EARLY STAGE RESEARCHER

Melby Johny

PROJECT: *Ultrafast electron dynamics in conformer selected amino acids*

Host institution: Duetches Elektronen- Synchrotron (DESY)

Supervisors: Prof. Dr. Jochen Küpper (DESY), Dr. Sebastian Trippel (DESY), Dr. Guiseppe Sansone (FRIEB), Dr. O. Kelly (PHOTEK)

Start date: April, 07, 2016

This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 641789

CURRICULUM VITAE

- April 2016 to present: ESR MEDEA, Controlled Molecule Imaging Group, Center for Free-Electron Science, Duetches Elektronen-Synchrotron (DESY), Hamburg
- May 2015 - March 2016: Project assistant in the Ultrafast Biophysics Group at Tata Institute of Fundamental Research (TIFR), Mumbai, India.
- December 2014 - April 2015: Performed Master's Thesis Project in the Ultrafast Biophysics Group at Tata Institute of Fundamental Research (TIFR), Mumbai, India.
- July 2010 - April 2015: 5 year Integrated M.Sc at International School of Photonics, Cochin University of Science and Technology (CUSAT), Cochin, India

Special experiences:

- Setting up of ultrahigh vacuum systems
- Conformer selection of molecules
- Handling Velocity Map Imaging (VMI) spectrometer and Time of Flight Spectrometer for electrons and ions.
- Simulations on VMI spectrometer
- Beam time preparations and working in beam time at PETRA III, LCLS and FLASH.
- Surface Enhanced Raman Spectroscopy, Time resolved Stimulated Raman Spectroscopy.
- Imaging techniques like Confocal Microscopy, TEM, SEM
- Self assembled peptide based nano-structures.

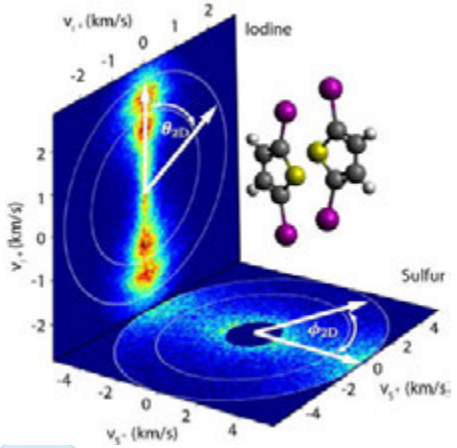
This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 641789

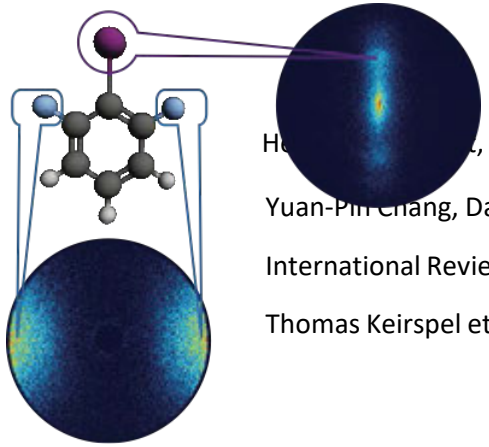
SCIENTIFIC SCOPE OF THE PROJECT

Ultrafast charge re-arrangement processes after ionisation of large (bio)molecules in gas phase.

- Preparation of “ideal” molecular samples by conformer selection of amino acids and small peptides in low temperature molecular beams.
- Quantum state measurements and wave packet dynamics
- Imaging ultrafast molecular dynamics in the molecular frame utilizing 3D aligned and oriented conformers of molecules.
- Understanding elementary chemical processes:

  isomerization, folding, binding, (photo)dissociation, charge migration…





H[illegible], Tamar Seideman, RMP 75, 543 (2003)

Yuan-Pin Chang, Daniel A. Horke, Sebastian Trippel, and Jochen Küpper

International Reviews In Physical Chemistry Vol. 34 , Iss. 4,2015

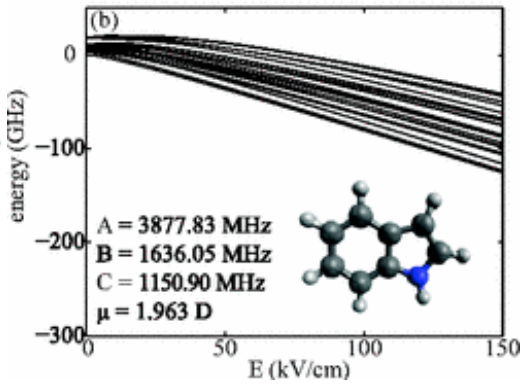
Thomas Keirspel et al, J. Phys. B: At. Mol. Opt. Phys. 48 (2015) 204002

This project has received funding from the European Union’s Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 641789

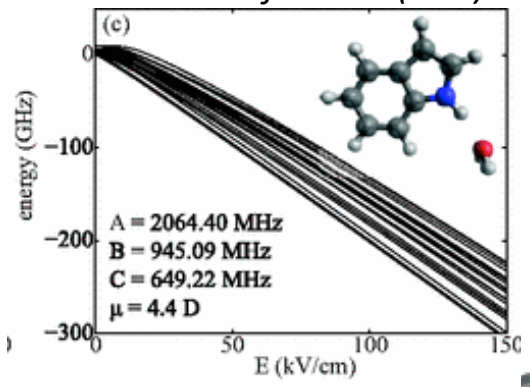
SCIENTIFIC ACTIVITIES AND GOALS IN PROGRESS- ***Photophysics of indole and indole-water cluster***

Indole—chromophore of the amino acid tryptophan and is solvated through H-bonding to form indole-$(H_2O)_1$

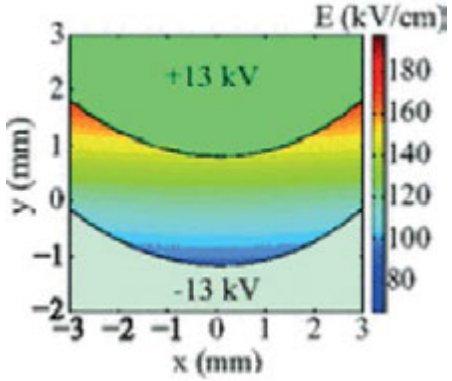
Stark curve of indole

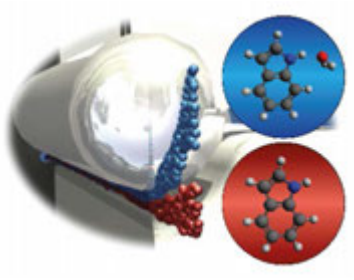


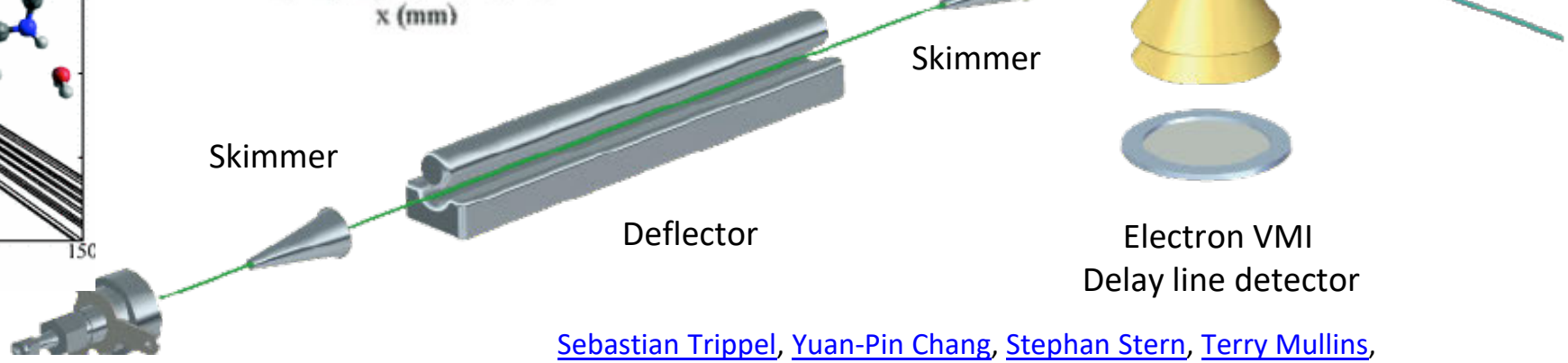
Stark curve of indole-$(H_2O)_1$



Experimental Setup







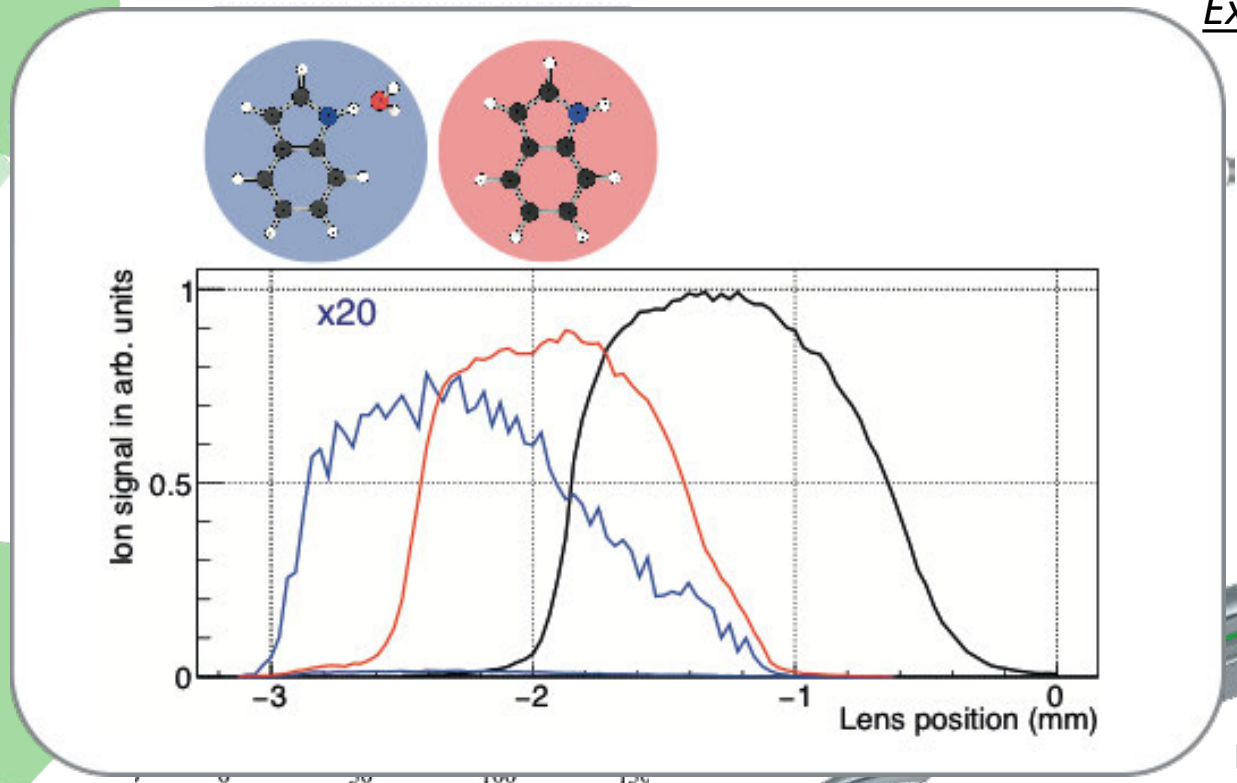
Sebastian Trippel, Yuan-Pin Chang, Stephan Stern, Terry Mullins, Lotte Holmegaard, and Jochen Küpper, Phys. Rev. A 86, 033202, 2012

This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 641789

SCIENTIFIC ACTIVITIES AND GOALS IN PROGRESS- ***Photophysics of indole and indole-water cluster***

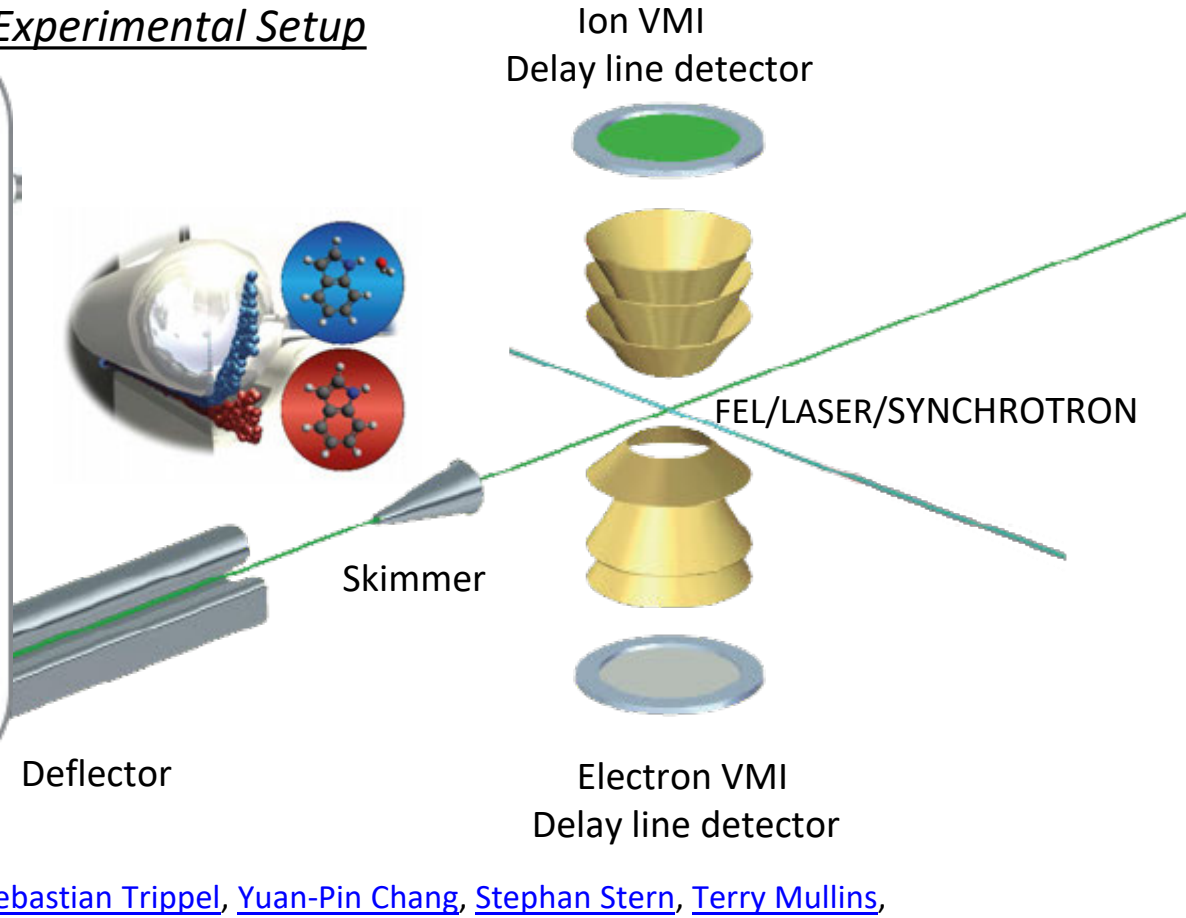
Indole—chromophore of the amino acid tryptophan and is solvated through H-bonding to form indole-$(H_2O)_1$

Stark curve of indole



Evan Lavie Valve, 250 Hz

Experimental Setup



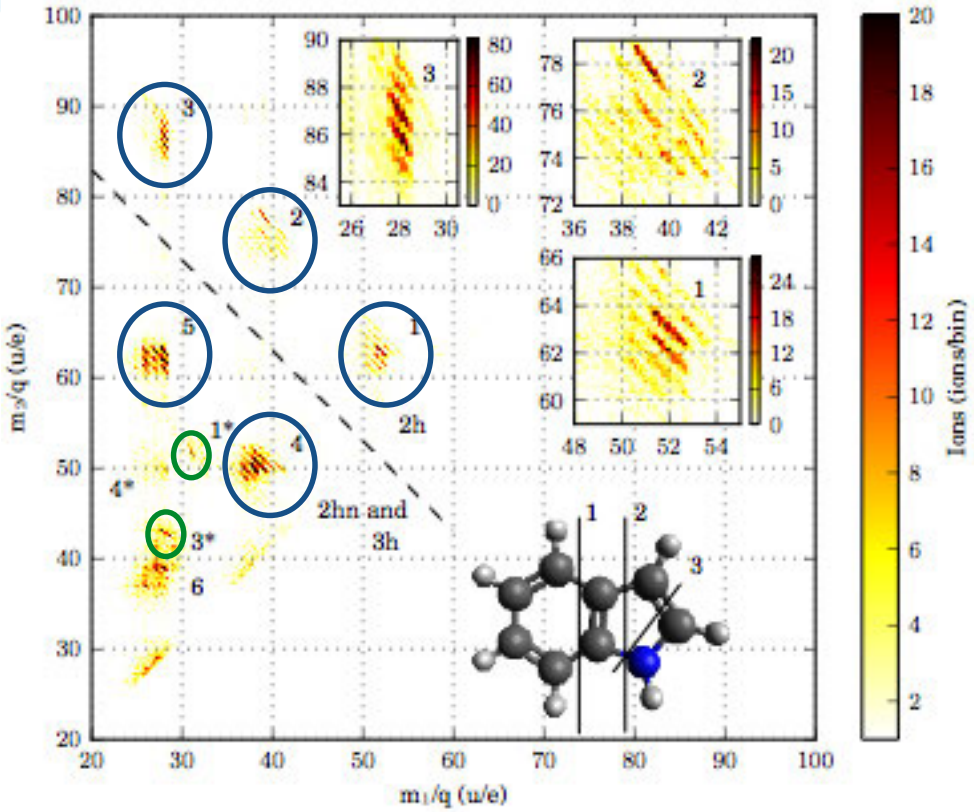
Sebastian Trippel, Yuan-Pin Chang, Stephan Stern, Terry Mullins, Lotte Holmegaard, and Jochen Küpper, Phys. Rev. A 86, 033202, 2012

This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 641789

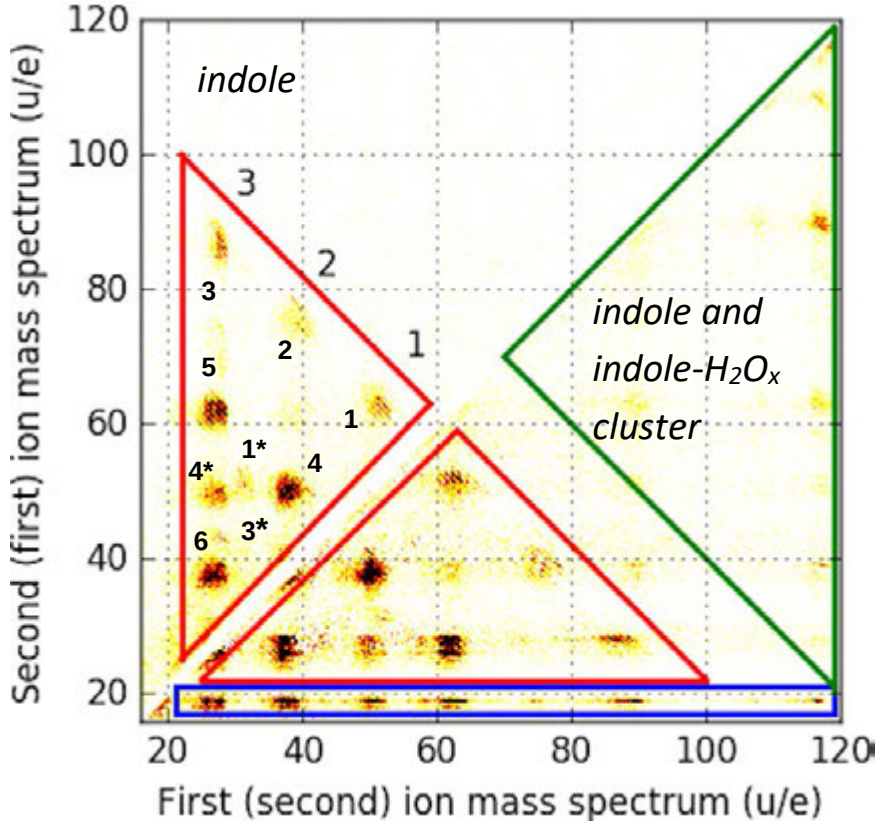
PETRA III beamtime PEPIPICO electron and ion dynamics

Photoelectron - **P**hotoi**o**n **P**hotoi**o**n **Co**incidence

indole monomer



indole - water



Indole

Indole-H_2O

Cluster

n → PIPICO island

n* → same fragmentation, different charge state

2h/3h → 2/3 hole

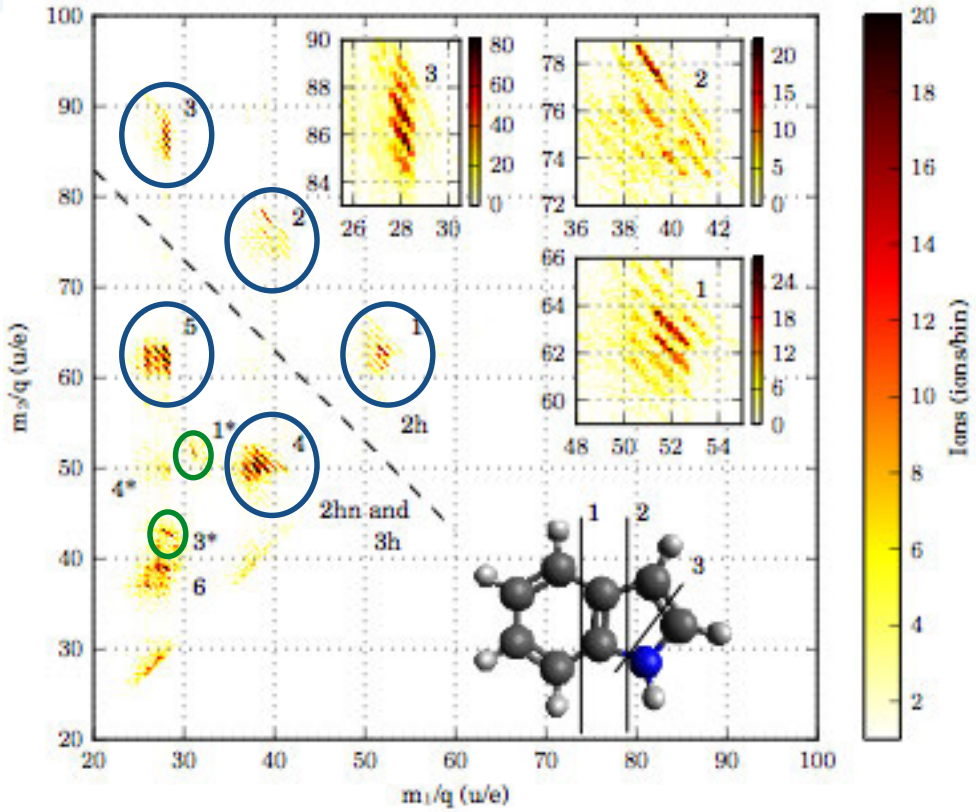
2hn → 2 hole & a neutral fragment

Thomas Kierspel et.al manuscript in preparation

This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 641789

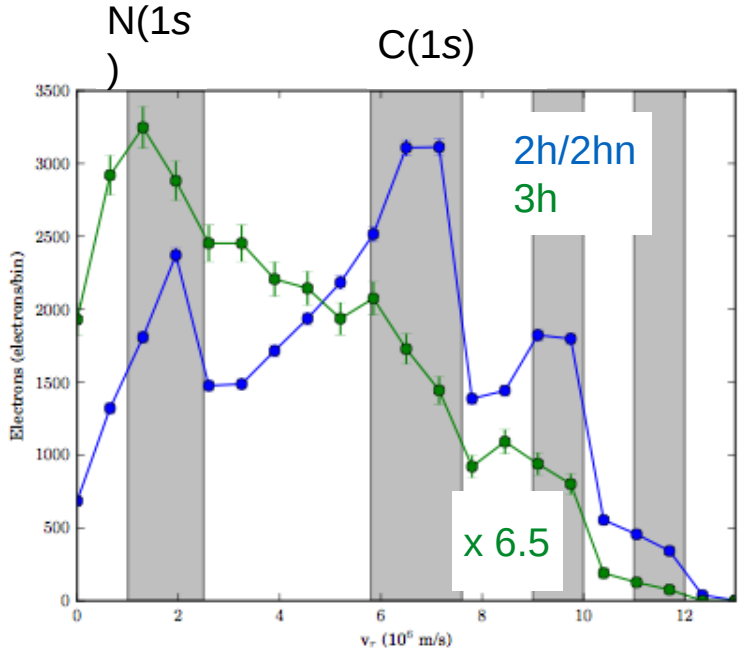
PIPICO indole monomer

Photoelectron - **P**hotoi**o**n **P**hotoi**o**n **Co**incidence



n → PIPICO island
n* → same fragmentation, different charge state
2h/3h → 2/3 hole
2hn → 2 hole & a neutral fragment

Electron coincidence



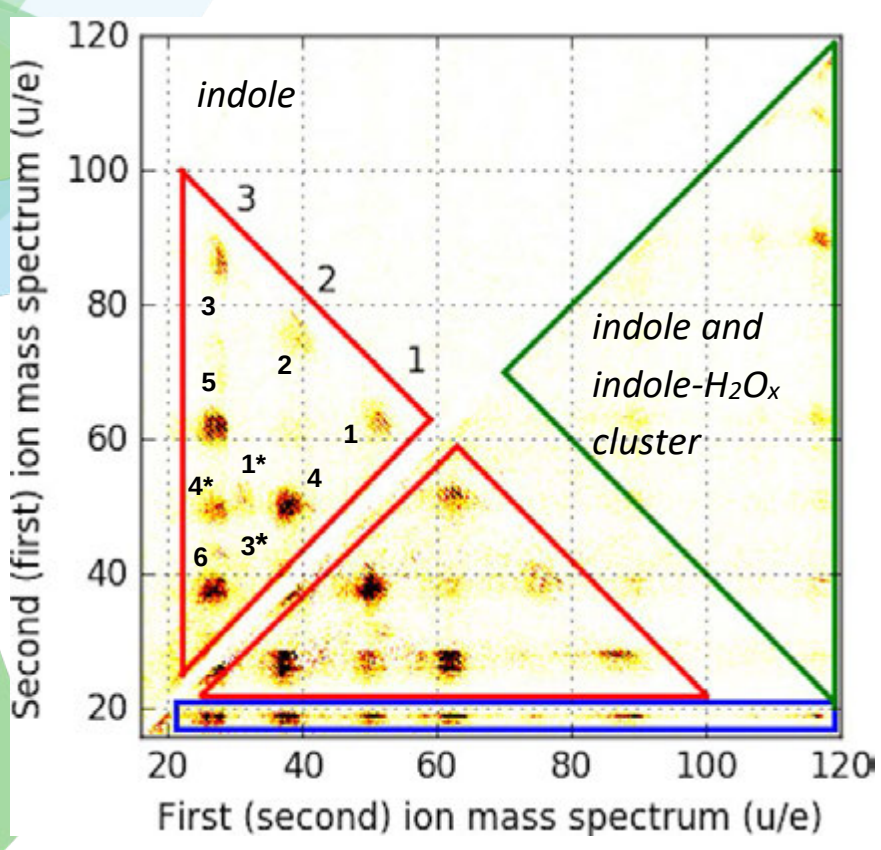
- 3h channels are dominated by N(1*s*) photoelectrons
- 3h channels show no strong C(1*s*) photoelectron contribution

Thomas Kierspel et.al manuscript in preparation

This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 641789

PIPICO indole - water

Photoelectron - **P**hotoi**o**n **P**hotoi**o**n **Co**incidence



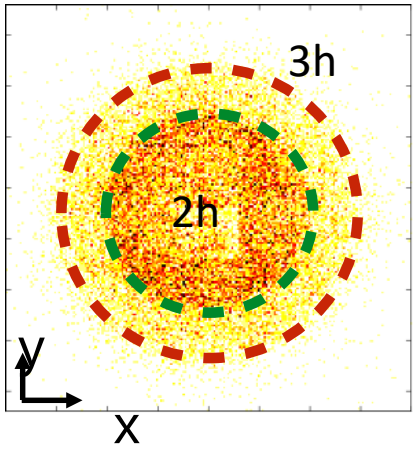
n → PIPICO island
n* → same fragmentation, different charge state

Indole

Indole-H_2O

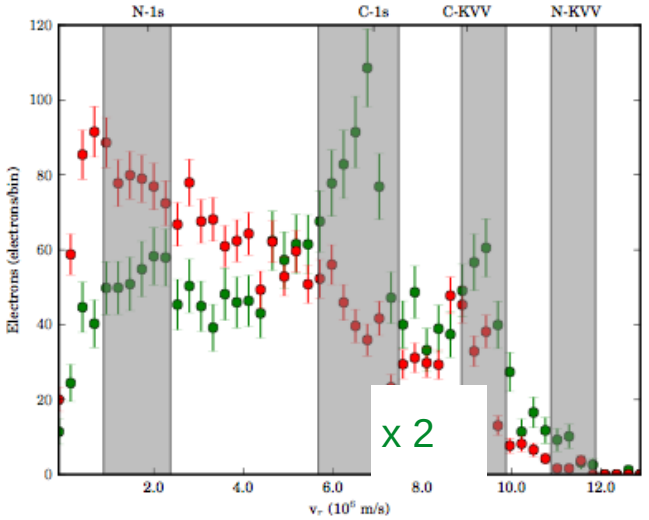
Cluster

Velocity map imaging (VMI) of hydronium



H_3O^+ (19)

Electron coincidence



- 3h channels are dominated by N(1*s*) photoelectrons
- 3h channels show no strong C(1*s*) photoelectron contribution

- *Charge and mass transfer to hydrogen bonded water*

Thomas Kierspel et.al manuscript in preparation

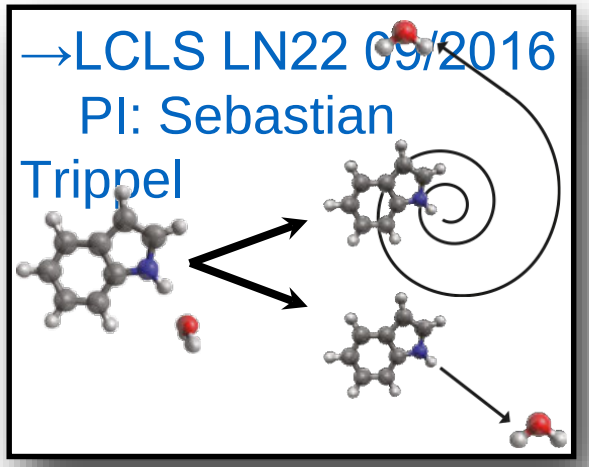
This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 641789

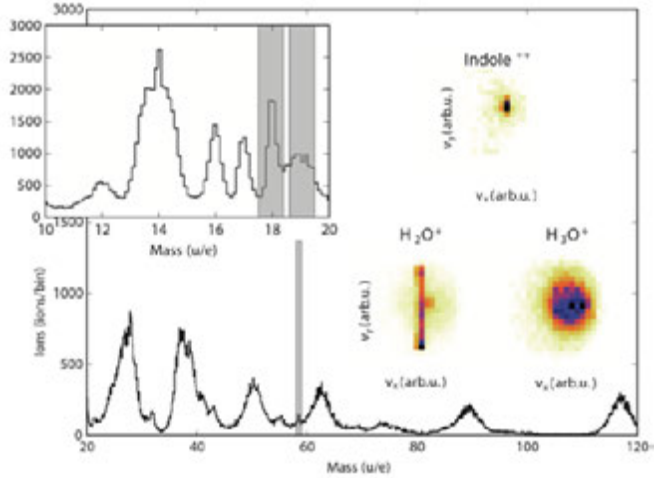
Summary and Future directions

- Disentangled the fragmentation of indole and indole-water upon coreshell ionization.
- Observed ionization and proton/hydrogen transfer from indole to H_2O as one of the dissociation pathway
- Different fragmentation channels for localized ionisation in indole and indole-H_2O

Future directions: LCLS Beamtime towards time-resolved studies of H-bond dynamics

- Unravel the hydrogen bond breaking dynamics using the combined time resolved photo-physics data.





This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 641789

SECONDMENTS, OUTREACH ACTIVITIES AND SOFT SKILLS TRAINING

Secondments

- PHOTEK (3 months in mid of 2017): Understanding the working of Double sided Velocity Mapping Imaging Spectrometer by performing Simulations. Experiments to improve the performance of high voltage switches in VMI spectrometers
- Unv. of Aarhus (2 months): Techniques for adiabatic and non-adiabatic alignment and orientation of molecules.

Outreach Activities

- Performed outreach activities in two different schools in the year 2016.
- Higher secondary students (17) and primary students (54).

Soft Skills Training

- Women's Carrier Day 2016 organised by PIER graduate school: Improvisation theatre techniques for scientific presentations, and scientific networking (30th June to 1st July).
- PIER graduate week 2016: Scientific and soft skill courses, innovation workshop.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 641789

CAREER DEVELOPMENT PLAN AND FUTURE ACTIVITIES

- Generation of optimised molecular beams for conformer selected amino acids and peptides.
- Implementation of techniques for adiabatic and non-adiabatic 3D alignment and orientation of individual conformers.
- Imaging electron-transfer and proton/hydrogen-transfer dynamics in indole with time and angle resolved photoelectron spectroscopy after excitation with femtosecond laser pulses.
- Atomically resolve the bond-breaking process using ultrafast diffractive imaging techniques

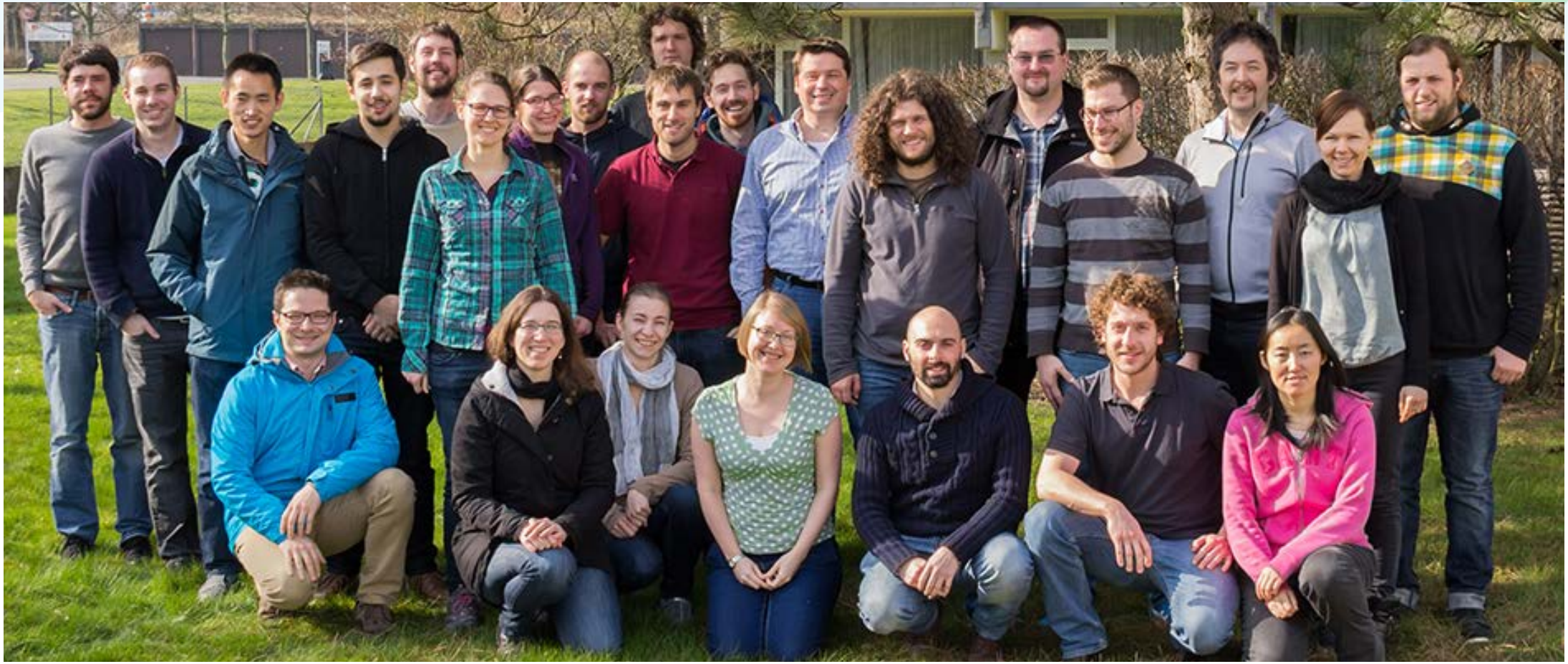
Chang,Horke,Trippel,Küpper International Reviews In Physical Chemistry Vol. 34 , Iss. 4,2015

Müller, Trippel, Długołęcki, Küppe,J. Phys. B: At. Mol. Opt. Phys. 48, 244001(2015)

Daria Popova-Gorelova, Jochen Küpper, Robin Santra, Phys. RevA94, 013412 92(2016)

This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 641789

ACKNOWLEDGEMENT



This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 641789

ACKNOWLEDGEMENT

Thanks to our collaborators

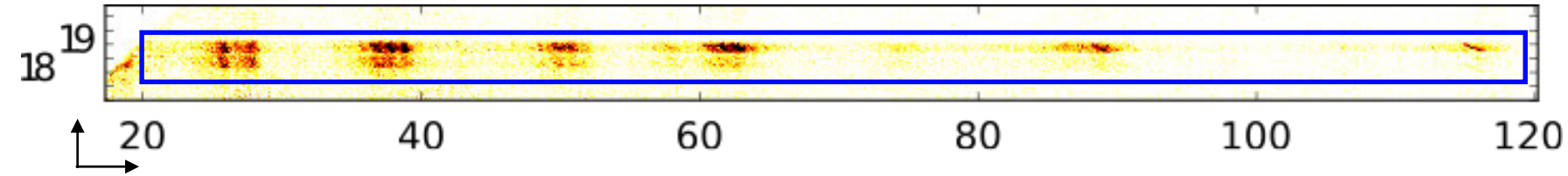
Denis Anielski[4], Rebecca Boll[4], Cédric Bomme[4], Benjamin Erk[4], Daniel Rolles[5], Evgeny Savelyev[4], Jens Viefhaus[4]

1) Center for Free-Electron Laser Science, DESY, Hamburg, Germany
2) The Hamburg Center for Ultrafast Imaging, University of Hamburg, Germany
3) Department of Physics, University of Hamburg, Germany
4) Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany
5) J.R. Macdonald Laboratory, Department of Physics, Kansas State University, Manhatten, USA

Thank you for your attention!

This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 641789

PIPICO — VMI images

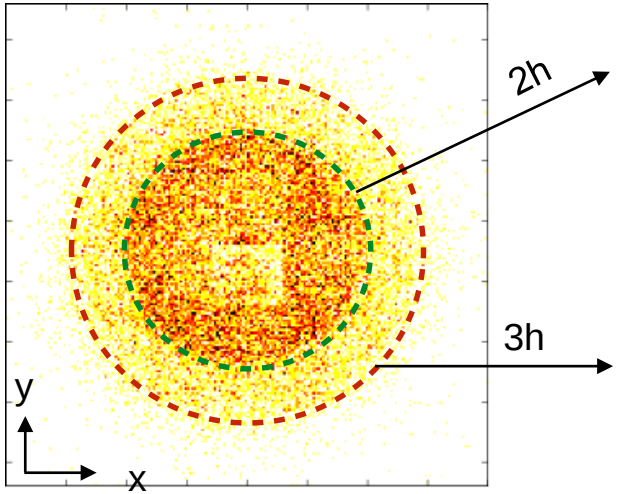


H_2O^+ (18)

H_3O^+ (19)

- charge and mass transfer to hydrogen bonded water
- different fragmentation channels for mass-transfer

Velocity map imaging (VMI) of hydronium



velocity