

Computational Photophysics



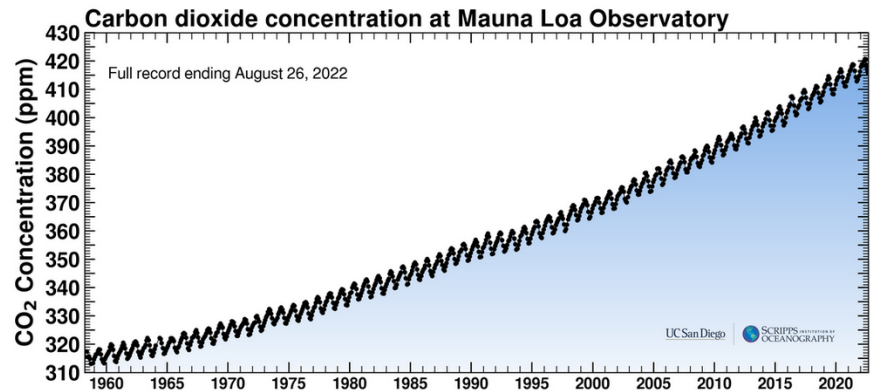
(links -> rechts: Gabriel Schöpfer, Dominik Jank, Jutta Schnizer, Rizalina Saragi, MO)

Milan Ončák

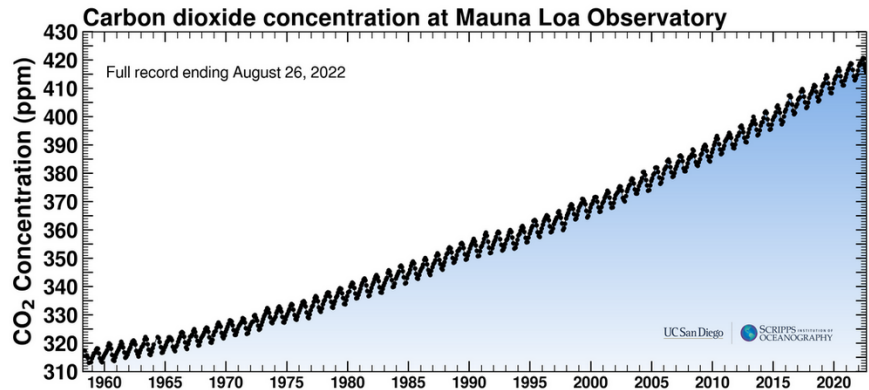
Institut für Ionenphysik und Angewandte Physik

11.1.2023, Bachelorarbeit-Präsentation

Klimawandel und die Rolle der Universitäten



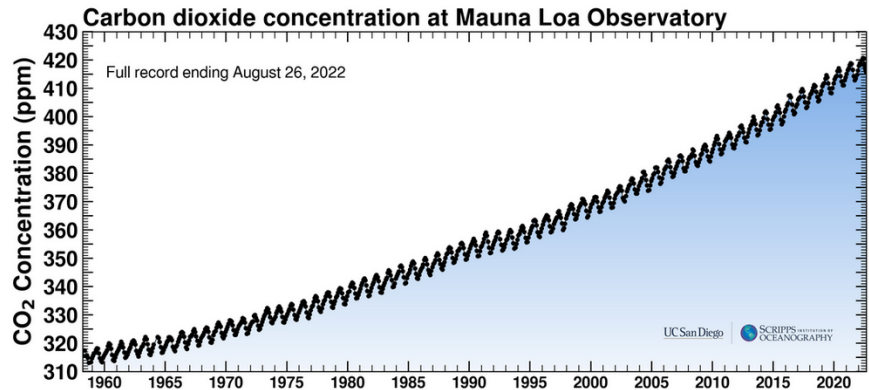
Klimawandel und die Rolle der Universitäten



Der einfacher Weg

- **Aufhören oder mindestens limitieren...**
 - ... Konsum von Fleisch und Tierprodukten
 - ... Fliegen
 - ... Nutzung von Autos
 - ... Kaufen neuer Elektronik, Kleidung usw.
- **Weniger Energieverbrauch**

Klimawandel und die Rolle der Universitäten



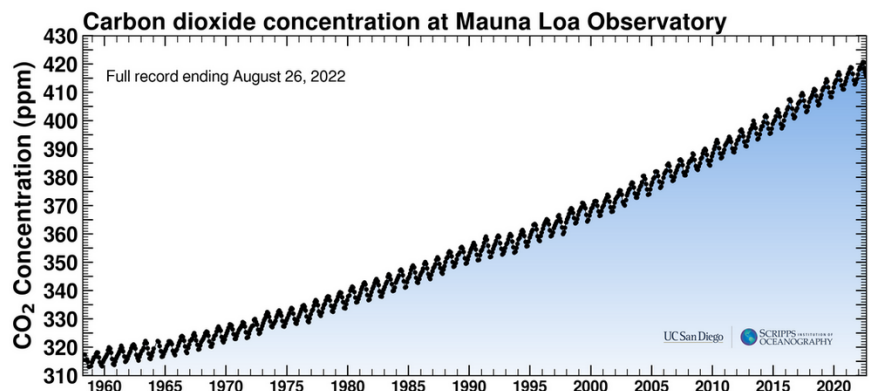
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Der harte Weg

- CO₂-Capture/Aktivierung
- Geoengineering
- Neue Energiequellen
- Entsäuerung der Meere
- Beeinflussung der atmosphärischen Chemie
- Effizientere chemische Prozesse
- ...

Klimawandel und die Rolle der Universitäten

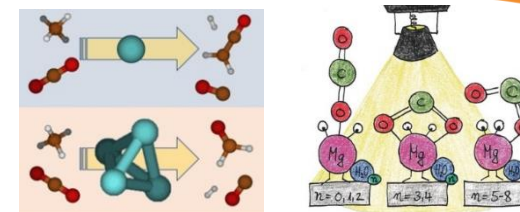


Der einfacher Weg

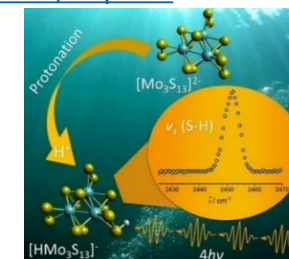
- Aufhören oder mindestens limitieren...
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Der harte Weg

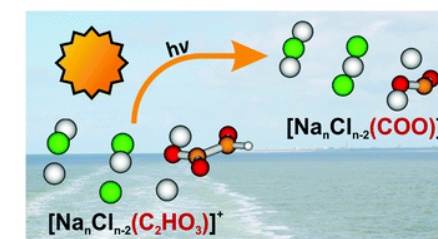
- CO₂-Capture/Aktivierung
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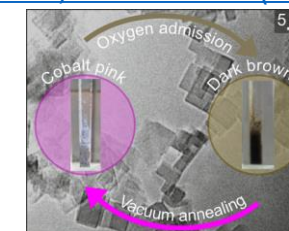
Angew. Chem. Int. Ed. 59, 7467-7471 (2020)
Chem. Eur. J., in press



Angew. Chem. Int. Ed., 60, 5074-5077 (2021)

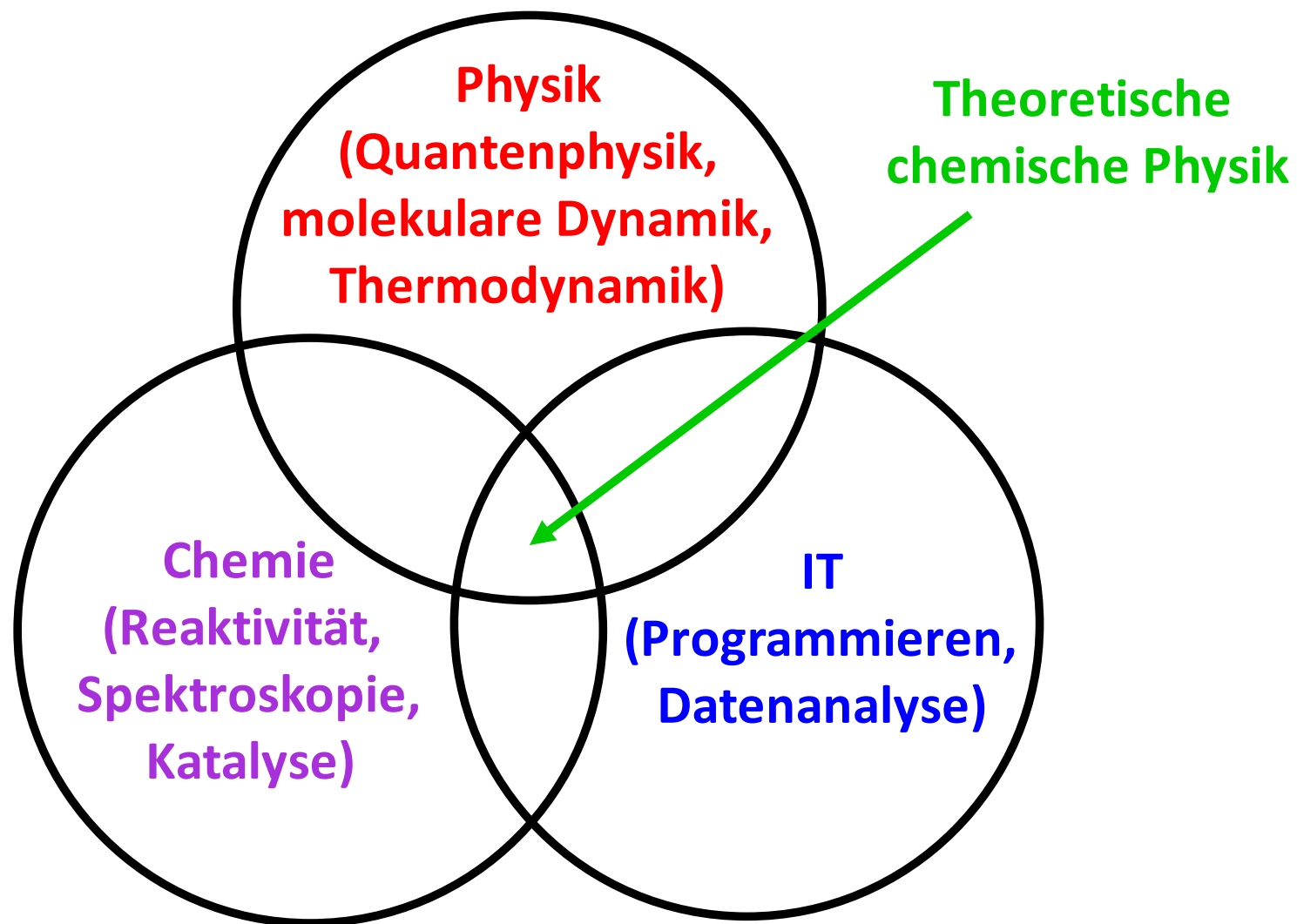


Phys. Chem. Chem. Phys. 20, 8143-8151 (2018)
Chem. Eur. J. 24, 12433-12443 (2018)

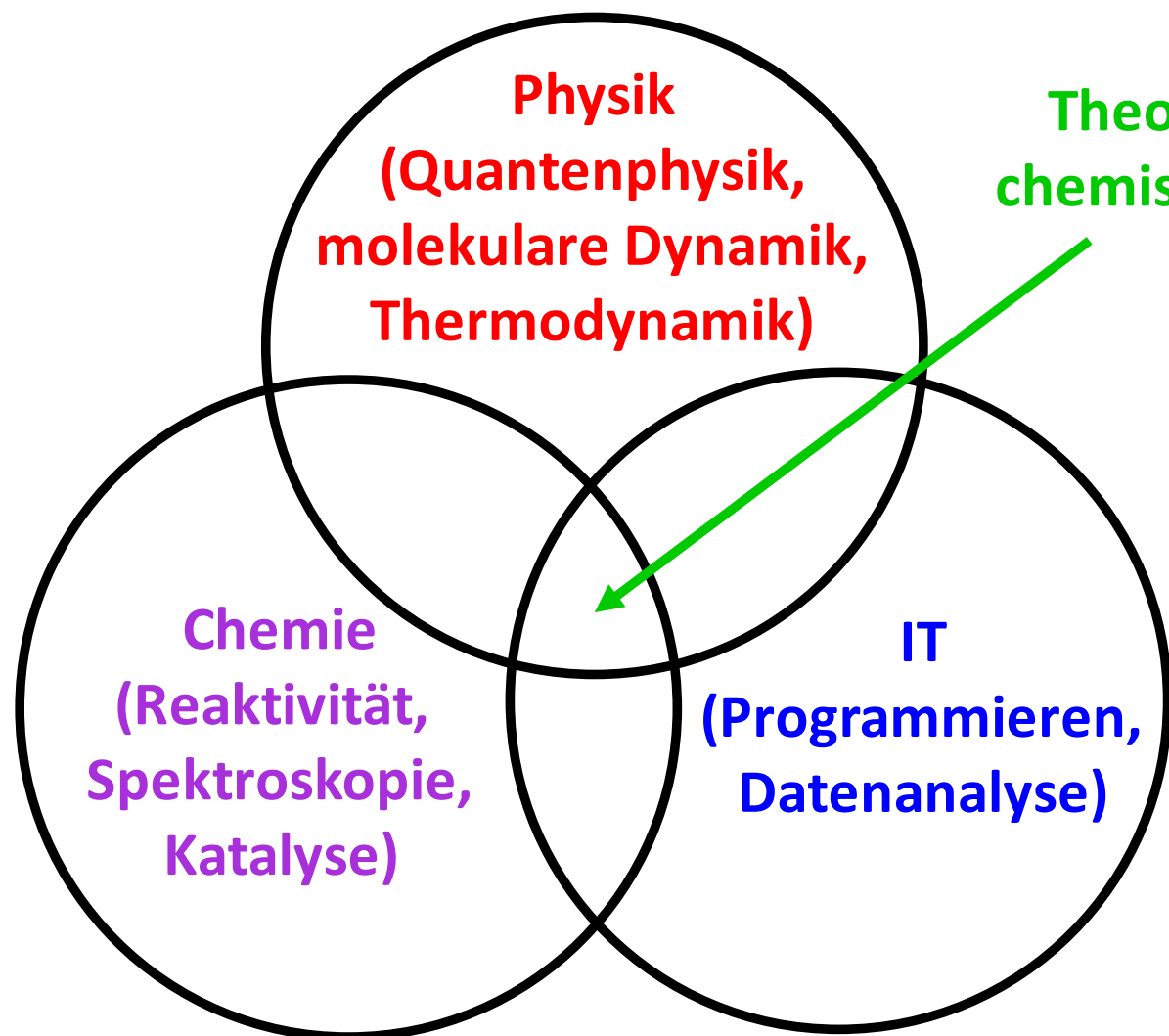


Chem. Eur. J., 26, 16049-16058 (2020)

Theoretische chemische Physik



Theoretische chemische Physik



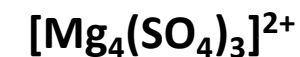
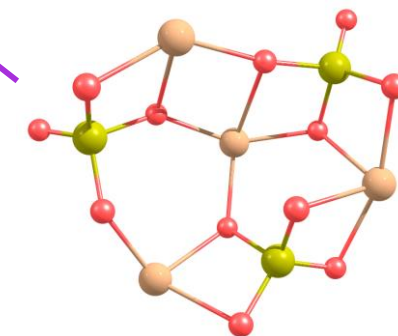
Theoretische
chemische Physik

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%nproc=14  
#BLYP/6-31g* scf=xqc DensityFit opt freq
```

comment

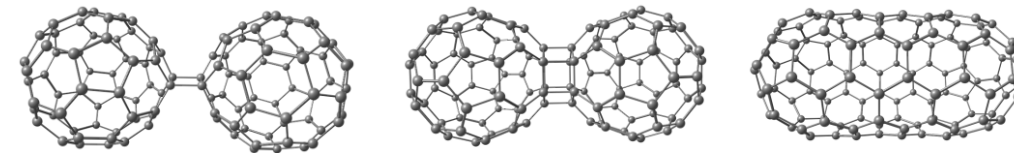
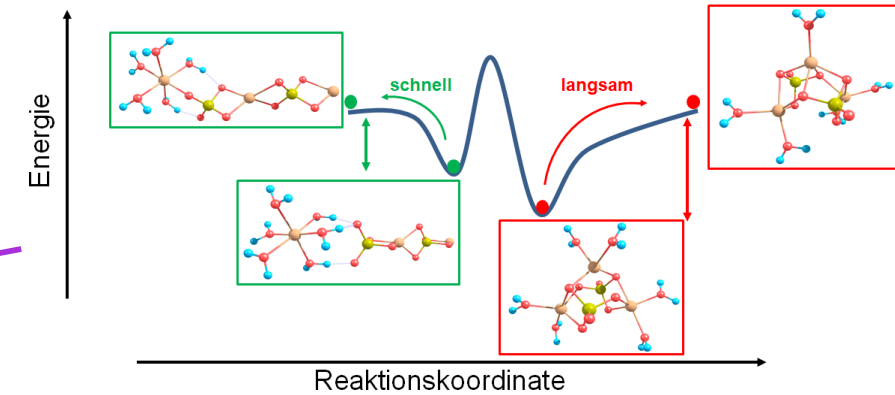
```
2 1  
O 2.512941 -1.671005 1.332481  
S 2.859590 -0.958565 0.019818  
O 2.861521 0.547767 0.279037  
Mg 2.205838 2.247039 -0.215428  
O 0.650547 3.206772 0.664220  
S -0.400592 2.272419 0.137839  
O 0.376747 1.611476 -1.079963  
O 4.006325 -1.425428 -0.704969  
O 1.477604 -1.271636 -0.761095  
Mg -0.188554 -0.339209 -1.199816  
O -0.959949 -1.852424 0.176473  
S -2.484257 -1.491221 -0.093930  
O -3.062284 -0.768880 1.102681  
O -2.204566 -0.252419 -1.073976  
O -0.734226 1.110248 1.053581  
O -1.727298 2.831269 -0.265149  
O -3.209540 -2.592617 -0.653979  
Mg -2.752237 1.109989 0.457234  
Mg 0.776751 -2.430077 0.826812
```

$$\hat{H}_{el}\Psi = E_{el}\Psi$$

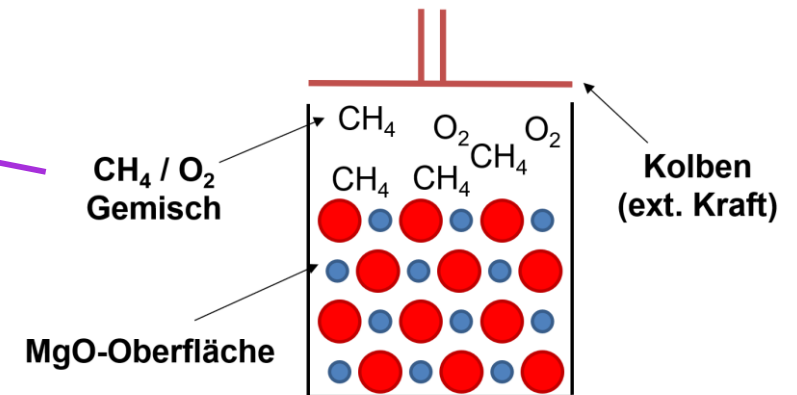


Ein paar mögliche Themen...

- Eigenschaften, Reaktivität und Dissoziation der Aerosole: $Mg_{n+1}(SO_4)_n(H_2O)^{2+}$, $[Pyruvat.Na_{n+2}Cl_n]^+$
- Wasserstoffentwicklung in $Zn^+(H_2O)_n$
- Genetische Algorithmen + Machine Learning: Effiziente Erkundung des Molekülraums
- *Nanoreaktor*: Effiziente Simulation der Phasenübergänge im Festkörper
- Der Alptraum der elektronischen Struktur: Astrochemisch relevante C_n^+ -Cluster



Wie sieht ein Fulleren-Dimer aus?



Neue Gruppe Erath-Dulitz

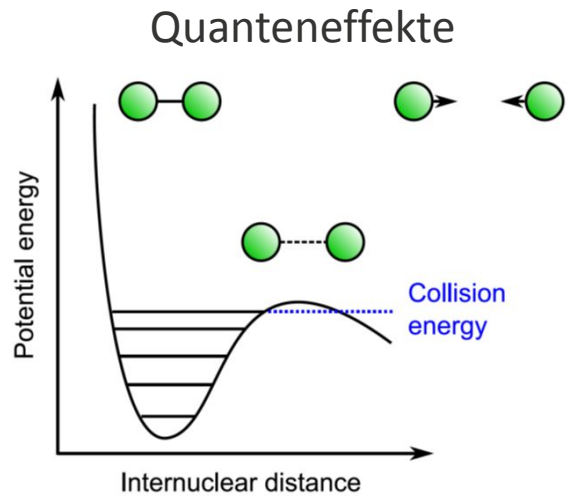
Gruppenretreat Wester-Gruppe, Matri a. Br. 2022



Kontakt:
katrin.erath-dulitz@uibk.ac.at

Forschungsinteressen

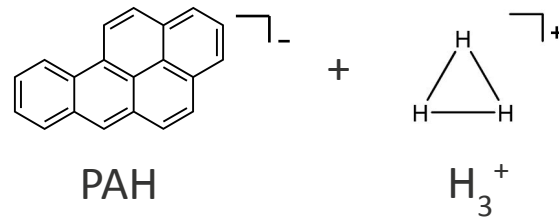
Produktion kalter Moleküle □ Chemie nahe 0 K



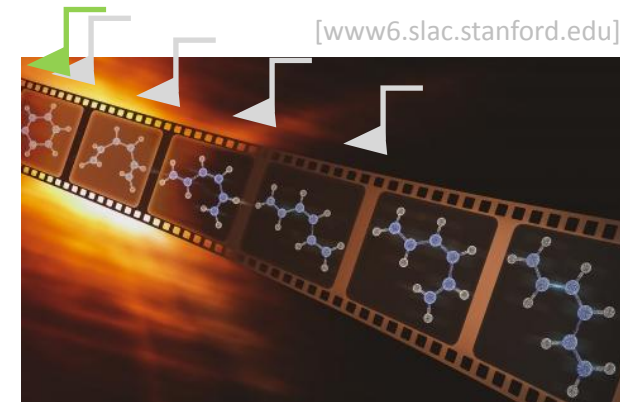
Chemie im All



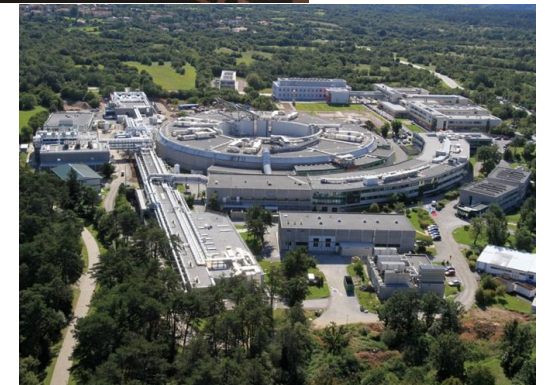
[Yury Dmitrienko]



Zeitaufgelöste Dynamik chemischer Reaktionen auf ultrakurzen Zeitskalen

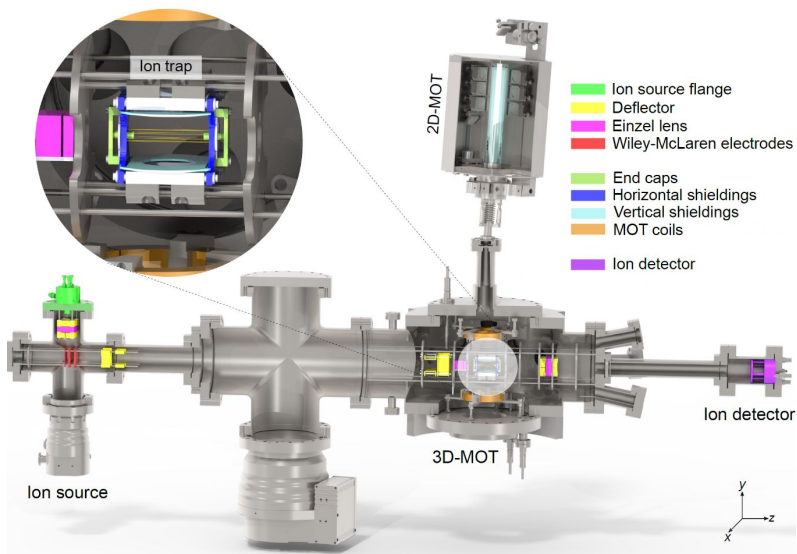


Freie-Elektronen-Laser FERMI, Triest

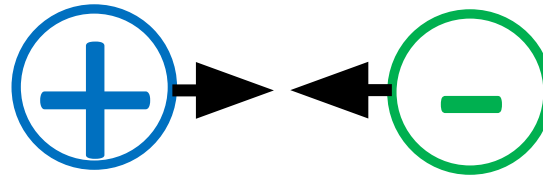


Aktuelle Forschungsthemen

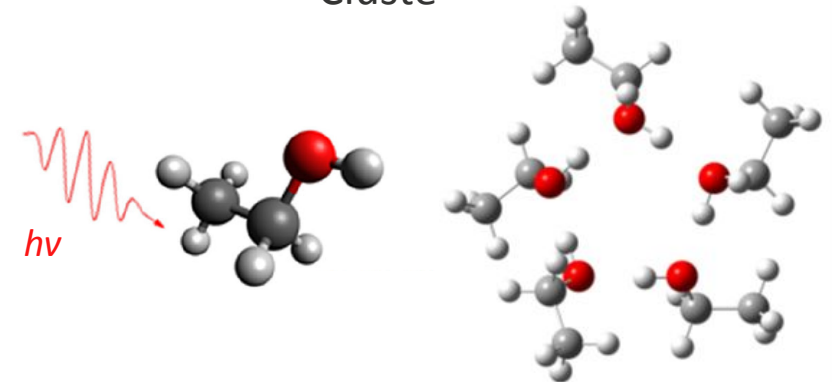
Kühlung von Ionen durch
Stöße mit ultrakalten Atomen



Kinetik von Reaktionen
zwischen Kationen und Anionen

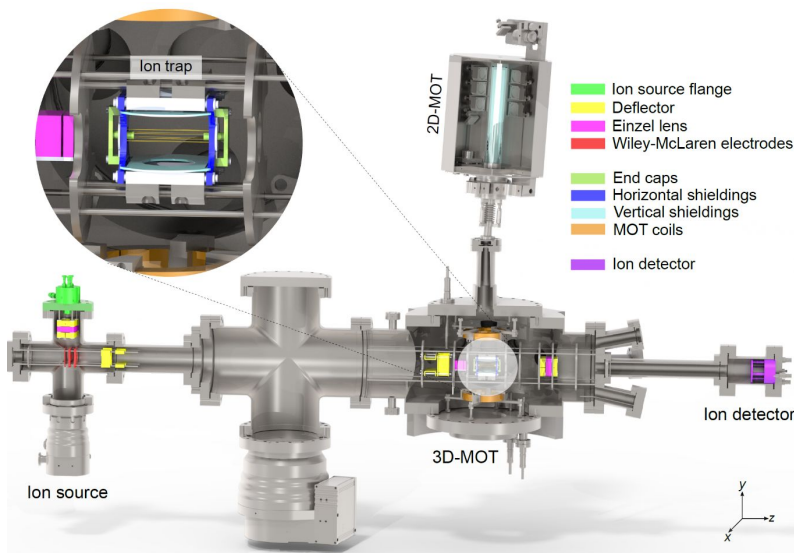


Zeitaufgelöste Spektroskopie zur
Reaktions-dynamik von Molekülen und
Clustern

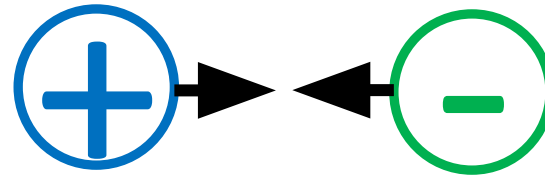


Mögliche Themen für Bachelorarbeiten 2023

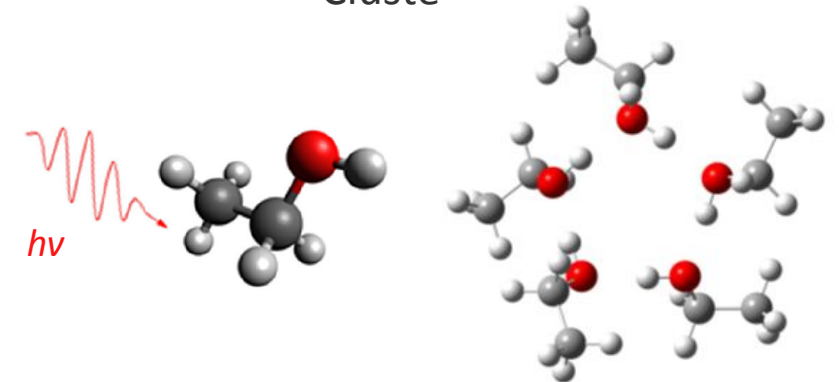
Kühlung von Ionen durch Stöße mit ultrakalten Atomen



Kinetik von Reaktionen zwischen Kationen und Anionen

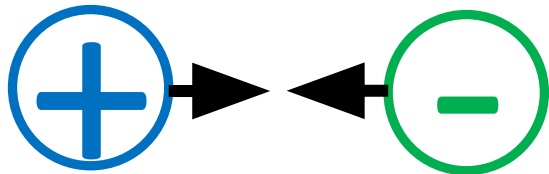


Zeitaufgelöste Spektroskopie zur Reaktions-dynamik von Molekülen und Clustern

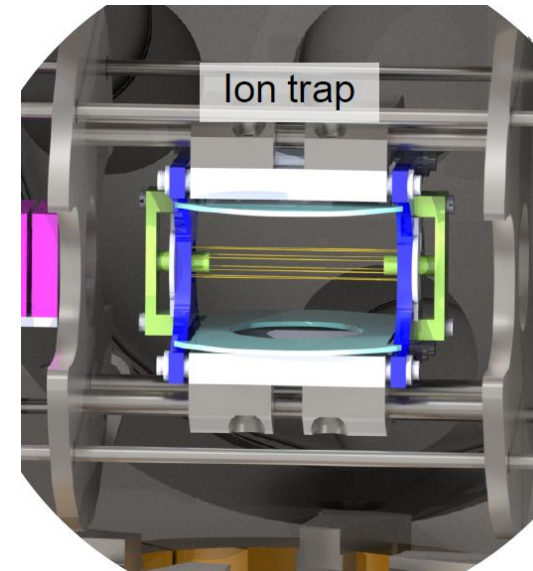


Mögliche Themen für Bachelorarbeiten 2023

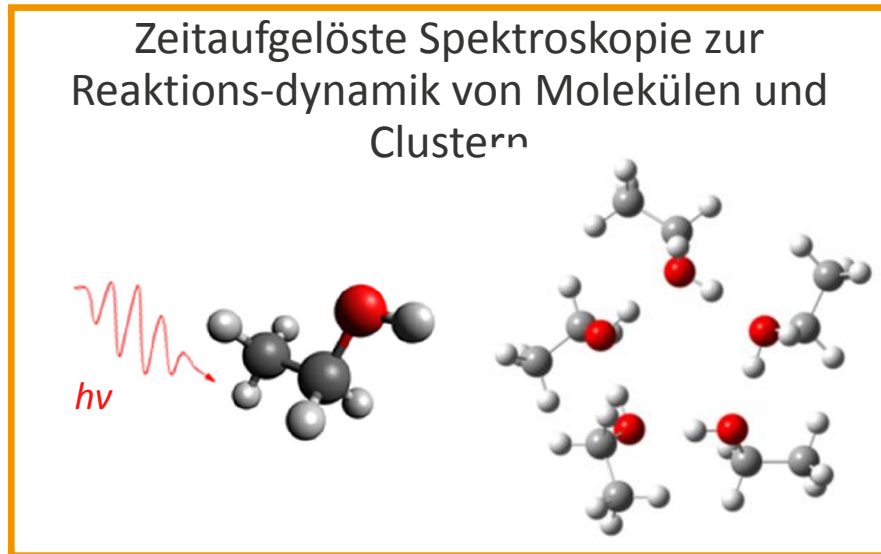
Kinetik von Reaktionen
zwischen Kationen und Anionen



Bestimmung von experimentellen
Parametern für eine Ionenfalle

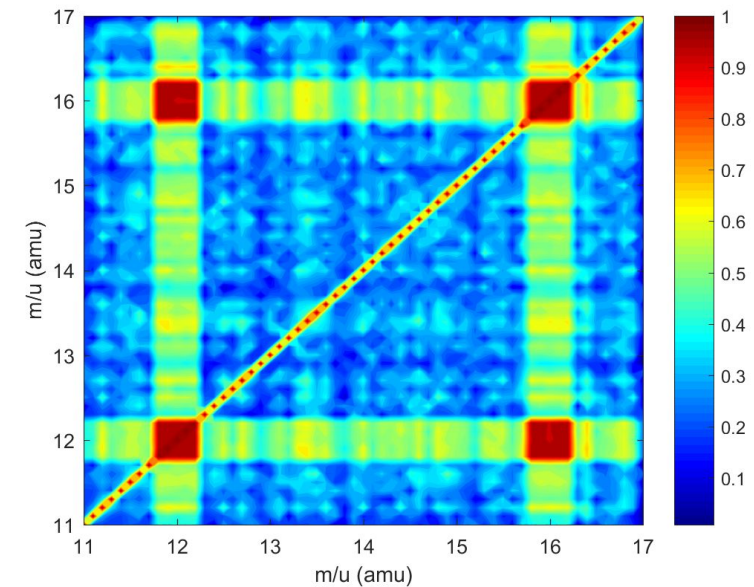


Mögliche Themen für Bachelorarbeiten 2023



Kovarianzanalyse von experimentellen Daten aus einer Strahlzeit

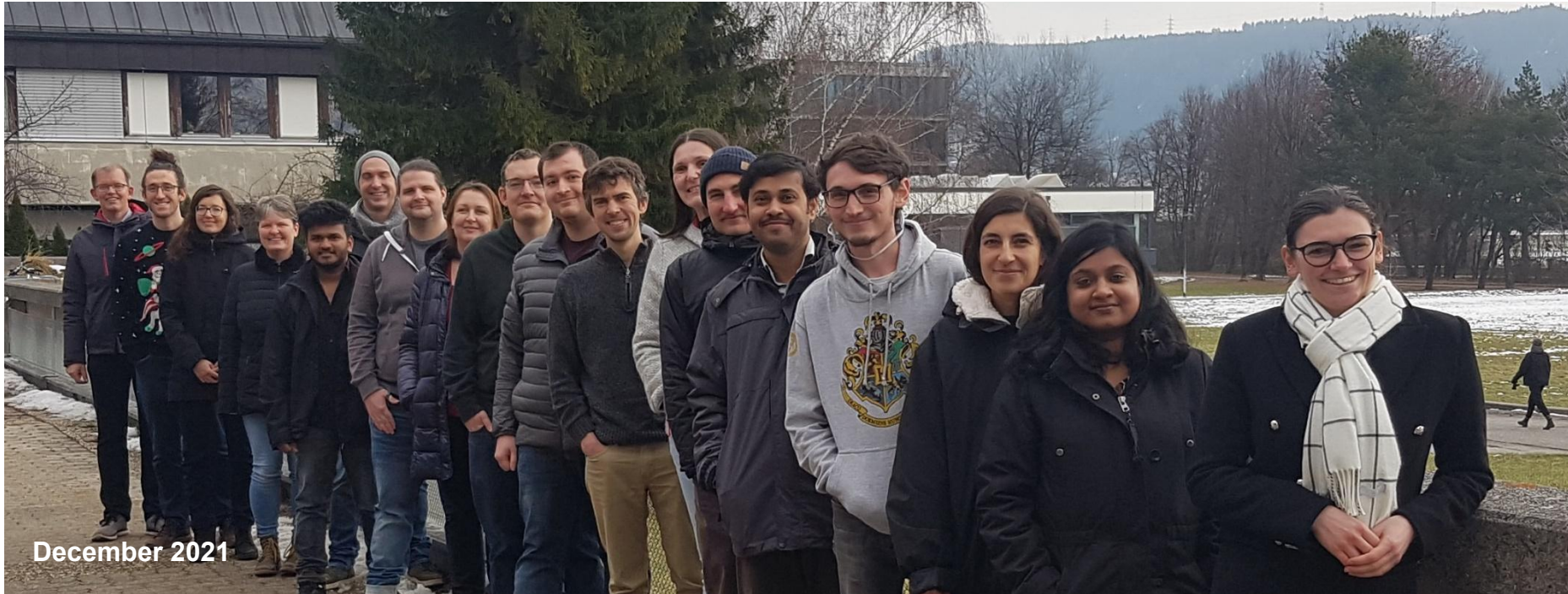
Beispiel: $\text{CO}^{2+} \rightarrow \text{C}^+ + \text{O}^+$



**Vielen Dank für die
Aufmerksamkeit!**



Molecular Systems group

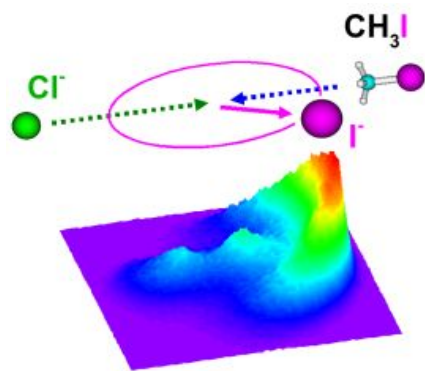


**Our research focus:
Quantum effects in the structure and interaction
of molecules and ions**

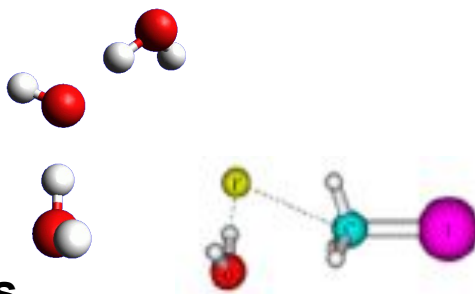


Dynamics and Spectroscopy of Charged Molecular Systems

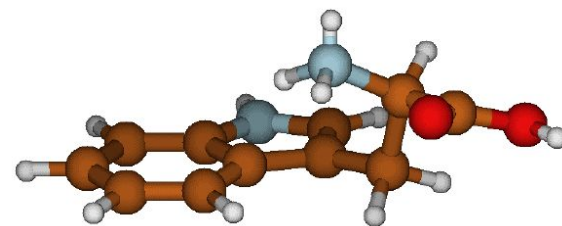
Ion-molecule reaction dynamics



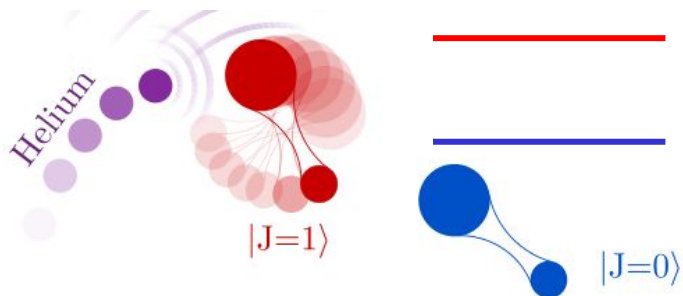
Micro-hydration effects



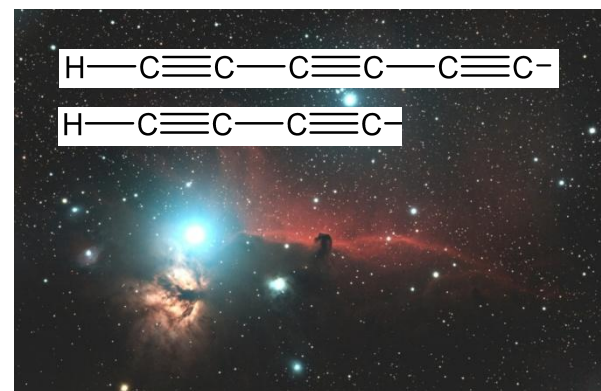
Biomolecular ions



Cold and state-controlled ions

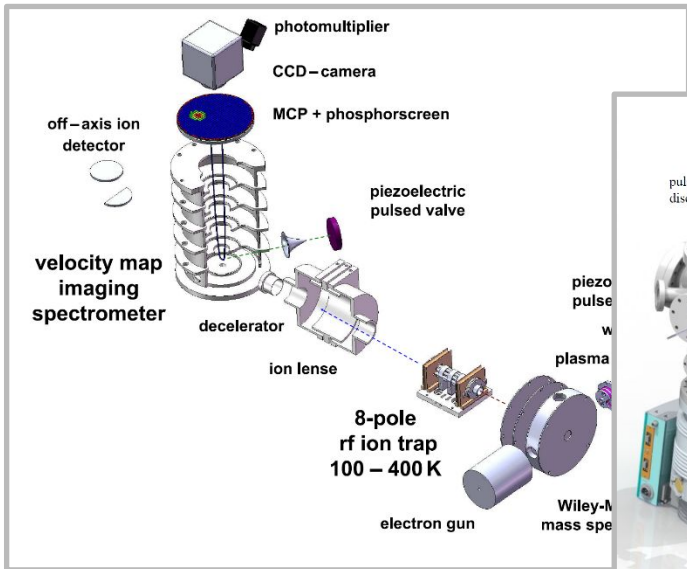


Interstellar ion formation

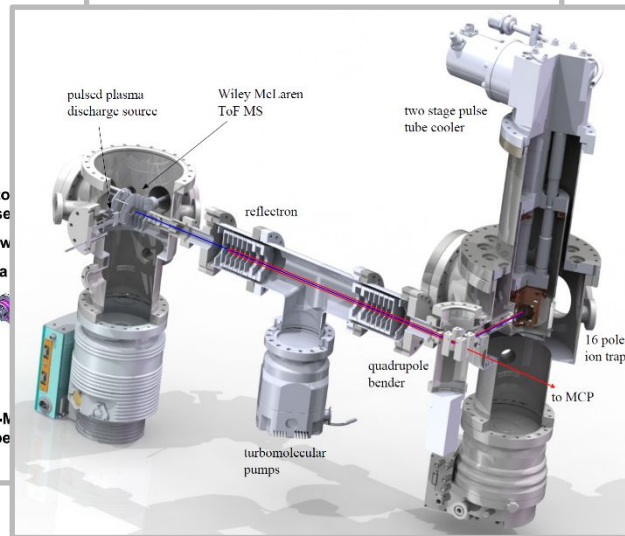


Dynamics and Spectroscopy of Charged Molecular Systems

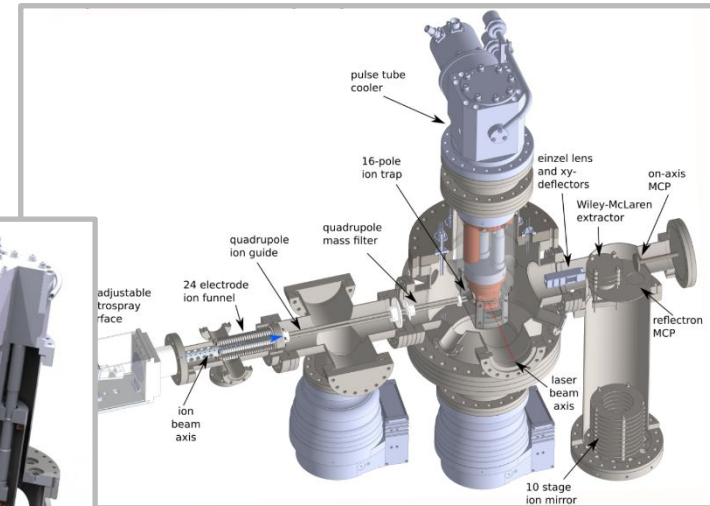
Experimentelle Aufbauten



Kreuzstrahlspektrometer
für Ionen-Molekül-
Reaktionsdynamik



6 Kelvin Ionenfalle
für Laborastrophysik an
interstellaren Ionen



3 Kelvin Elektrospray-
Ionenfalle für Spektroskopie an
Biomolekülen und Clustern

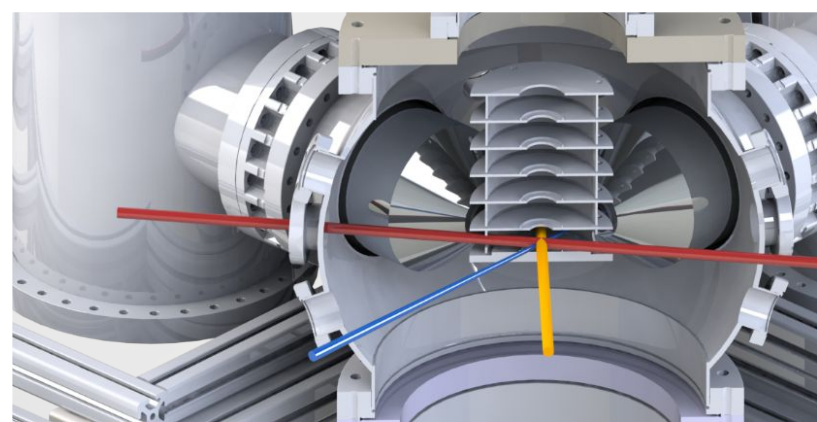
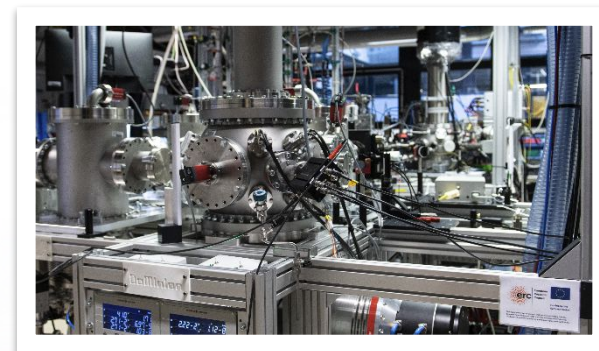
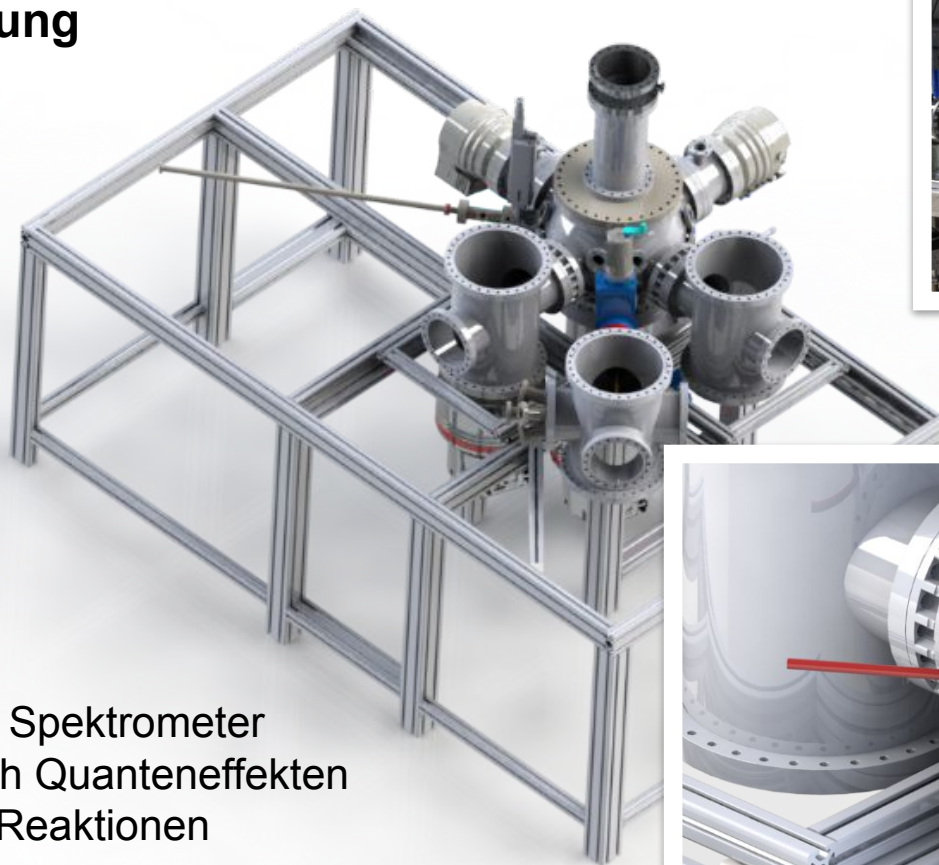


Dynamics and Spectroscopy of Charged Molecular Systems

Neue Entwicklung



DoMIInlon



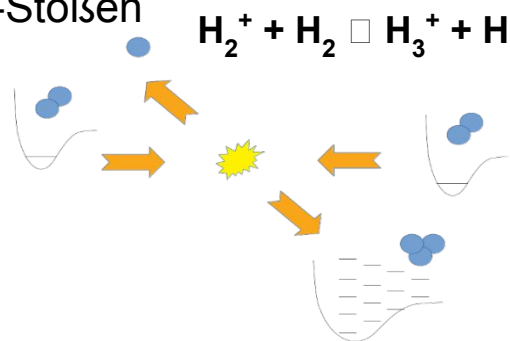
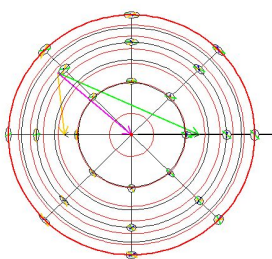
Hochauflösendes Spektrometer
für die Suche nach Quanteneffekten
in Ionen-Molekül-Reaktionen



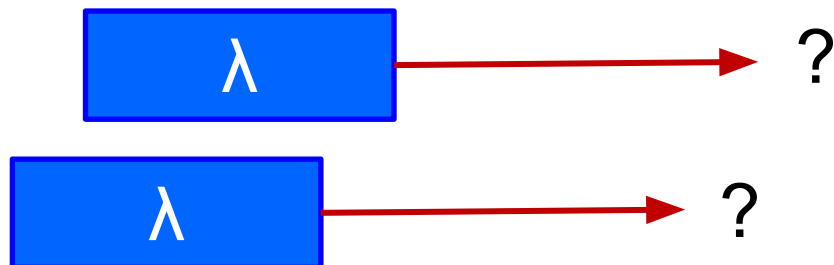
Dynamics and Spectroscopy of Charged Molecular Systems

Mögliche Themen für Bachelorarbeiten 2023

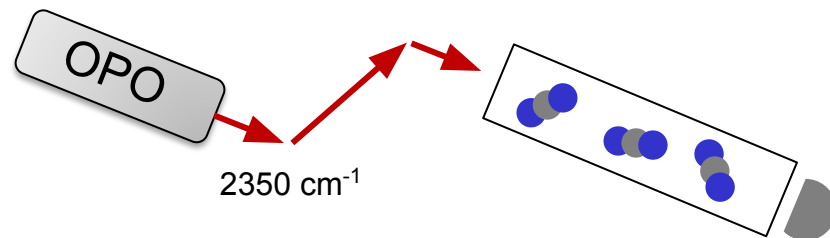
Quantenzustands-Auflösung in
Ionen-Molekül-Stößen



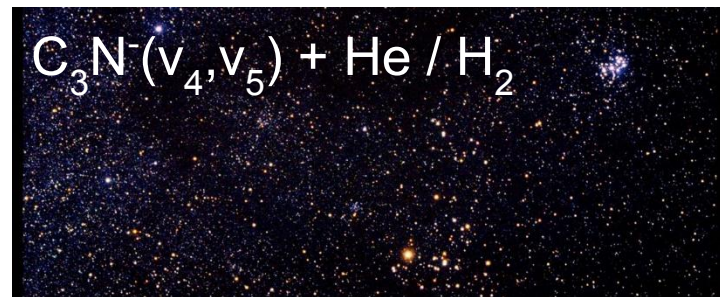
Aufbau und Test zweier Dioden-Laser



Hochauflösende Infrarotspektroskopie
von Kohlendioxid



Interstellare Stöße mit oder ohne
thermisches Gleichgewicht





Dynamics and Spectroscopy of Charged Molecular Systems

Bei Interesse, einfach melden:

roland.wester@uibk.ac.at

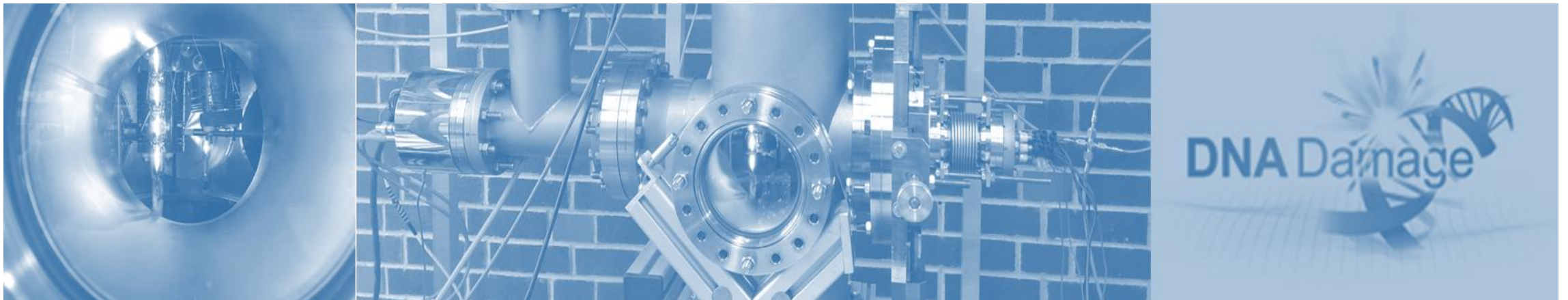
Vielen Dank für die Aufmerksamkeit!



Collaborations

Szeged
Heidelberg
Prag
Stockholm
Bordeaux
Orlando
Albuquerque

Inelastic Electron Scattering – WG Denifl



Jiakuan Chen, MSc

(PhD Candidate – AG Denifl)



About the Inelastic Electron Scattering Group

The Group

- 5 PhD Students, 1 master student, and a student coworker.

Research fields

Gas Phase studies

- Low energy electron ($E_{\text{kin}} < 15$ eV) attachment to biomolecules, *radiosensitizers* and polymeric compounds

Clusters

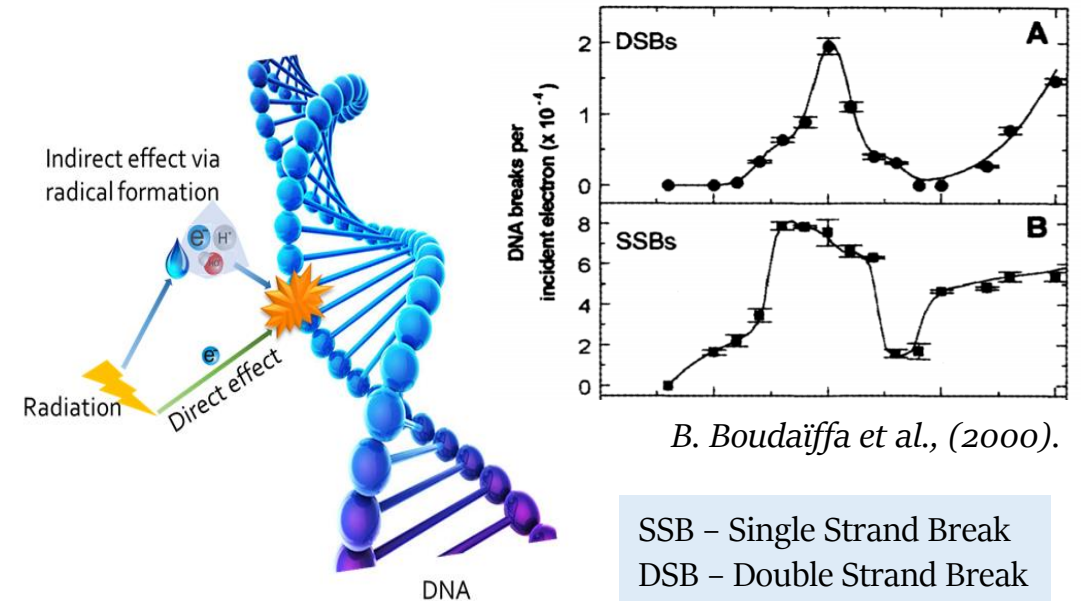
- Rare gas clusters and/or molecular clusters

Applications:

- Radiation chemistry, atmospheric chemistry, astrochemistry, material sciences

Motivation

Biological effect of radiation and low energy electrons

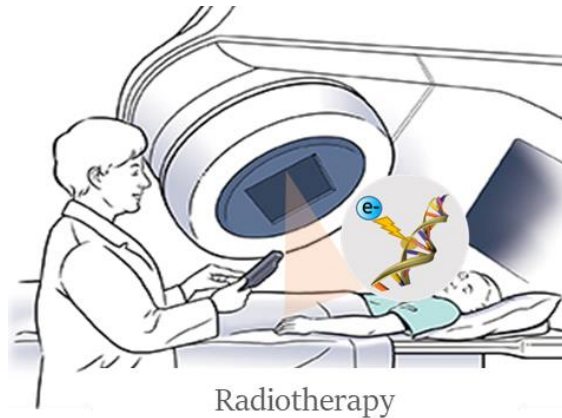
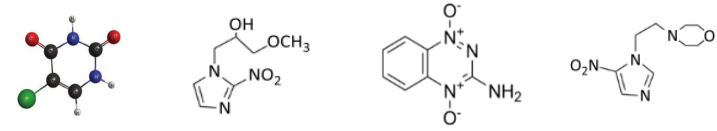


SSB – Single Strand Break
DSB – Double Strand Break

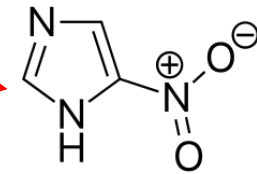
Overcoming in cancer treatment

Combination Therapy

Radiotherapy + chemotherapy

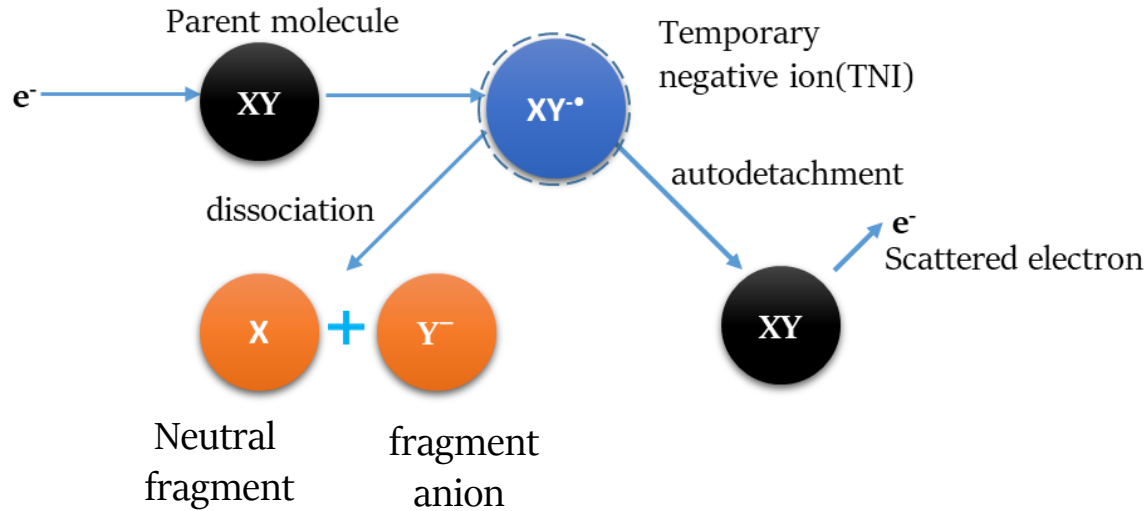


Incorporation of chemical agents



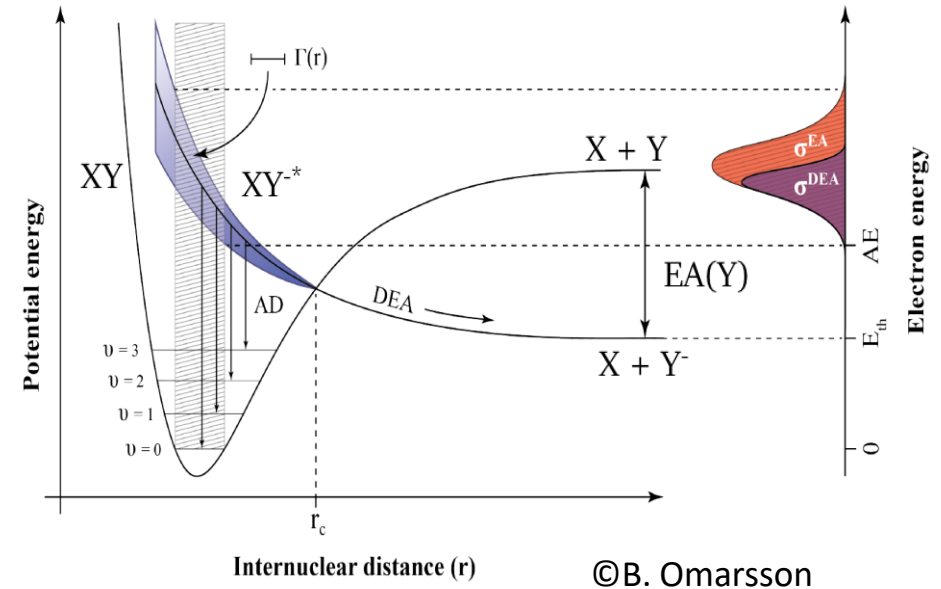
Radiosensitizers

Dissociative Electron Attachment (DEA)

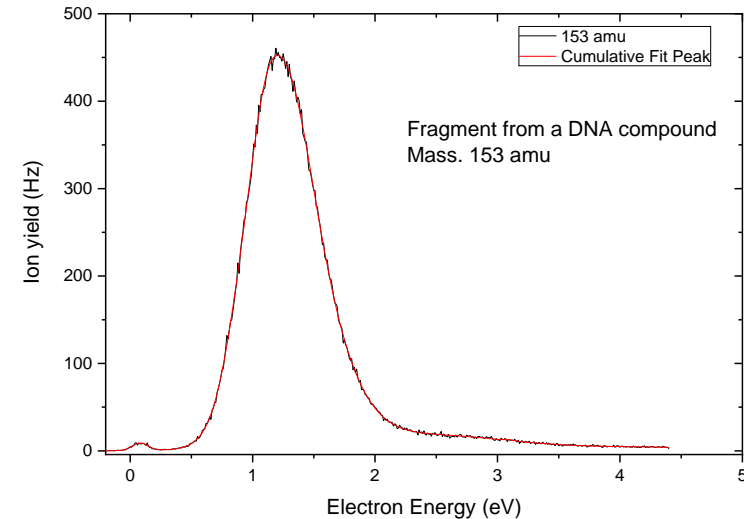


Results in bond cleavages:

Single bond, double bond or complex decompositions into multiple fragments

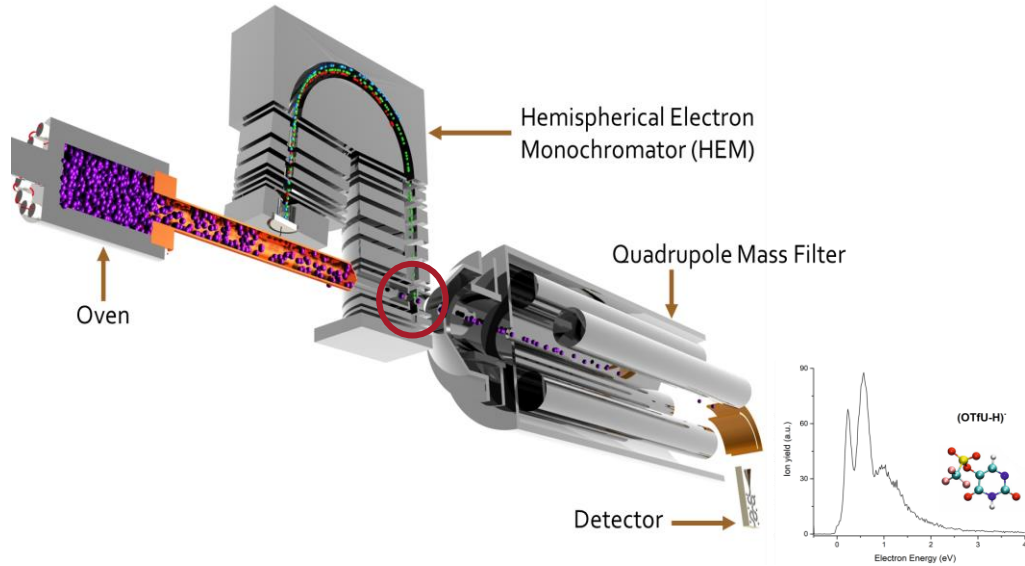


Potential Energy Diagram illustrating electron attachment

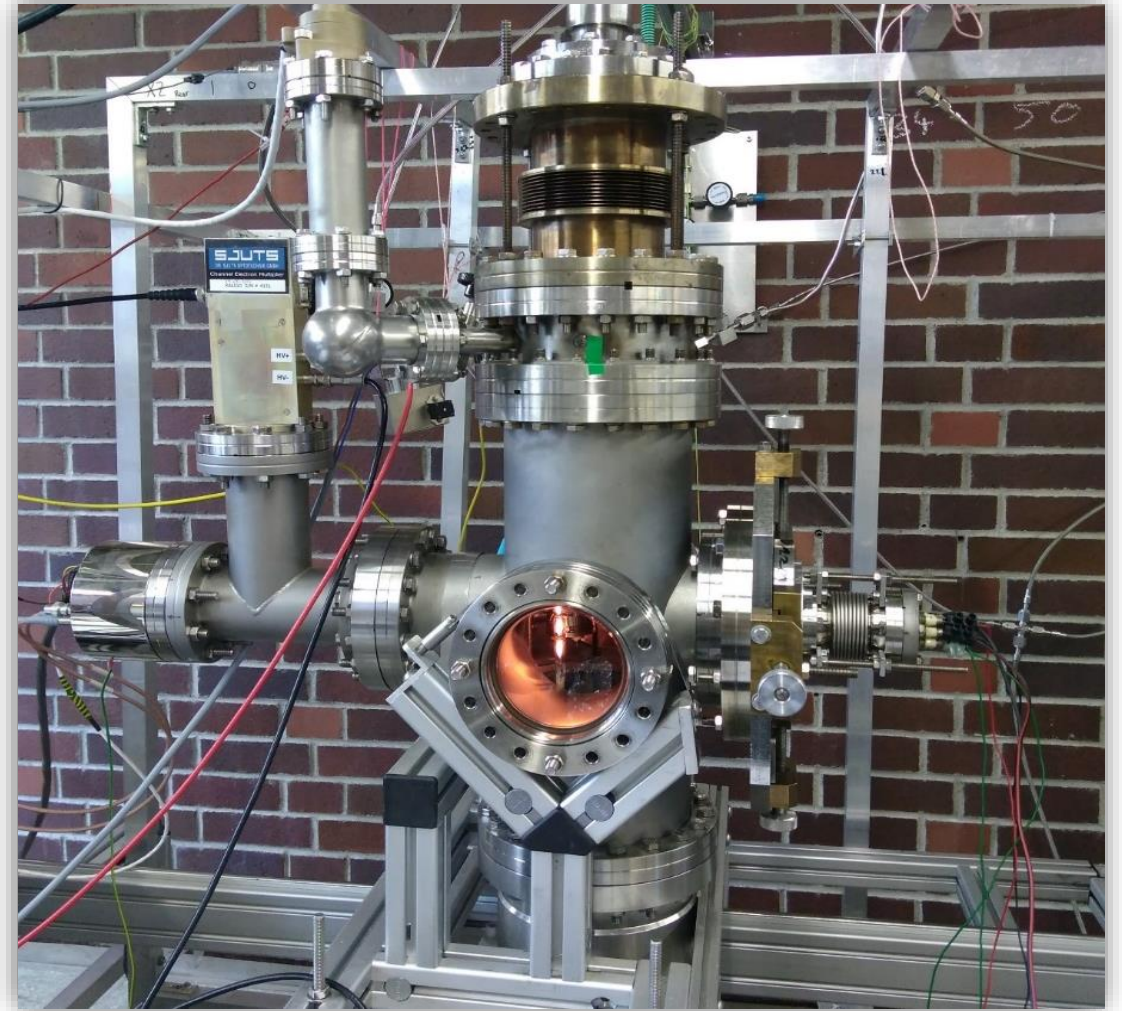


Experimental Setups

Crossed Electron-Molecular Beam setup ([WIPPI](#))

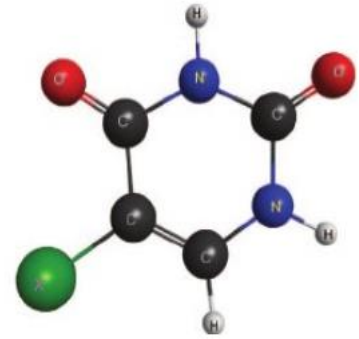


Hemispherical electron monochromator coupled to a quadrupole mass spectrometer in order to detect with high energy resolution ($<100\text{meV}$) the product ions upon inelastic electron interaction.



Possible topic in this year

- Electron attachment to a radiosensitiser (modified uracil).



https://www.uibk.ac.at/ionen-angewandte-physik/ag-denifl/

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Studies Research Connect About us

Institute for Ion Physics and Applied Physics - WG Denifl

WG Denifl: Inelastic Electron Scattering

Welcome at the homepage of the working group Inelastic Electron Scattering. The working group investigates fundamental questions concerning the interaction of low-energy (<100 eV) electrons with atoms, molecules and clusters. This interaction is highly relevant for the description of biological processes like for example radiation damage of cells and for material sciences, where these processes can play a fundamental role on molecular scales.

You are interested to research in these fields? [Follow here.](#)



Institute for Ion Physics and Applied Physics

- > Inelastic Electron Scattering
- Research: topics
- Research: projects
- Coworkers
- Publications
- Open positions

Acknowledgement



Prof. Dr. Stephan Denifl



Patrick Ziegler



Debasish Parida



Jiakuan Chen



Muhammad Saqib



Farhad Izadi



Vy Nguyen



Lara Schorr



Prof. Dr. Milan Oncak
(Computational Photochemistry)
UIBK



Prof. Dr. Janusz Rak
University of Gdansk,
Poland

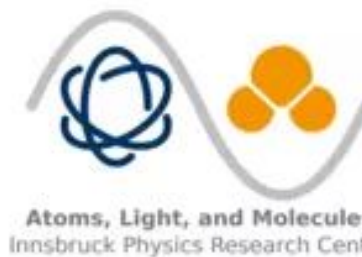
Chemische Physik – AG Beyer



Ethan Cunningham
Sandra Forndran
Jessica Hartmann
Shan Jin
Marcos Juanes San José
Sarah Madlener
Maximilian Müntst
Markus Nötzold
Manuel Rainer
Magdalena Salzburger
Simone Schirra
Christian van der Linde

FWF

Der Wissenschaftsfonds.



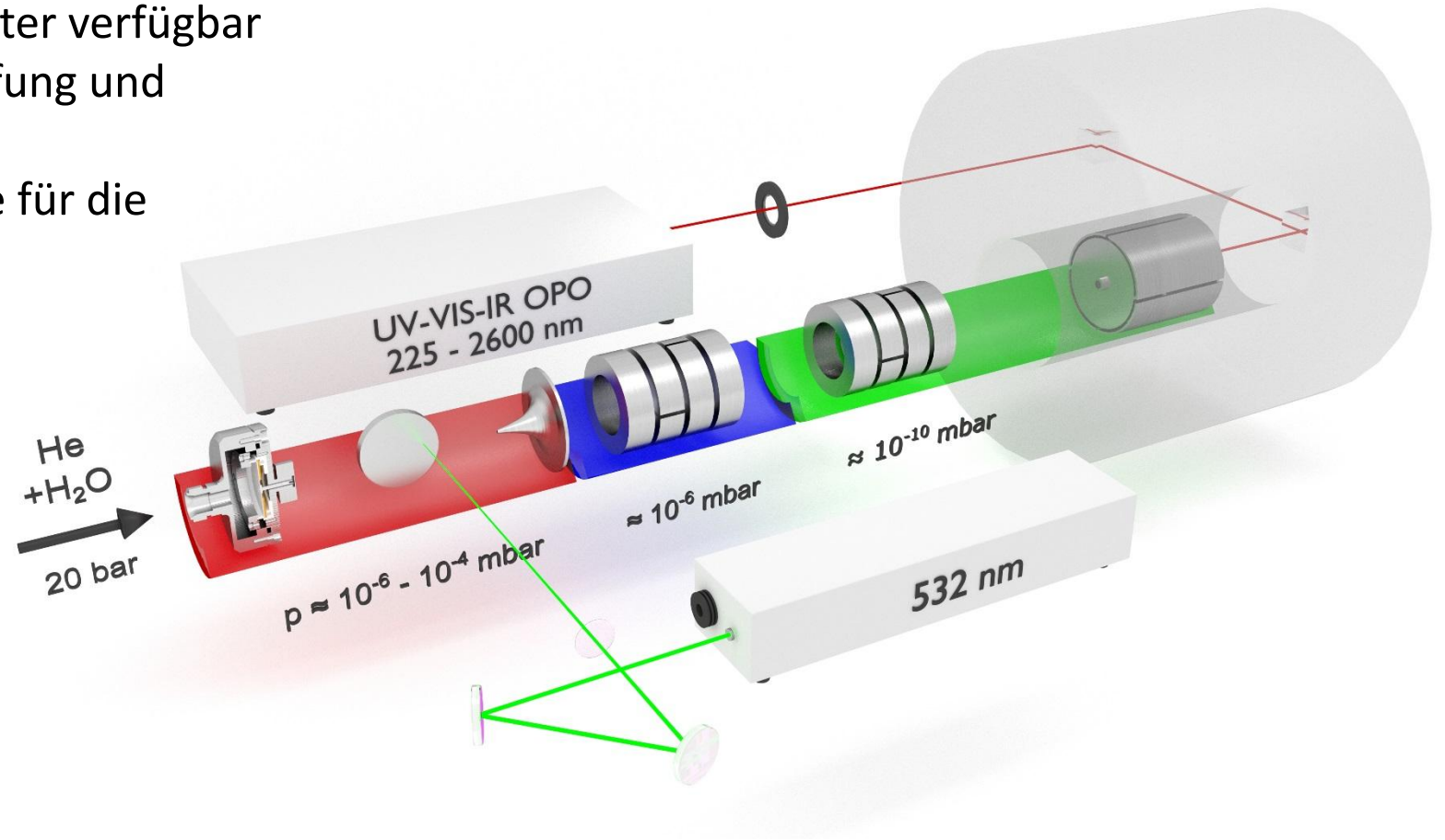
FWF



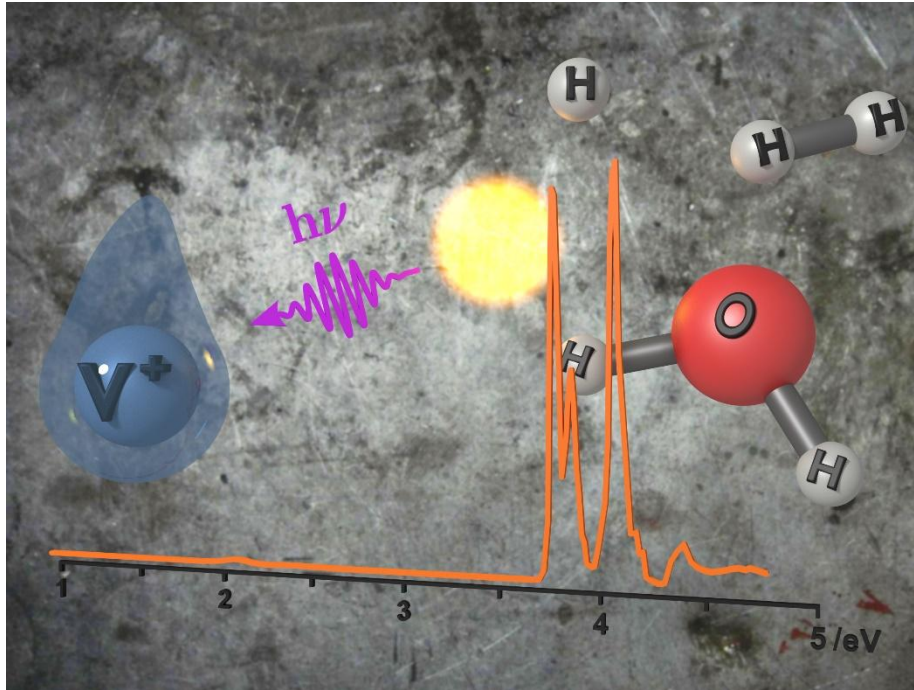
Clusterphysik im Massenspektrometer

- Zwei FT-ICR Massenspektrometer verfügbar
- Clusterquellen: Laserverdampfung und Elektrosprayionisation
- Durchstimmbare Lasersysteme für die Spektroskopie

$$\omega_c = \frac{z}{m} B_0$$



Bachelor-/Masterarbeit: Photochemische Wasserspaltung



Motivation: Wasserstoffwirtschaft, Klimaneutralität

Ziele:

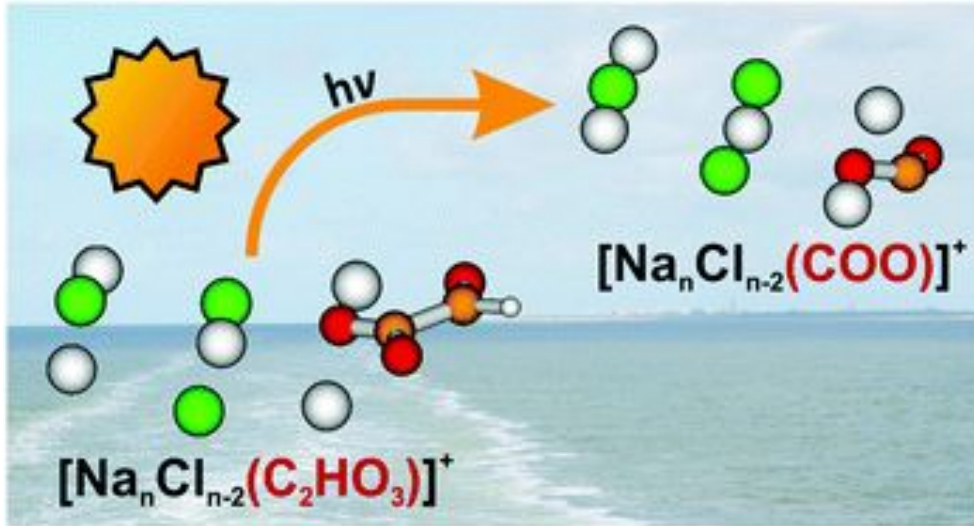
- Untersuchung der beteiligten elektronischen Zustände
- Rolle des Metallions
- Energiebilanz

Durchführung:

- Wassercluster mit einem Metallion aus Laserverdampfung
- Anregung mit Laserlicht führt zur Freisetzung von Wasserstoff

In nächster Zeit geplante Metalle: Aluminium, Eisen

Bachelor-/Masterarbeit: Labormodelle für Aerosole



Bildnachweis: Photochemistry of glyoxylate embedded in sodium chloride clusters, a laboratory model for tropospheric sea-salt aerosols - Physical Chemistry Chemical Physics (RSC Publishing)

Motivation: Atmosphärenchemie, Klima

Ziele:

- Aufklären von Reaktionen beim *atmospheric processing*
- Physikalisch-chemische Eigenschaften von Salzclustern

Durchführung:

- Salzcluster aus Elektroprayionisation
- Anregung mit Laserlicht - Spektroskopie, Photochemie
- Stöße mit reaktiven Molekülen

In nächster Zeit geplante Experimente:

- Reaktionen von Salzclustern mit Fluoressigsäure
- Photochemie von dotiertem Natriumchlorid

K-Regio-Projekt GALANT: Analytik hochreiner Gase

- Untersuchung von Reaktionswegen zur selektiven chemischen Ionisation
- Nachweisgrenzen $< \text{pptv}$ erwünscht, d.h. $< 1:10^{12}$
- Entwicklung und Optimierung von Ionenquellen
- Anwendungen in der Hochtechnologie: Elektronik, Halbleiter, Bildschirme, chemische Industrie

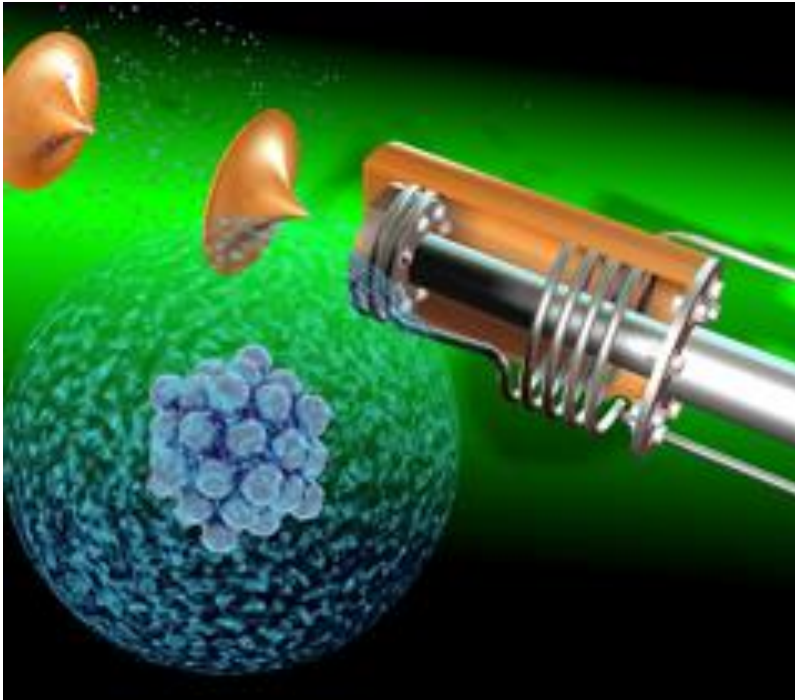
Bachelor-/Masterarbeit: Optimierung von Ionenquellen



Nano-Bio-Physics

Main research focus:

formation and analysis of ionic molecules, clusters and complexes embedded in superfluid helium nanodroplets



- **Laser spectroscopy** in combination with mass spectrometry
- Collision induced dissociation in combination with **mass spectrometry**
- Deposition of **nanoparticles** on surfaces

➤ Laser spectroscopy in combination with mass spectrometry

Topic: On the search of the carriers of the diffuse interstellar bands

Open positions:

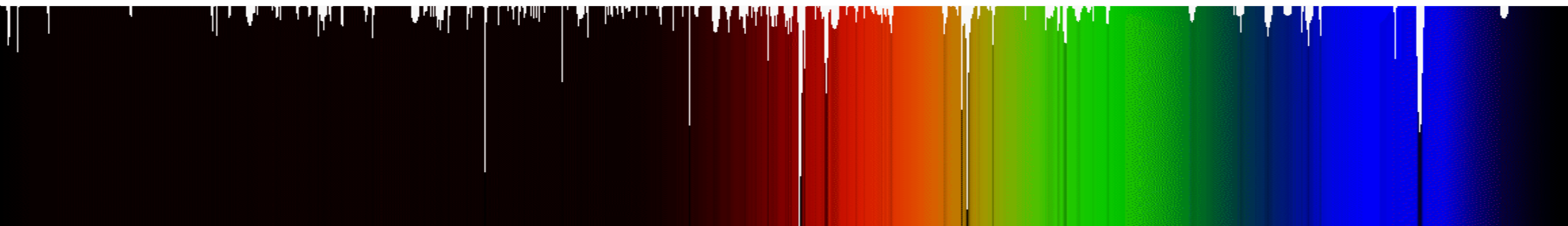
- Construction and assembly of a two-part oven system which allows to evaporate two different samples in a single vacuum chamber (Bachelor project; time: Jan/Feb 2023)
- Spectroscopy of $(C_{60}\text{-metal})^+$ complexes (Bachelor project; time: spring 2023)



Post-Doc:
Elisabeth Gruber
E.Gruber@uibk.ac.at



PhD student:
Lisa Ganner



➤ Laser spectroscopy in combination with mass spectrometry

Topic: Messenger spectroscopy of photoactive (metal)organic molecules

Open position:

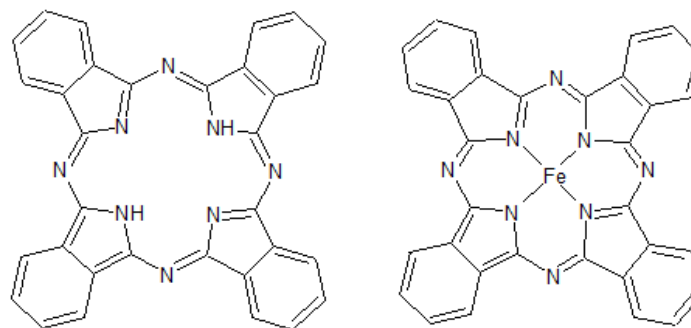
- Spectroscopy of metal-phthalocyanine cation complexes
(Bachelor project; time: Jan/Feb 2023)



Post-Doc:
Elisabeth Gruber
E.Gruber@uibk.ac.at



PhD student:
Stefan Bergmeister



➤ Mass spectrometry

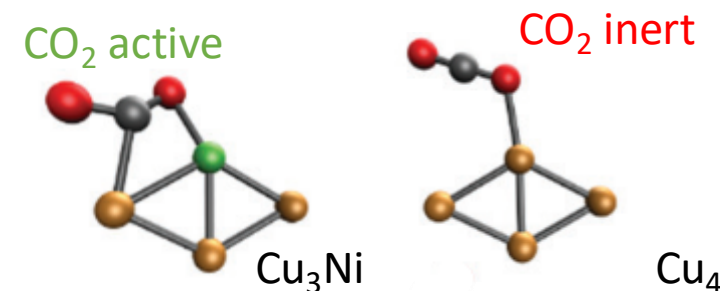
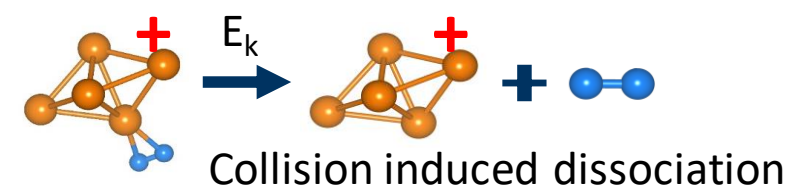
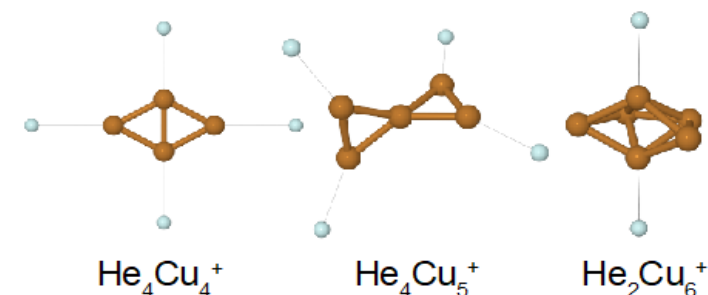
Topic: Metal clusters as a model system to study catalytic reactions, such as CO₂ activation

Open positions:

- Define the structure of Ni clusters by He tagging
(Bachelor project; time: from Feb 2023)
- Characterize size-dependent binding dissociation energy of CO₂ and metal clusters
(Master project; time: from Feb 2023)
- Formation and structural characterization of bimetallic clusters.
Each atom matters!
(Master project; time: from Feb 2023)



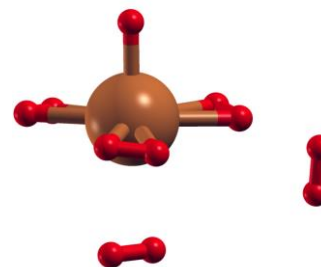
Post-Doc: Olga Lushchikova
Olga.Luschikova@uibk.ac.at



➤ Mass spectrometry

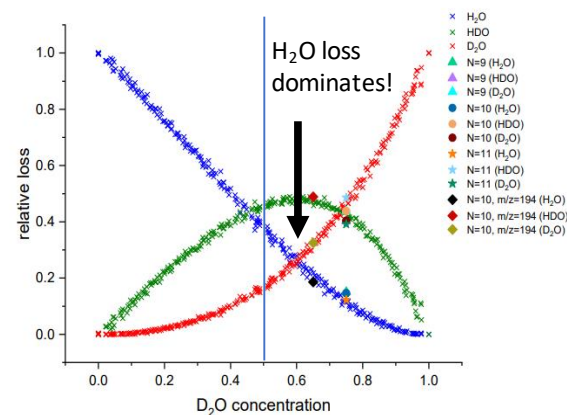
Spin off projects

- H_2 storage on Cu^- at ultracold temperature
(Bachelor project; time: Jan/Feb 2023)



More than 100 H_2 molecules?

- Investigation of a novel isotope effect in cold mixed NH_3/ND_3 clusters
(Bachelor project; time: Jan/Feb 2023)



Post-Doc: Olga Lushchikova
Olga.Lushchikova@uibk.ac.at



PhD student: Siegfried Kollotzek
Siegfried.Kollotzek@uibk.ac.at

➤ Deposition of nanoparticles on surfaces

Topic: Deposition of size-selected clusters grown in helium nanodroplets

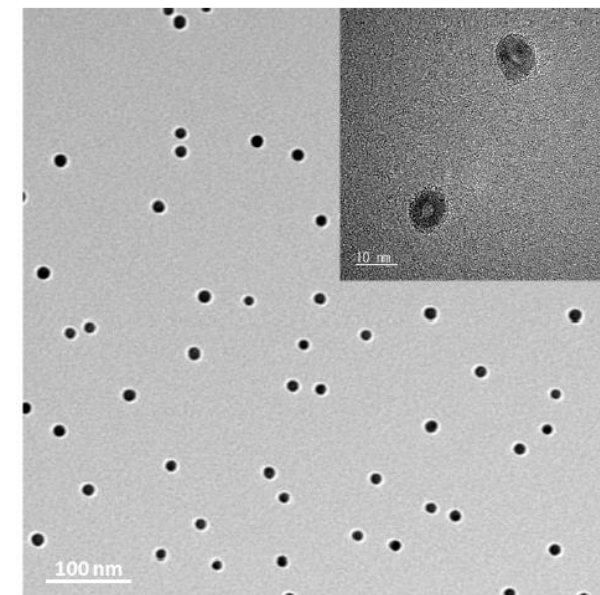
Time: start anytime between spring and autumn (Master project)

- deposit gold nanoparticles on different substrates
- characterize the resulting size-distributions
- test modification of surface characteristics (e.g. optical behaviour, electrical conductivity or biocompatibility)

Methods: experimental setup (clustersource, electrostatic sector, gold-oven), microscopy (TEM, AFM), 4-point-probe, spectroscopy



PhD student: Anna Maria Reider
Anna-Maria.Reider@uibk.ac.at
Paul.Scheier@uibk.ac.at



- Deposition of nanoparticles on surfaces

Topic: Magnetron Sputter Deposition – Aluminium coatings for antennas

Time: February (Bachelor project)



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Paul.Scheier@uibk.ac.at

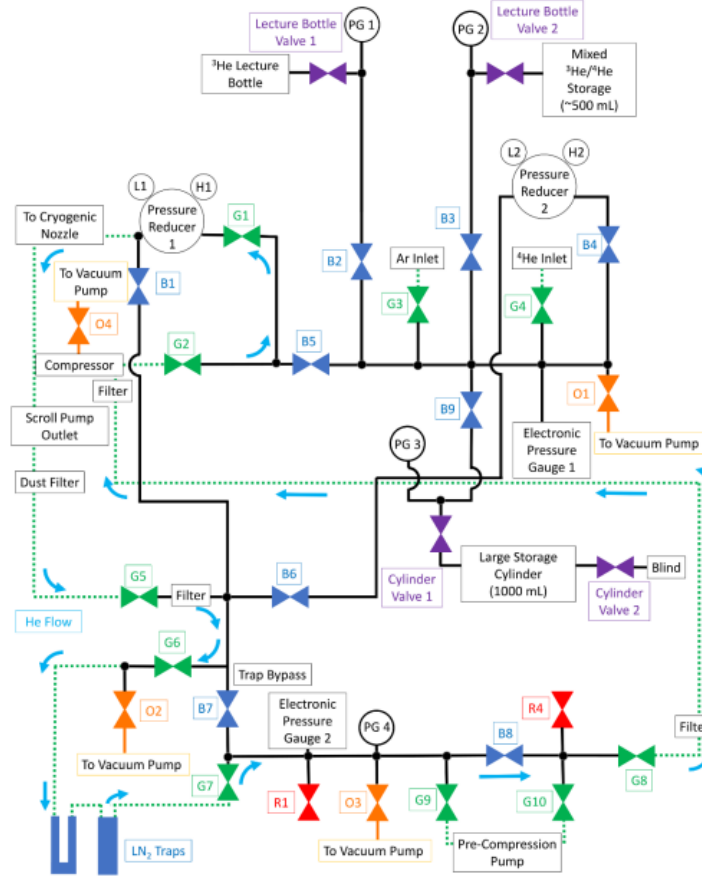
Master student: Daniel Fürhapter
(mechatronics)

- Deposition of aluminium films on glass
- Characterization of surface roughness and electrical conductivity of the film depending on experimental parameters
- Outlook: application for antennas at the Institute of Mechatronics

Method: Magnetron Sputtering, AFM, 4-point-probe

➤ Assembly and testing of a helium recycler

Master project; time: start anytime



Senior Scientist:
Fabio Zappa



Prof. Paul Scheier
Paul.Scheier@uibk.ac.at