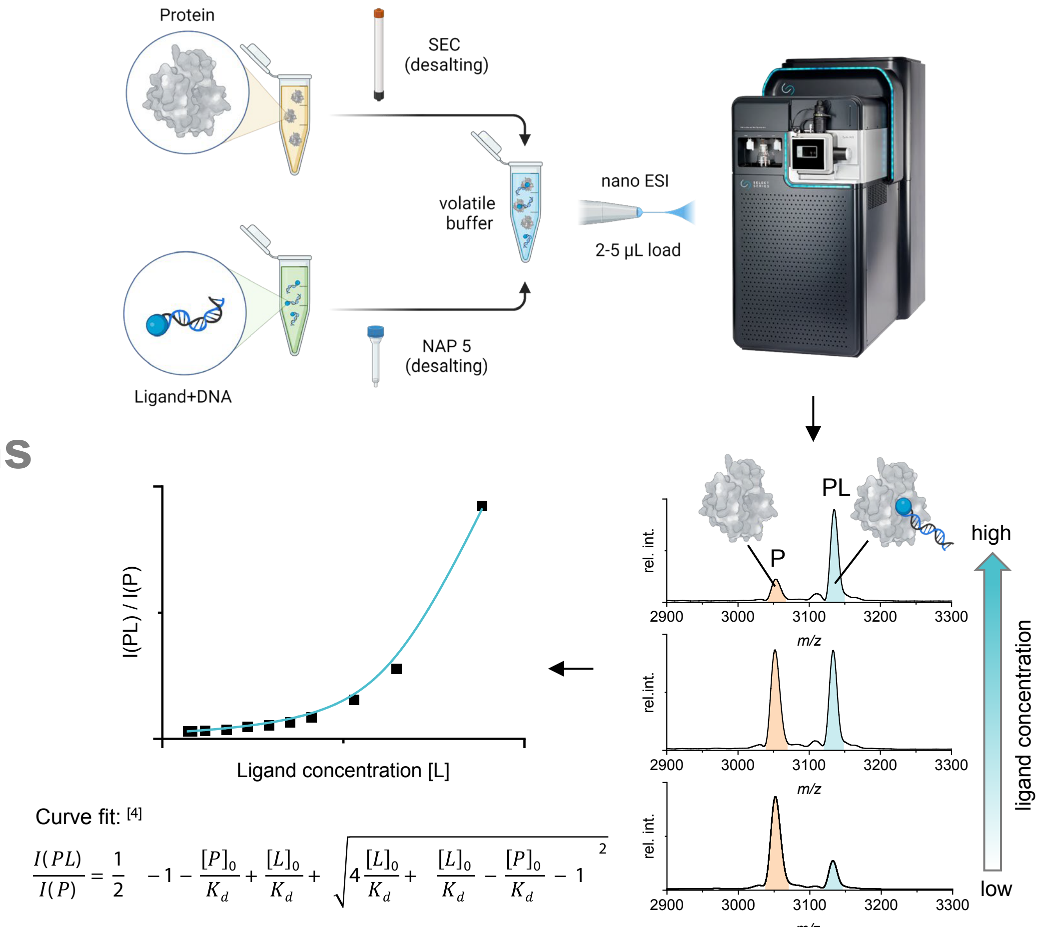
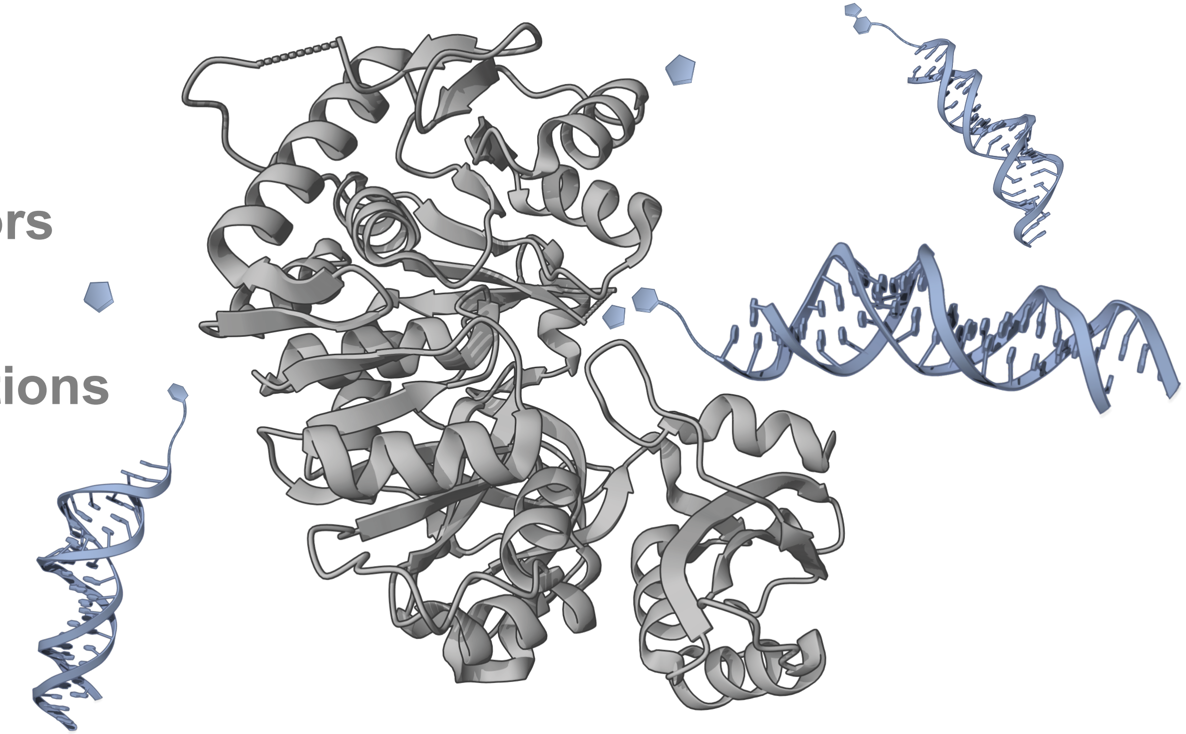


$$\frac{I(PL)}{I(P)} = \frac{1}{2}\left(-1-\frac{[P]_0}{K_d}+\frac{[L]_0}{K_d}+\sqrt{4\frac{[L]_0}{K_d}+\left(\frac{[L]_0}{K_d}-\frac{[P]_0}{K_d}-1\right)^2}\right)$$

Collaboration with the Renato Zenobi's group @ ETH

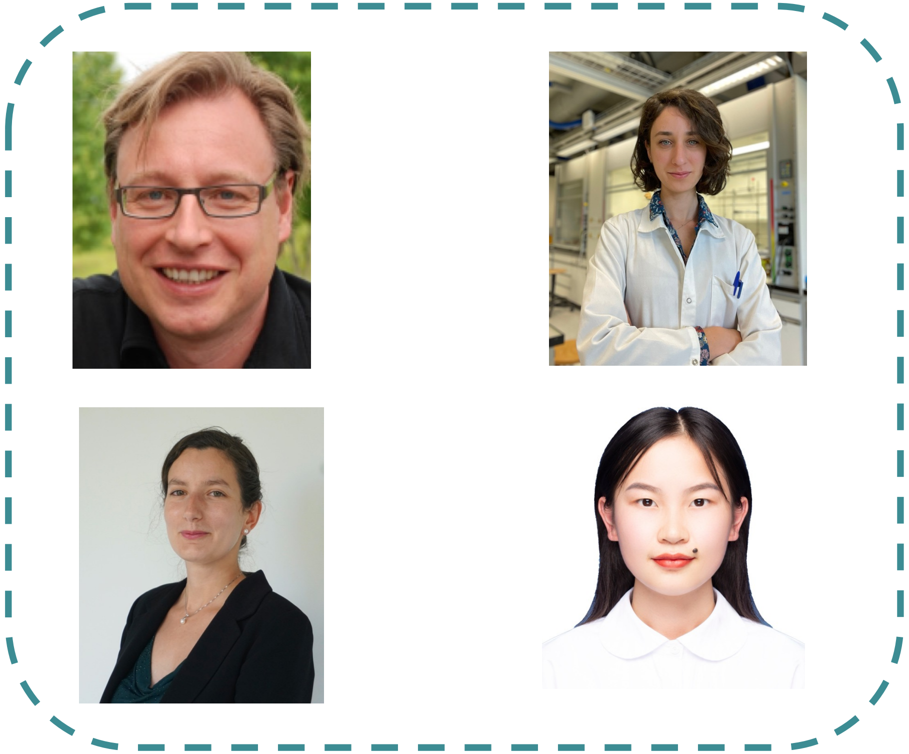
DNA-encoded Chemical Libraries @ ETH Zurich

- Design and Construction of DELs
- Screening for Internal Targets & Collaborators
- Development of new, DNA compatible Reactions
- Hit Validation Strategies
- **Enzymatic Reactions on DNA**

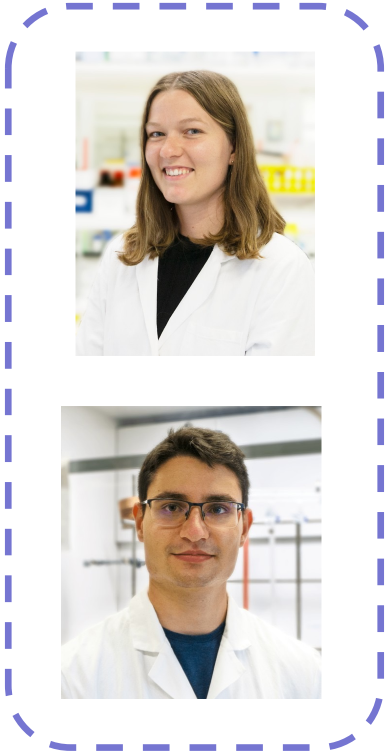


Collaboration with the Rebecca Buller's group @ ZHAW

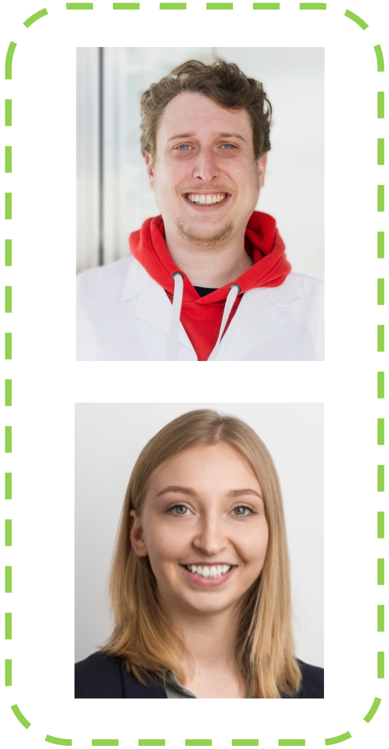
The Scheuermann Lab



Chemists



Pharmacists



Biologists

Current staff:

PI, senior scientist, 2 Postdocs, 5 PhD students, 3 master students

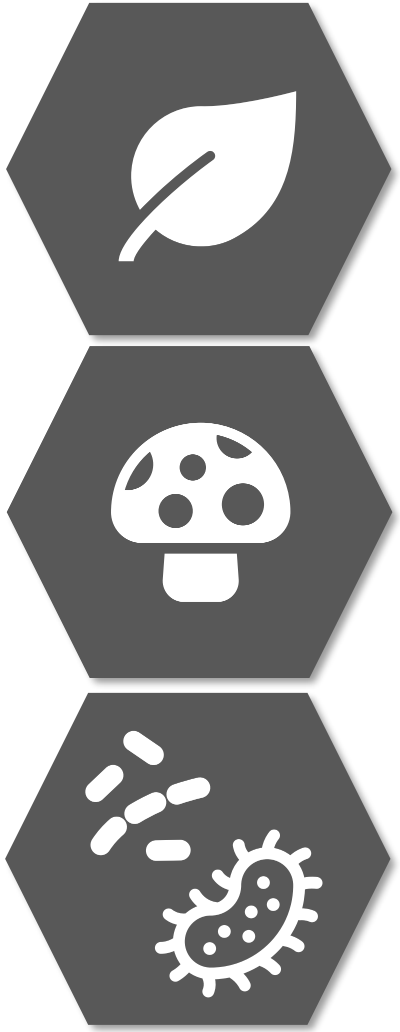
ETH zürich

Novel systems for sustainable biosynthesis of therapeutic natural products

Fraley Research Group
Institute of Pharmaceutical Sciences, ETH Zürich
VCS Research Group Introduction
22. May 2024

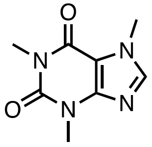
Using biology to amplify the accessible chemical space for medicinal chemistry efforts

Natural products and their impact on our daily lives



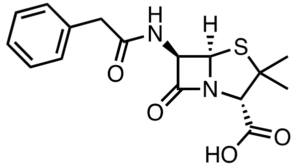
Caffeine
Stimulant

Coffea arabica



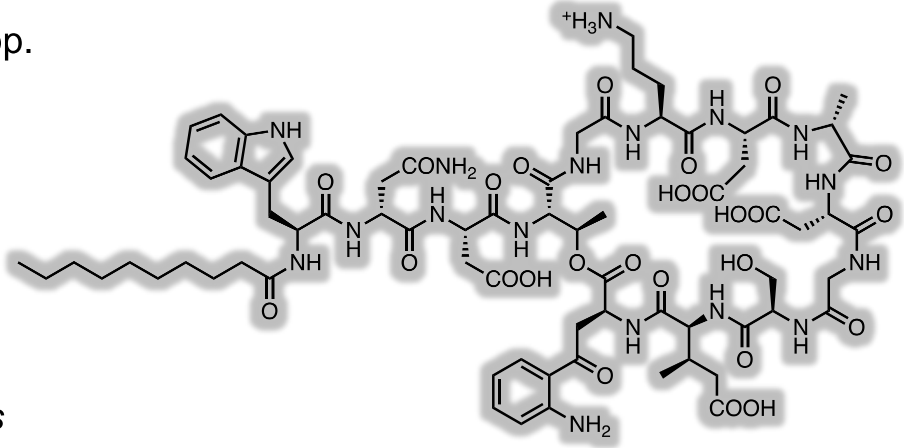
Penicillin
Antibiotic

Penicillium spp.



Daptomycin
Antibiotic

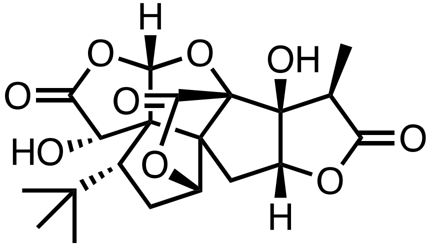
Streptomyces roseosporus

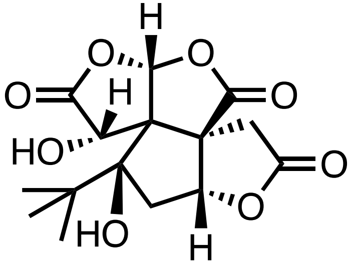


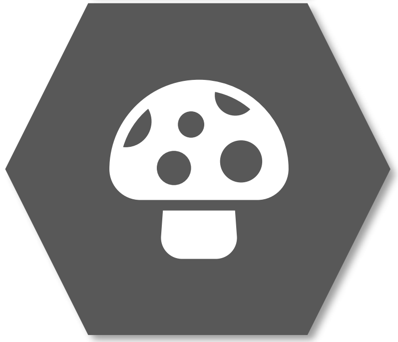
Micklefield, J. *Cell Chem. Biol.* (2004)

Overview and introduction to our research area

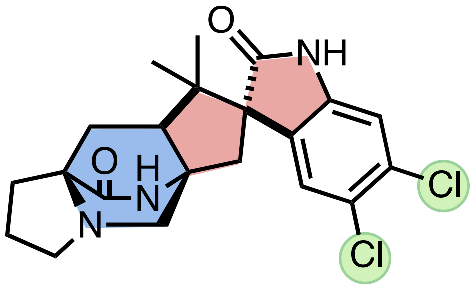
Historical plant-based therapeutics



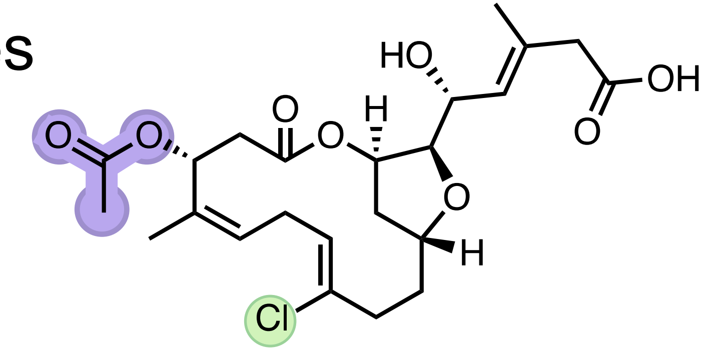


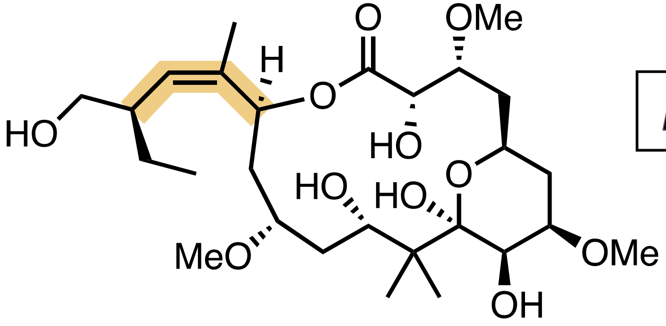


Fungal indole alkaloids

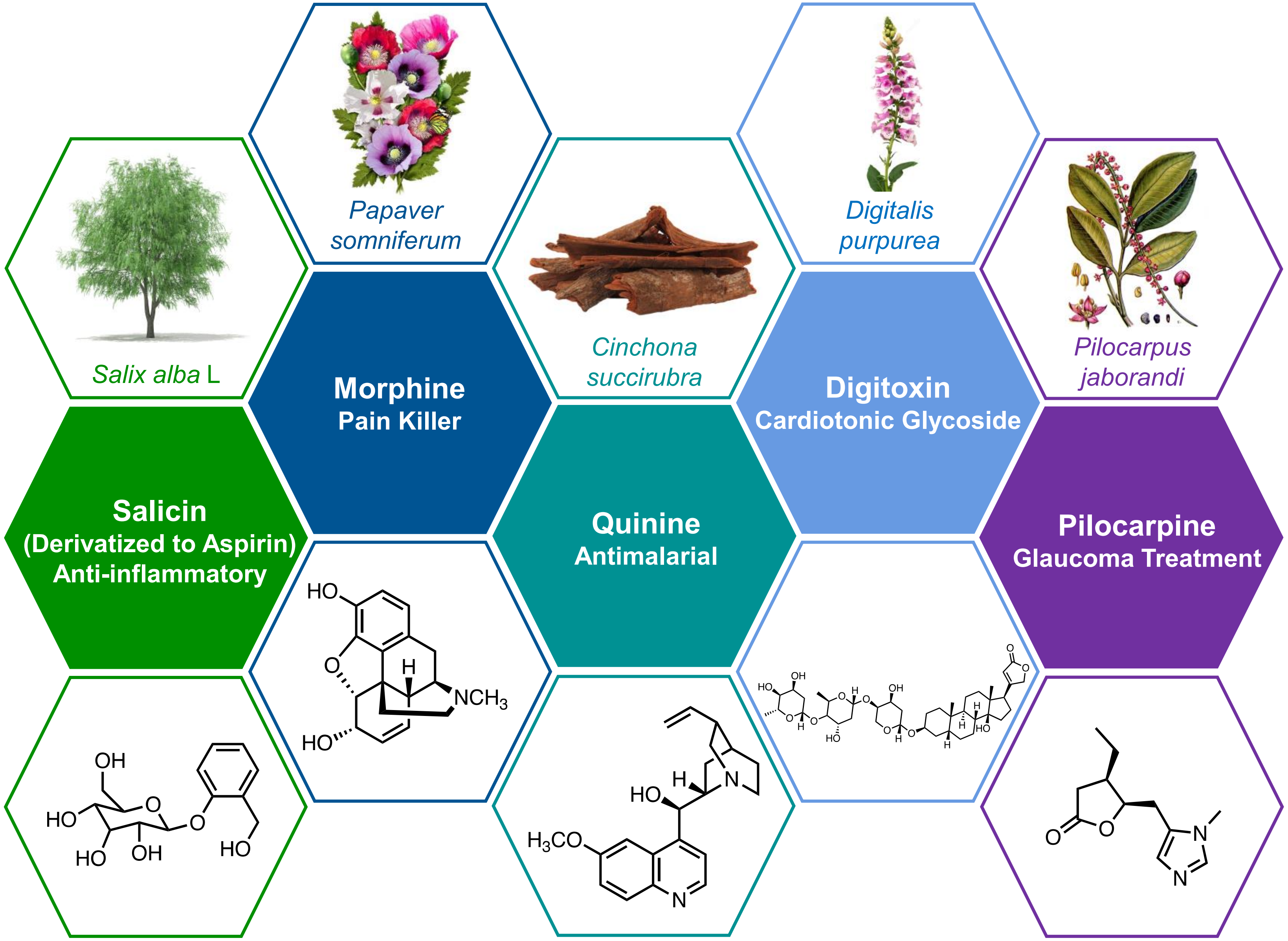


Polyketides from symbiotic bacteria



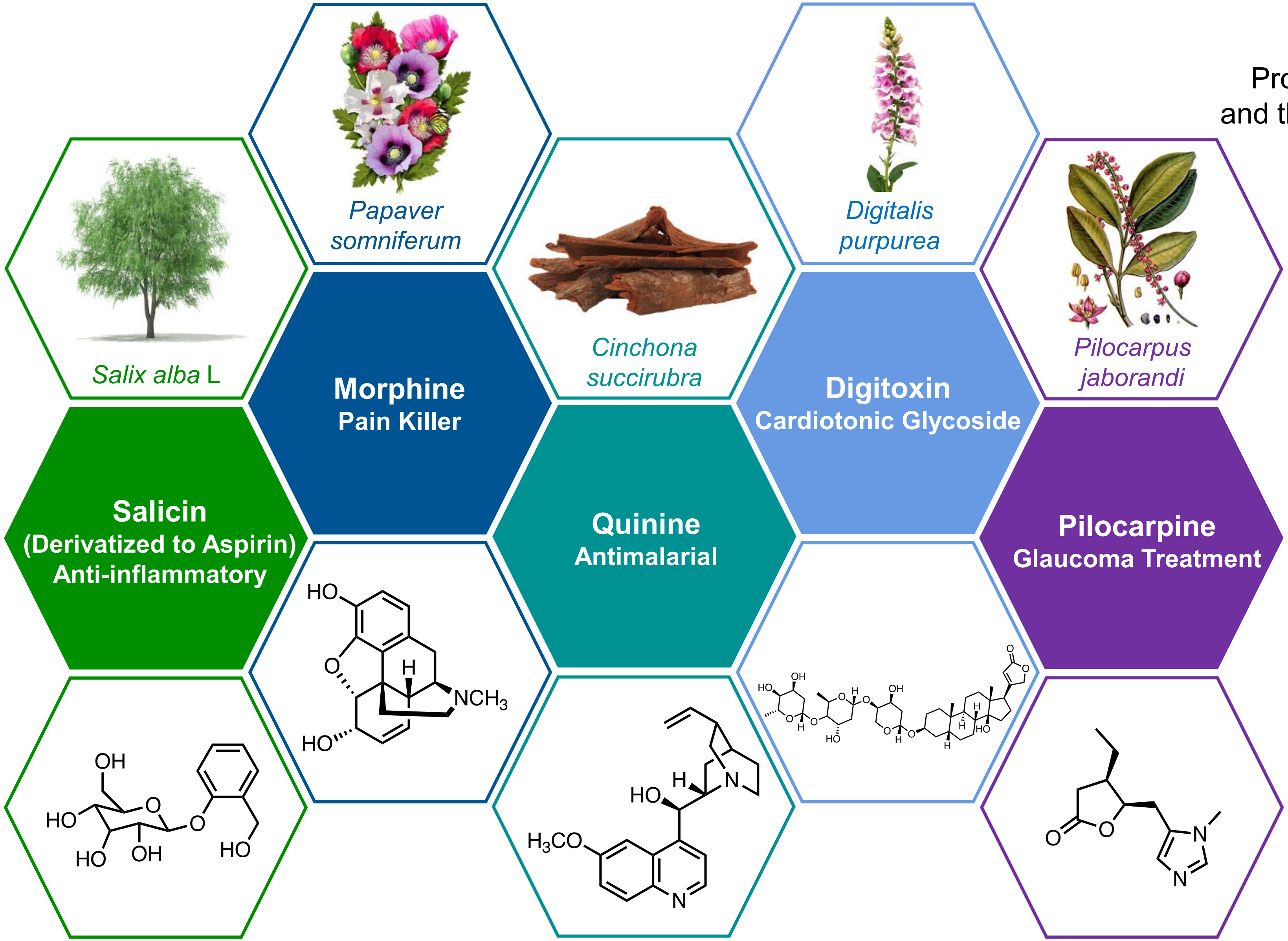


Significance of plant-based medicines

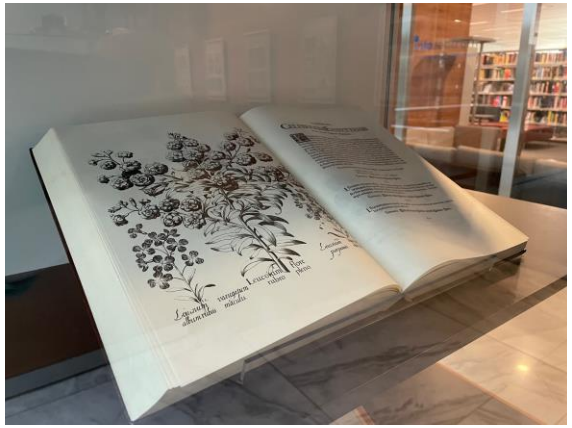


Dias, D. A.; Urban, S.; Roessner, U. *Metabolites.* (2012).

Significance of plant-based medicines



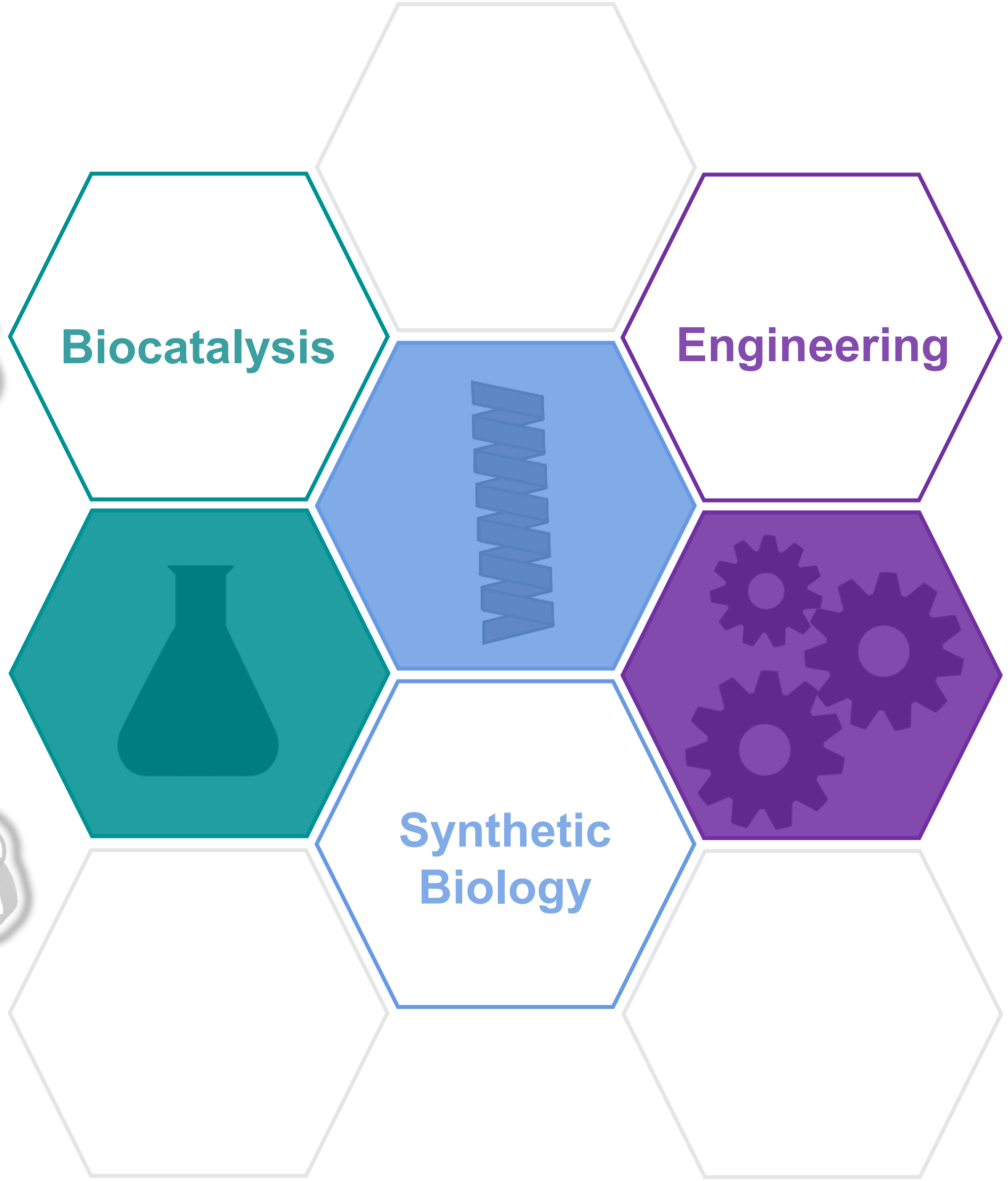
For more information:
Prof. Carl G. Hartwich's Herbal Book Collection
and the Pharmacognostic Collection (both in HCI)



Dias, D. A.; Urban, S.; Roessner, U. *Metabolites.* (2012). https://chab.ethz.ch/en/outreach/collections/pharmacognostic-collection.html

Our approach to sustainable production

Our approach to sustainable production

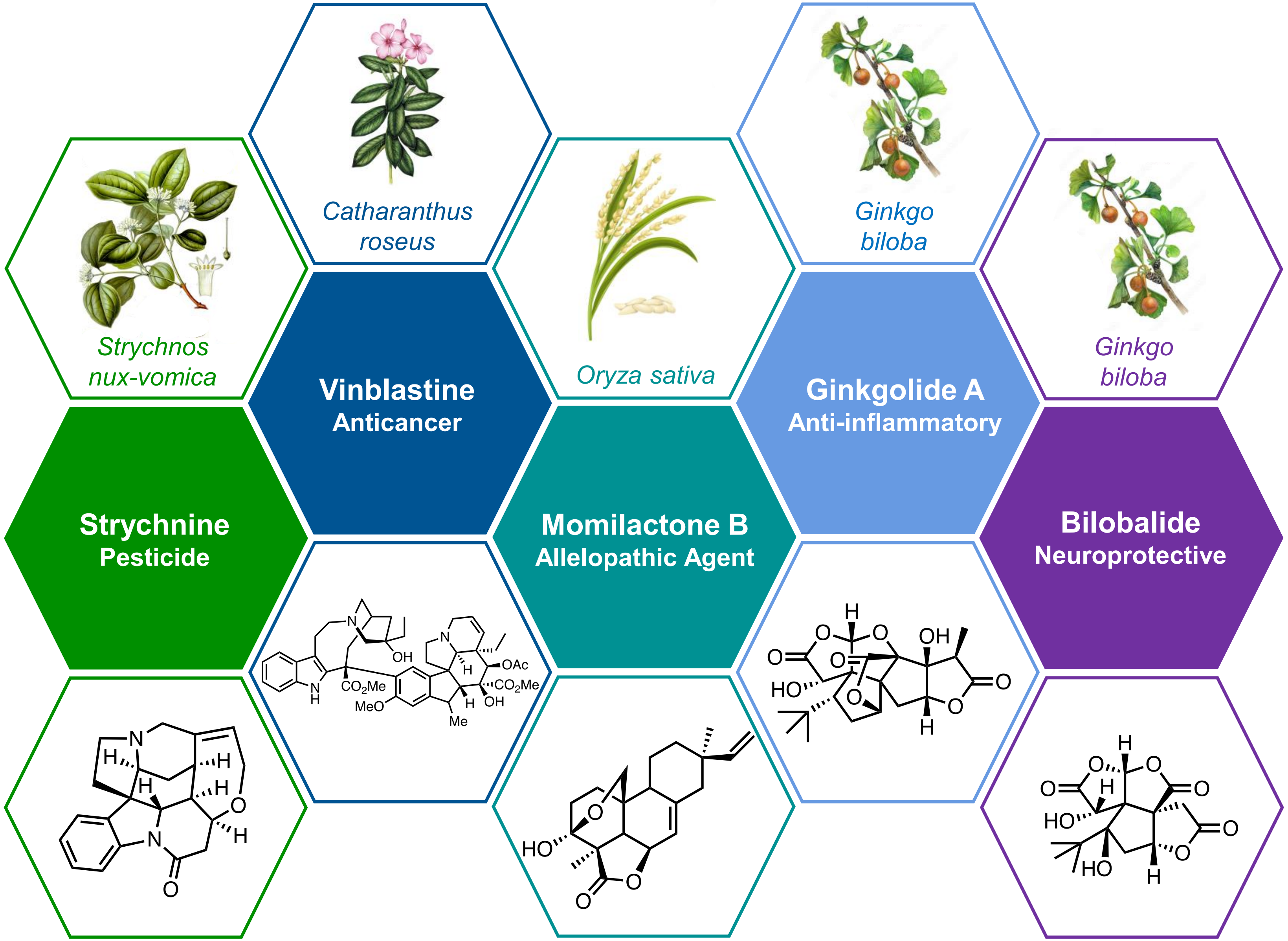


Environmentally friendly chemistry

Efficient and Selective reactions

Sustainable production of bioactive molecules

Coming full circle on the way to sustainable biotechnology

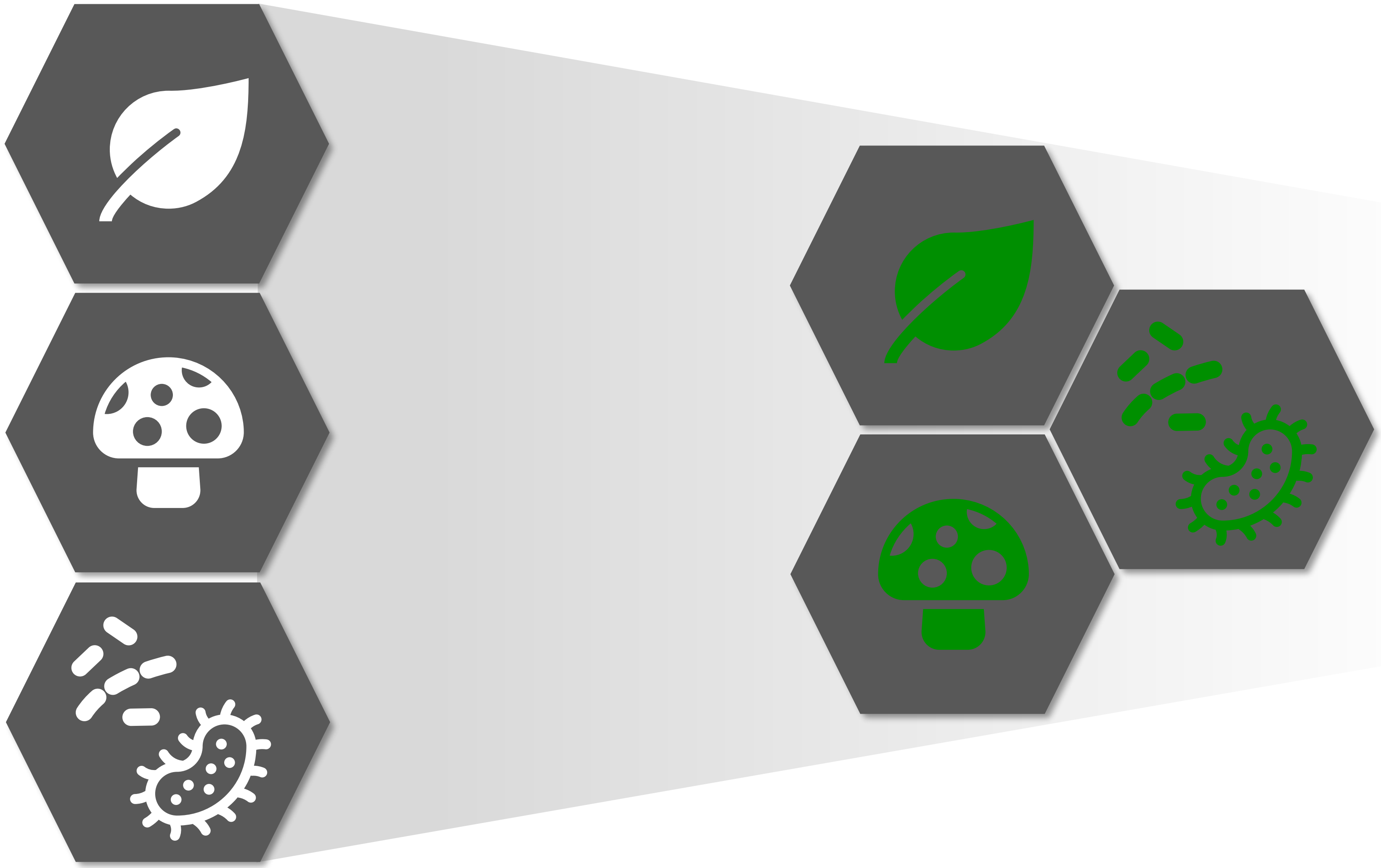


Our team has discovered a laboratory cultivable plant source for complex bioactive terpenoids.

- Heterologous system for challenging enzymatic targets such as plant cytochromes P450.
- Subsequent biochemical discovery and engineering for terpene diversification.
- Opens avenues for biotechnological production of plant-based therapeutics.

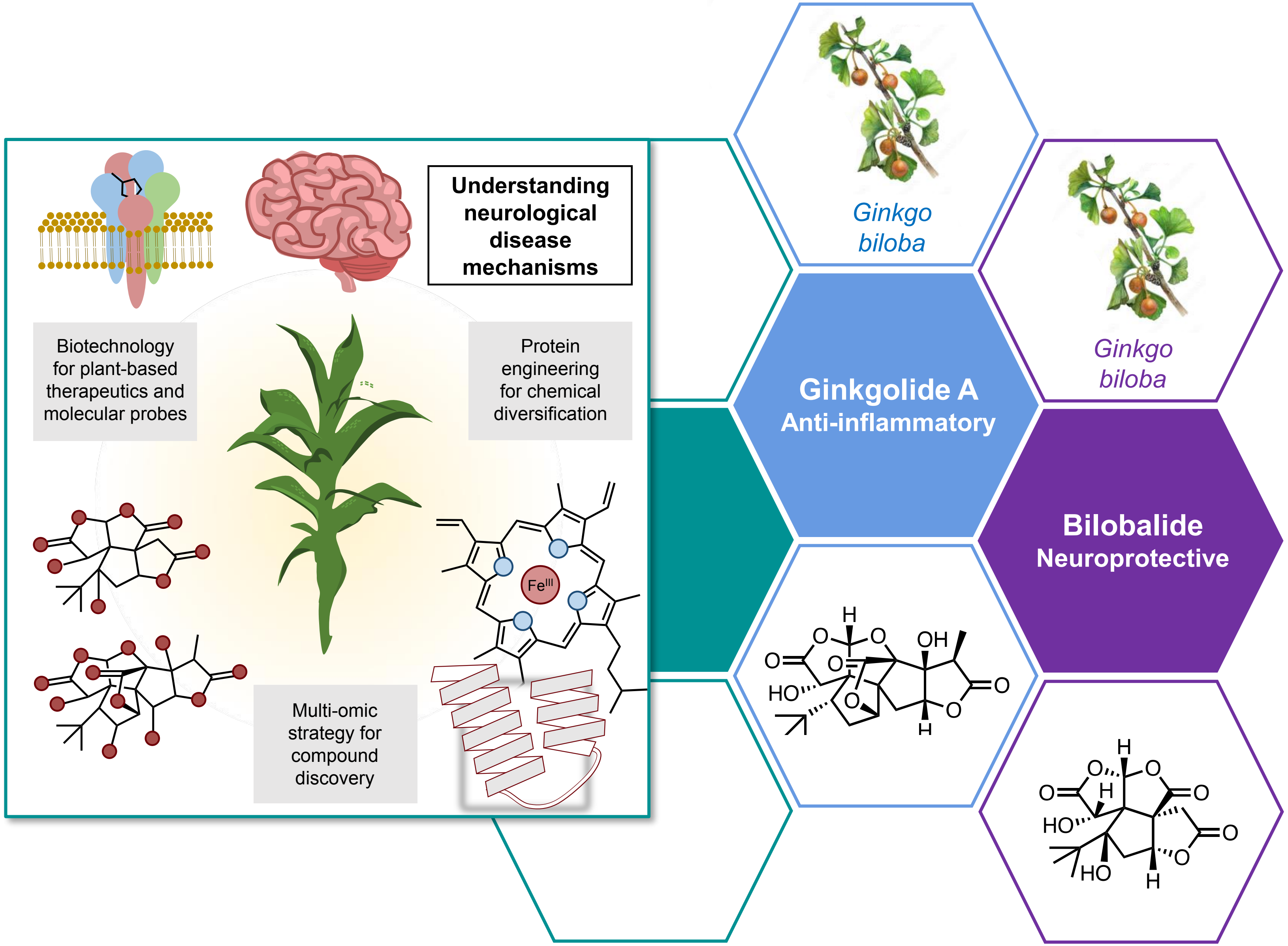
Hong, B.; Grzech, D.; Caputi, L.; Sonawane, P.; et al. *Nature*. (2022). Caputi, L.; Franke, J.; Farrow, S.C.; et al. Science. (2018)
Mao, L.; Kawaide, H.; Higuchi, T.; et al. *Proc. Natl. Acad. Sci.* (2020). Forman, V.; Luo, D.; Geu-Flores, F.; Lemcke, R.; et al. *Nat. Commun.* (2022).

Coming full circle on the way to sustainable biotechnology



Leveraging plant defensive mechanisms and microbial interactions for sustainable terpenoid chemistry

Ginkgolides as a prime target for biotechnological production

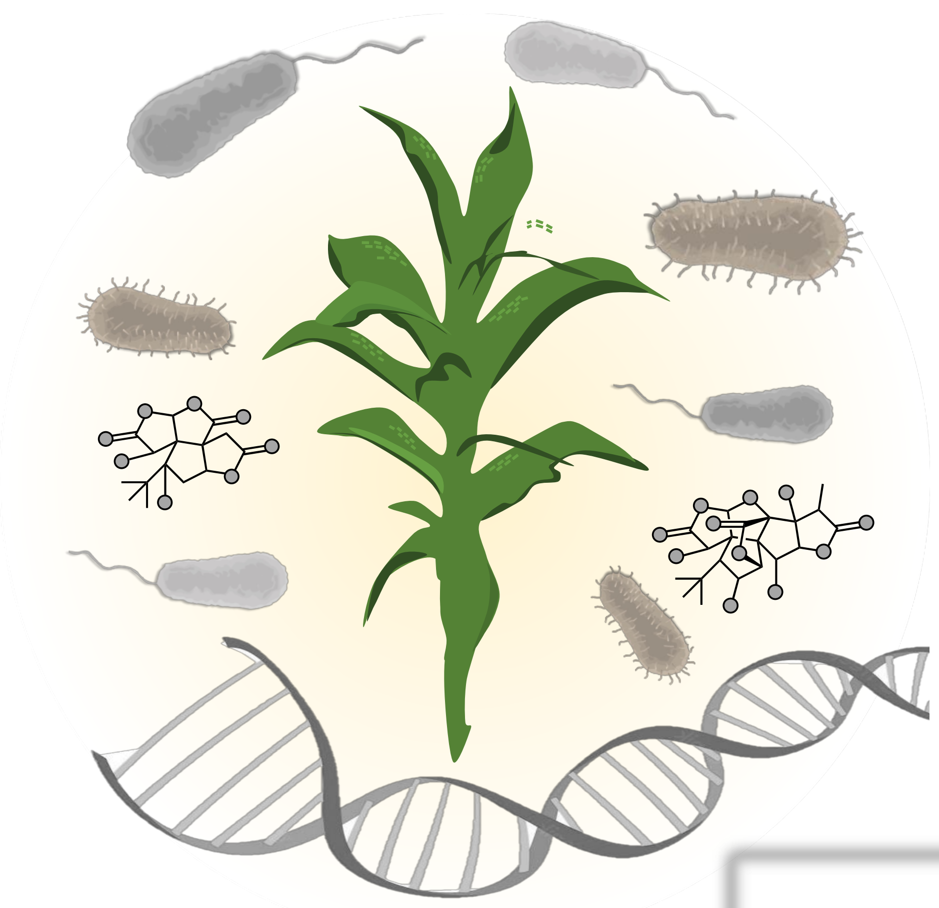


Ginkgo extract is one of the most popular natural supplements consumed worldwide, valued at over 10 bn USD.

Our biotechnology platform will produce its main constituents in a more sustainable manner.

Hong, B.; et al. *Nature*. (2022). Caputi, L.; et al. Science. (2018). Mao, L.; et al. *Proc. Natl. Acad. Sci.* (2020). Forman, V.; et al. *Nat. Commun.* (2022). Horn, A.; Pascal, A.; Lončarević, I. *Crit. Rev. Plant Sci*. (2021)

Acknowledgements for preliminary plant biotechnology projects



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Austausch und Mobilität
Echanges et mobilité
Scambi e mobilità
Exchange and mobility

ETH zürich

UNESCO BIOSPHÄRE
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LUZERN SCHWEIZ

For more information please see the Fraley Group website: **https://fraley.ethz.ch/**