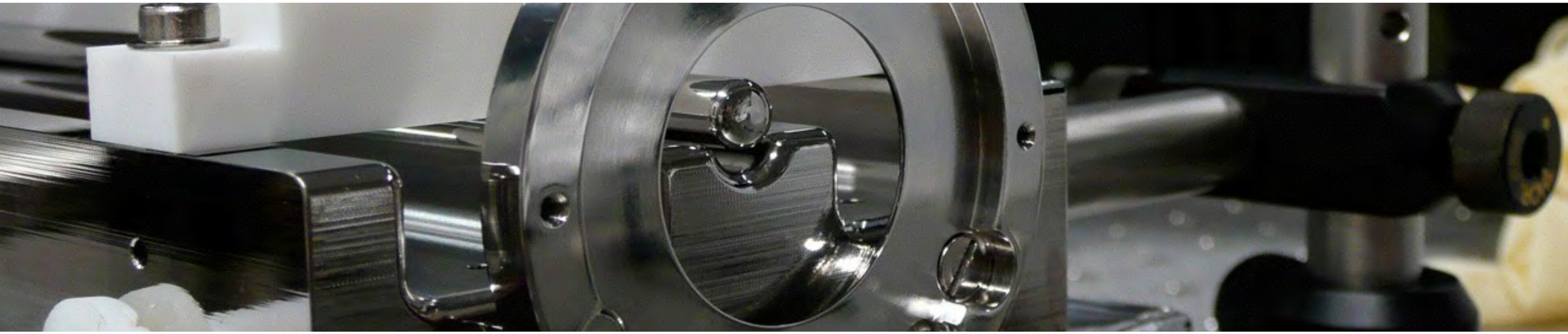
Presentation of the DESY node
DESY–CFEL – Controlled Molecule Imaging
DESY–FLASH – CAMP @ FLASH

Jochen Küpper

Center for Free-Electron Laser Science (CFEL), DESY, Hamburg, Germany
Department of Physics, University of Hamburg, Germany
The Hamburg Center for Ultrafast Imaging (CUI), Germany
Daniel Rolles – Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany



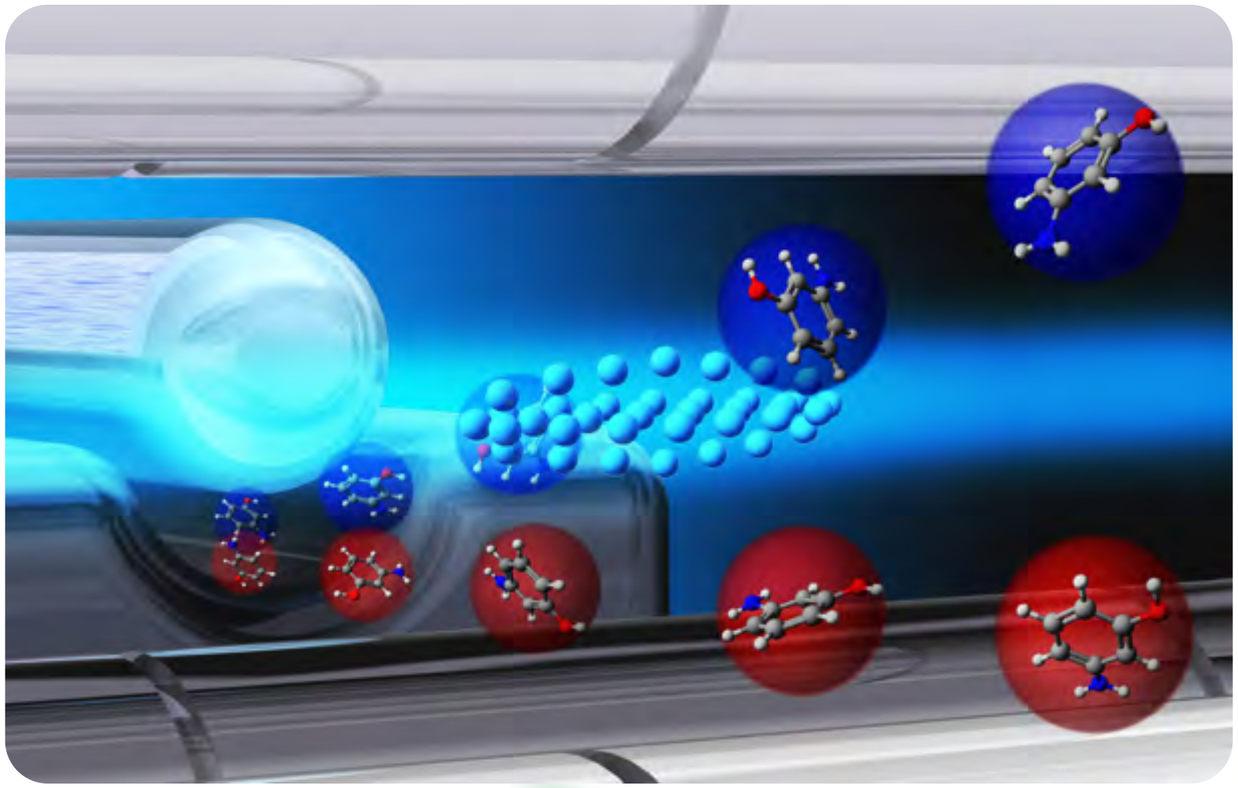
CUI THE HAMBURG CENTER FOR ULTRAFAST IMAGING

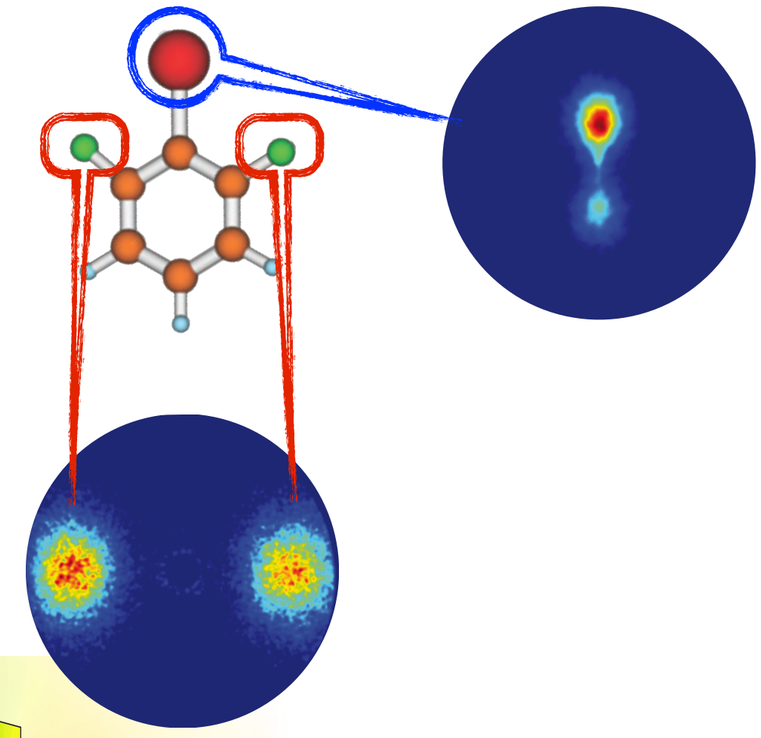
Universität Hamburg
DER FORSCHUNG | DER LEHRE | DER BILDUNG

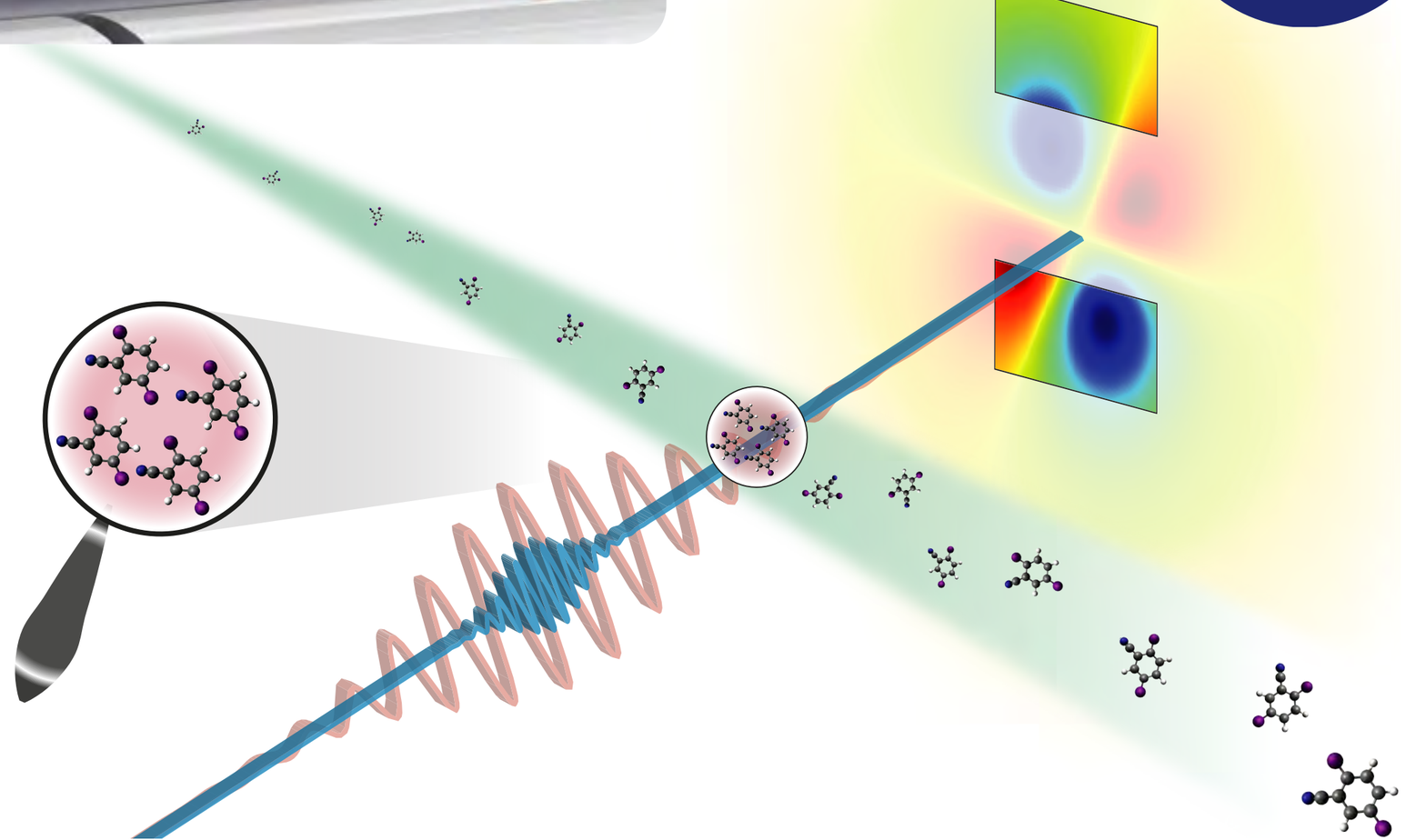
CFEL SCIENCE
Controlled Molecule Imaging

DESY
HELMHOLTZ ASSOCIATION

Complex molecules in the gas-phase
Understanding the structure-function relationship







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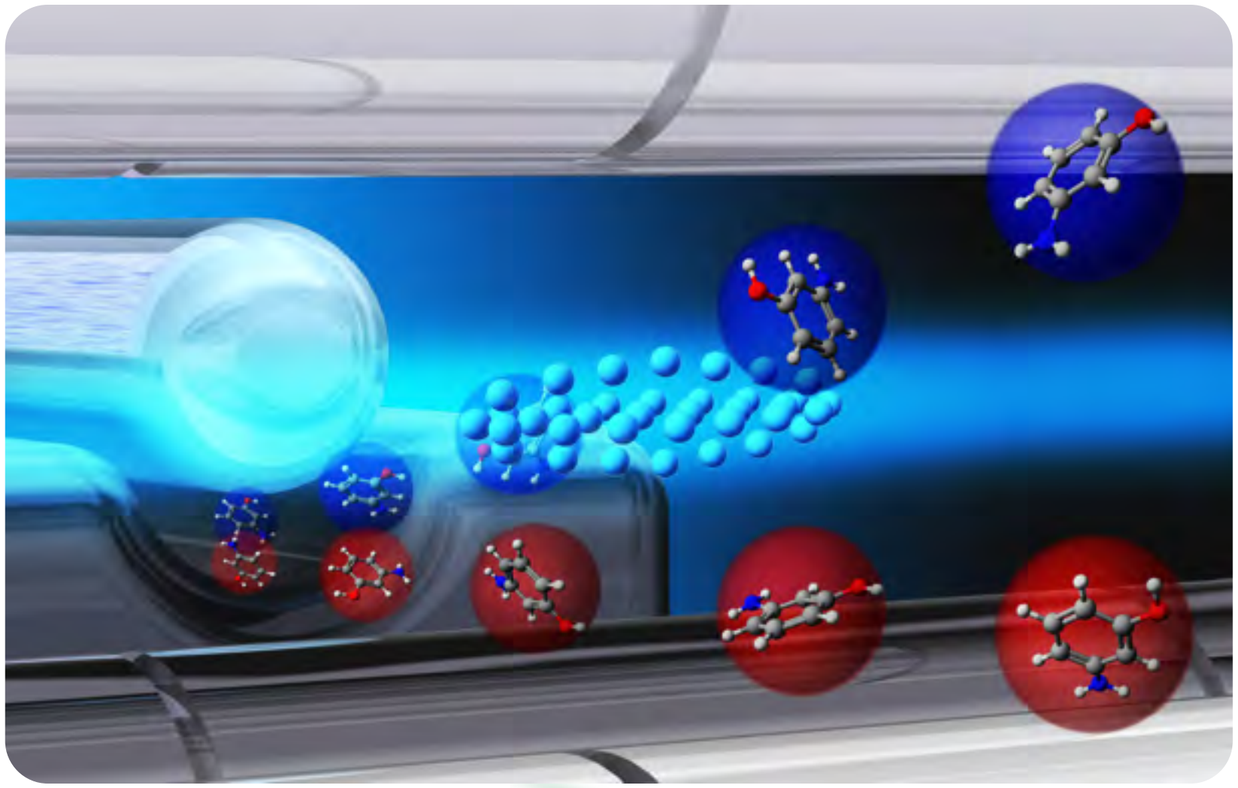
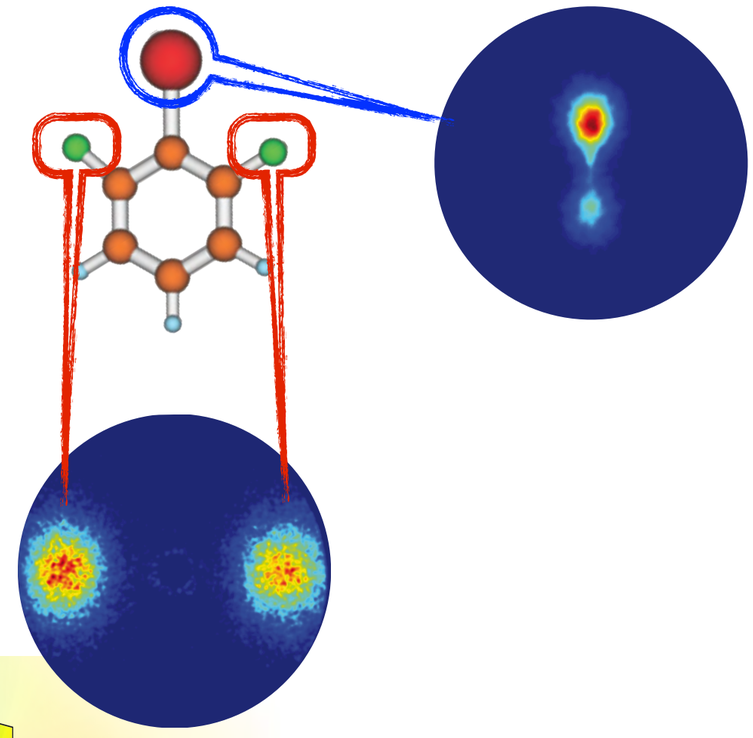
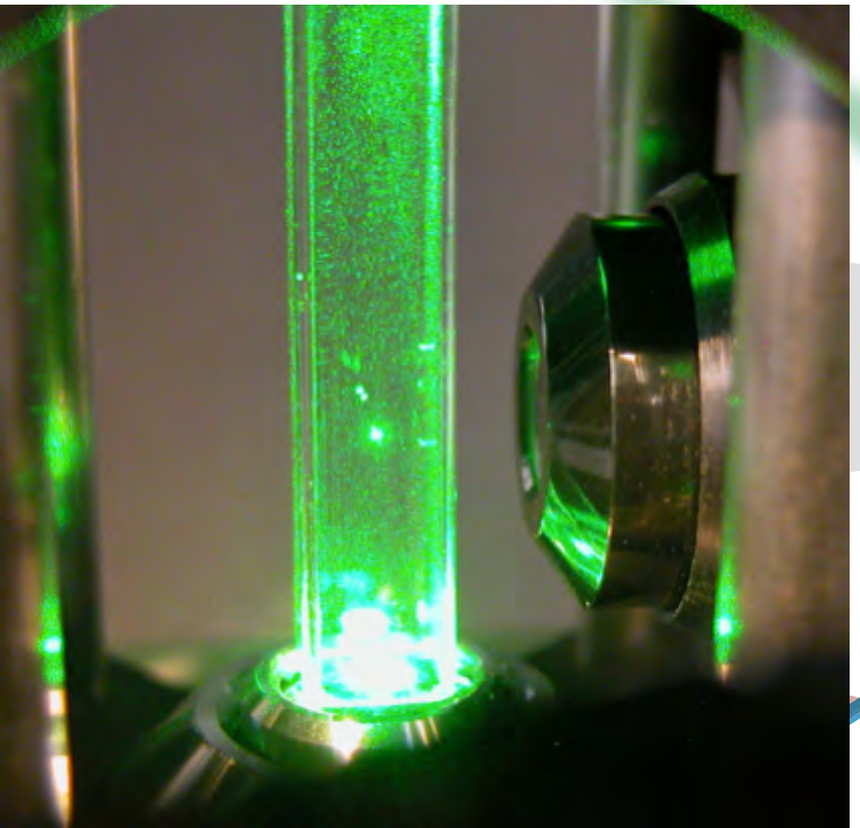
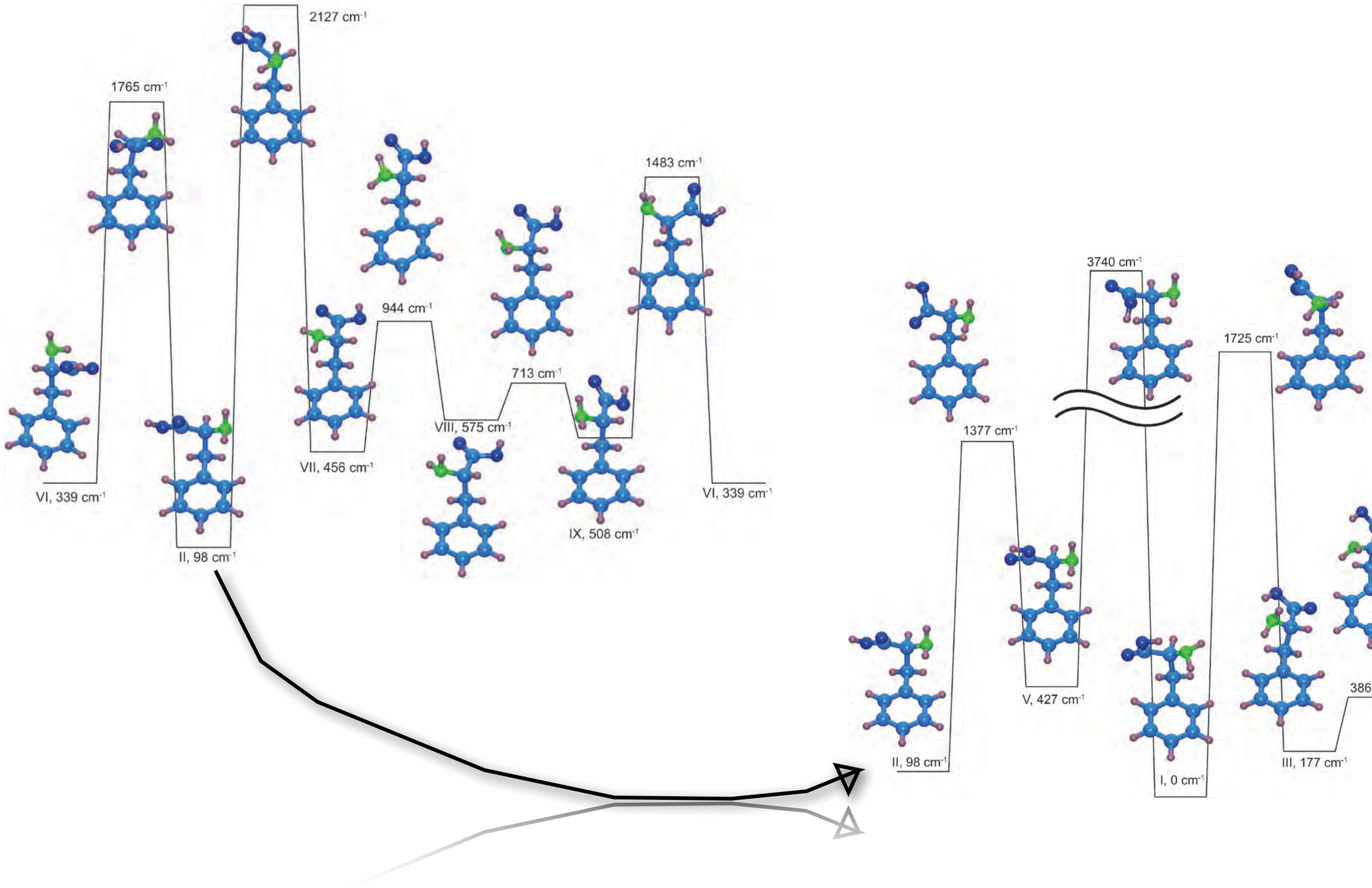






The structure-function relationship of electronic dynamics
Conformers of amino acids: glycine and phenylalanine



von Helden, Compagnon, Blom, Frankowski, Erlekam, Oomens, Brauer, Gerber, Meijer, *Phys. Chem. Chem. Phys.* **10**, 1248 (2008)
Miller, Clary, Meijer, *J. Chem. Phys.* **122**, 244323 (2005)

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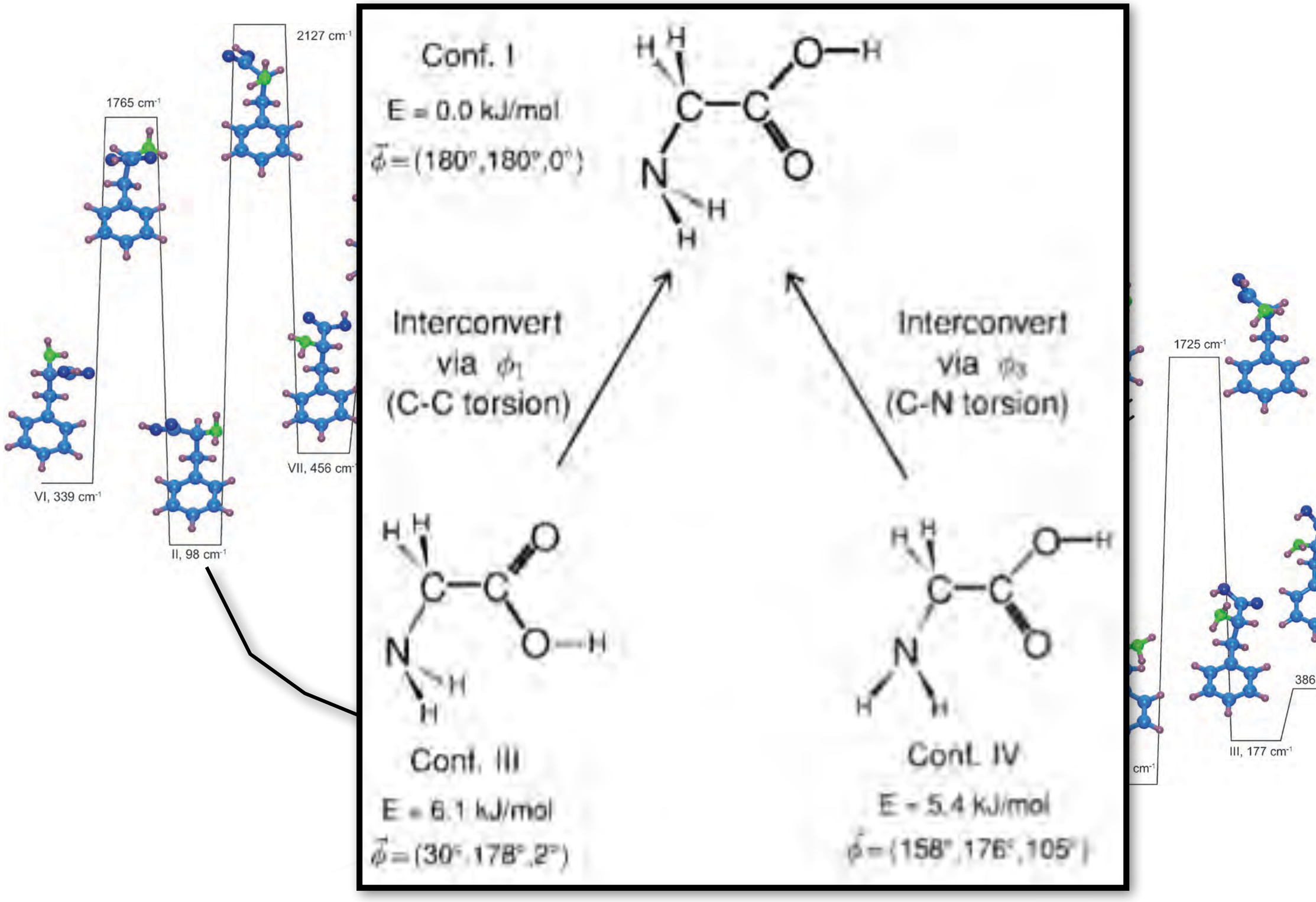

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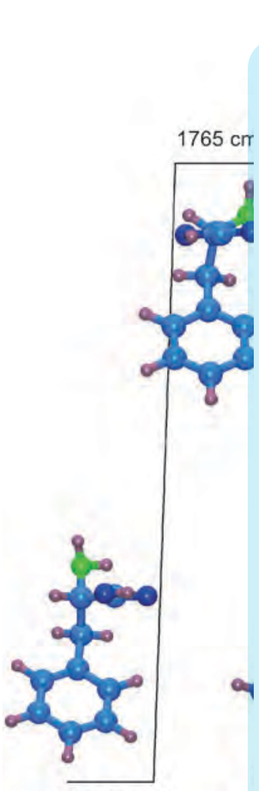
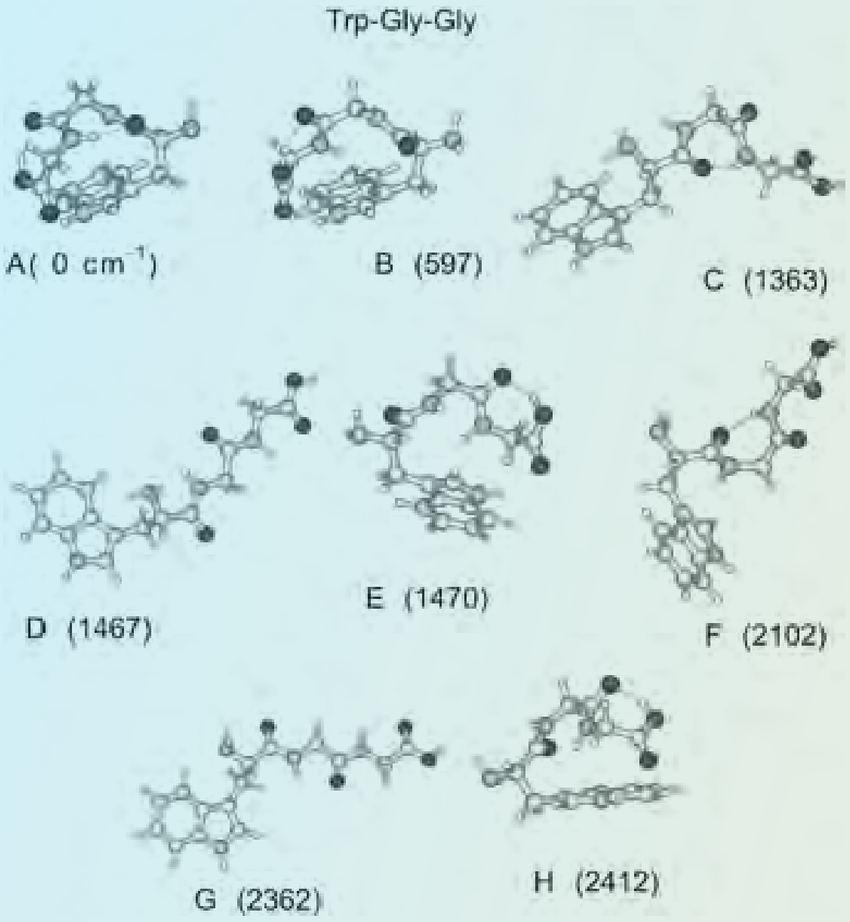
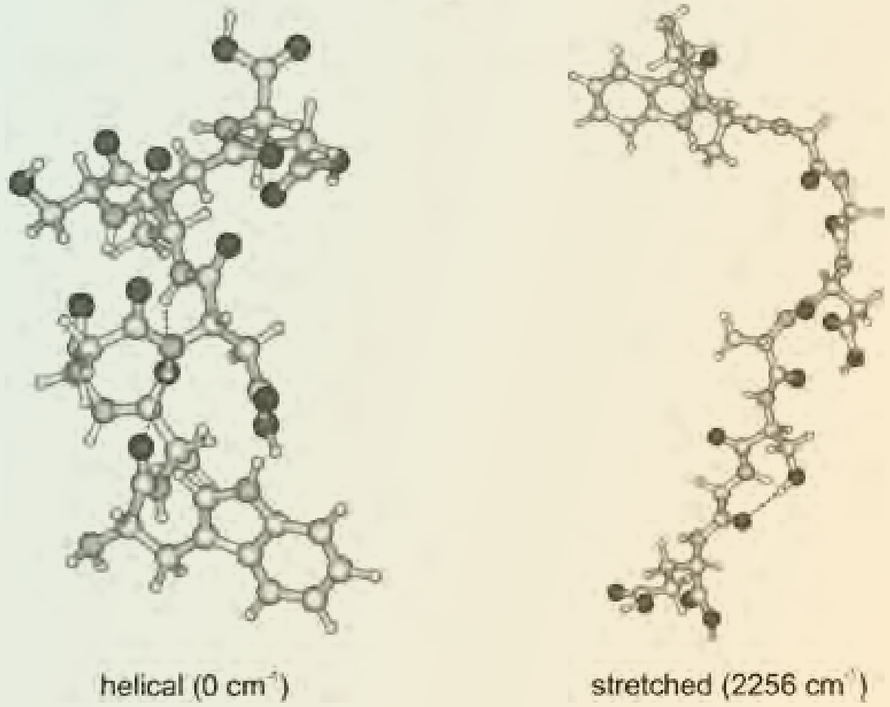
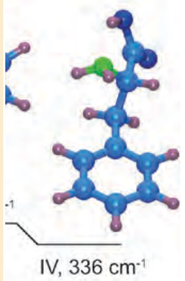
The structure-function relationship of electronic dynamics
Conformers of amino acids: glycine and phenylalanine

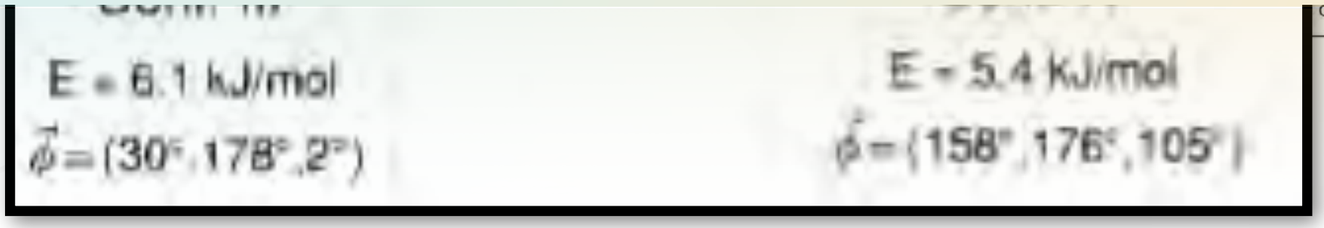
and bigger....











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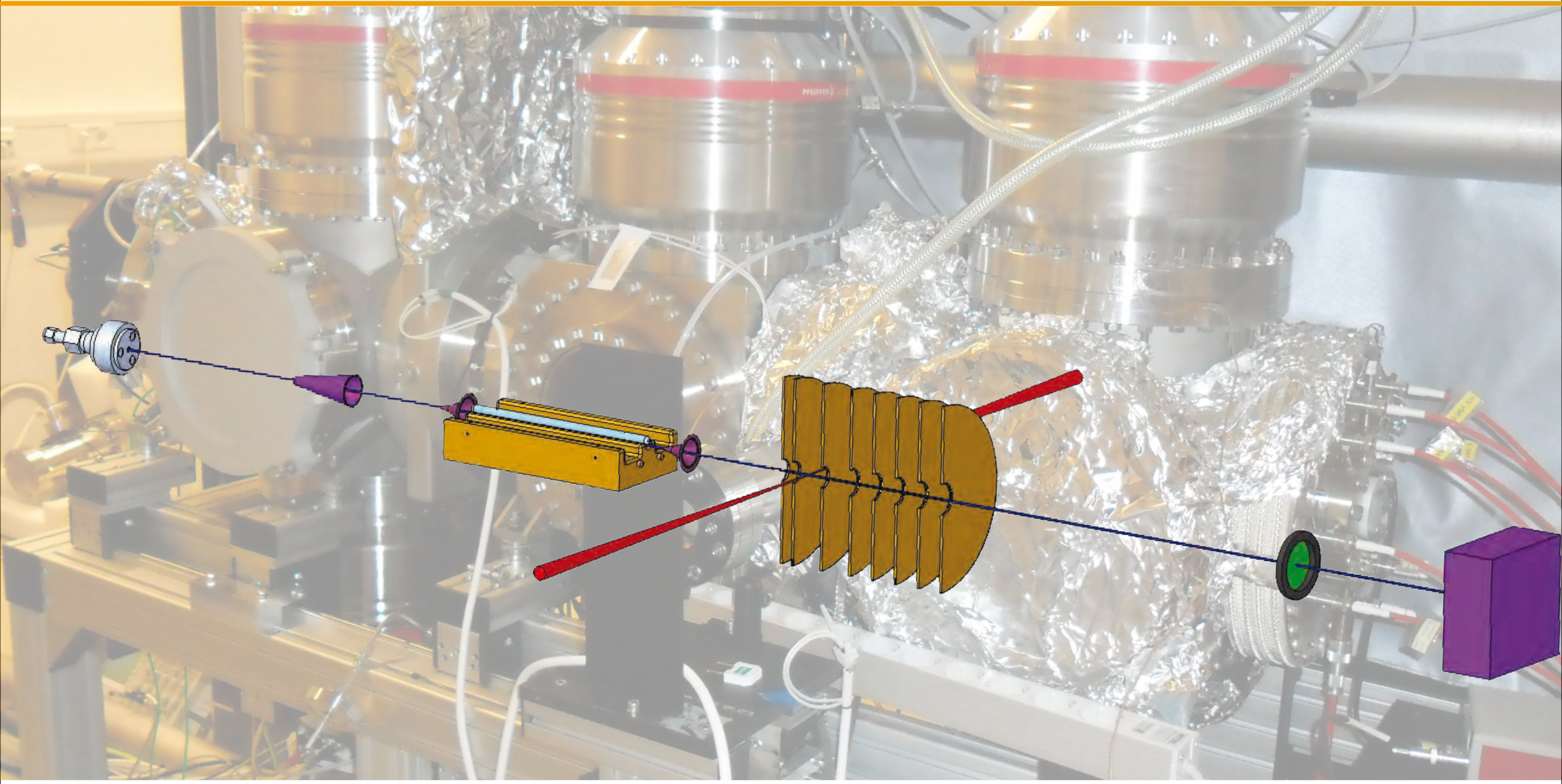
Toward time-resolved *imaging of chemical dynamics* kHz-rate manipulation experiments



Trippel, Mullins, Müller, Kienitz, Długołęcki, JK, *Mol. Phys.* **111**, 1738-1743 (2013, Bretislav Friedrich Festschrift)

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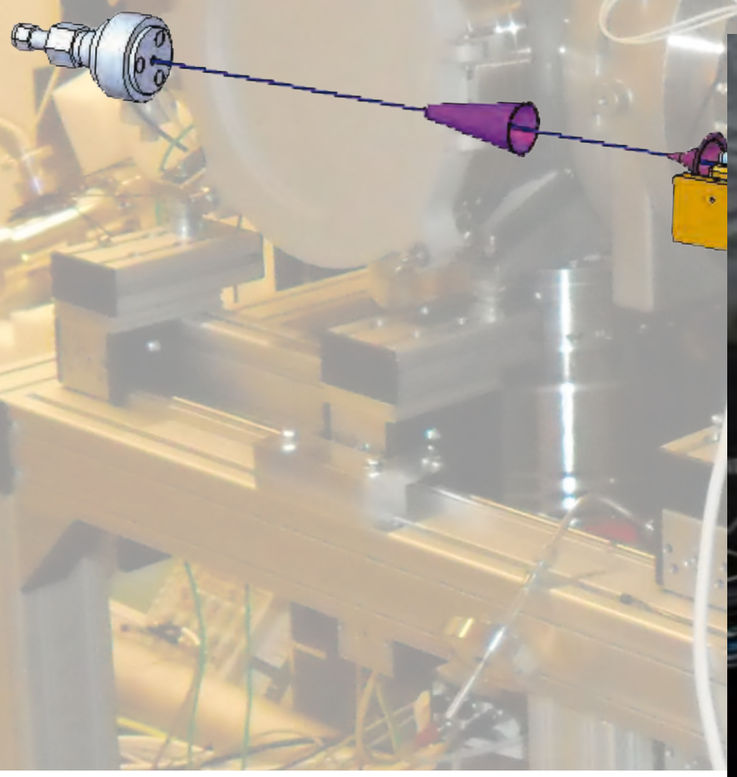

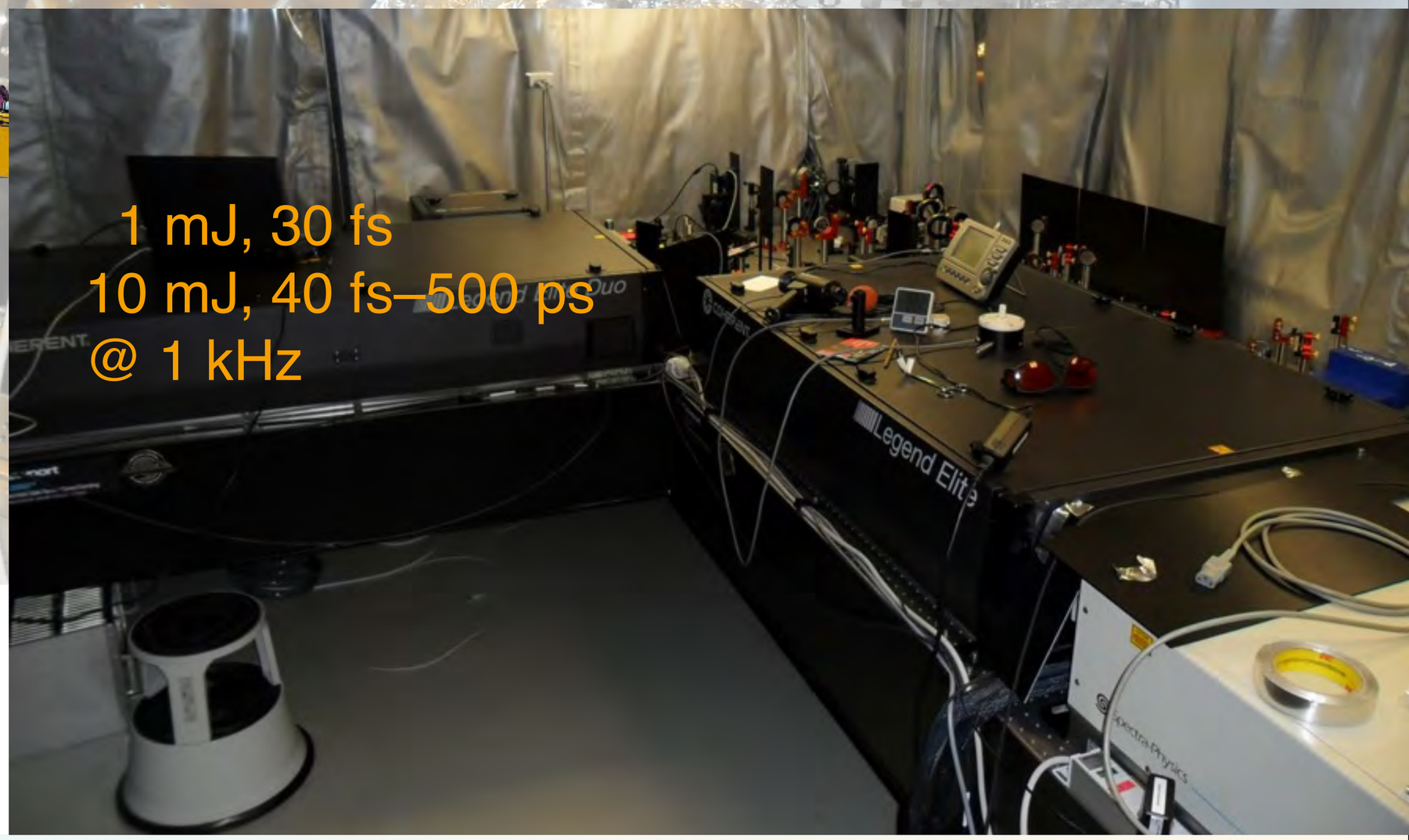

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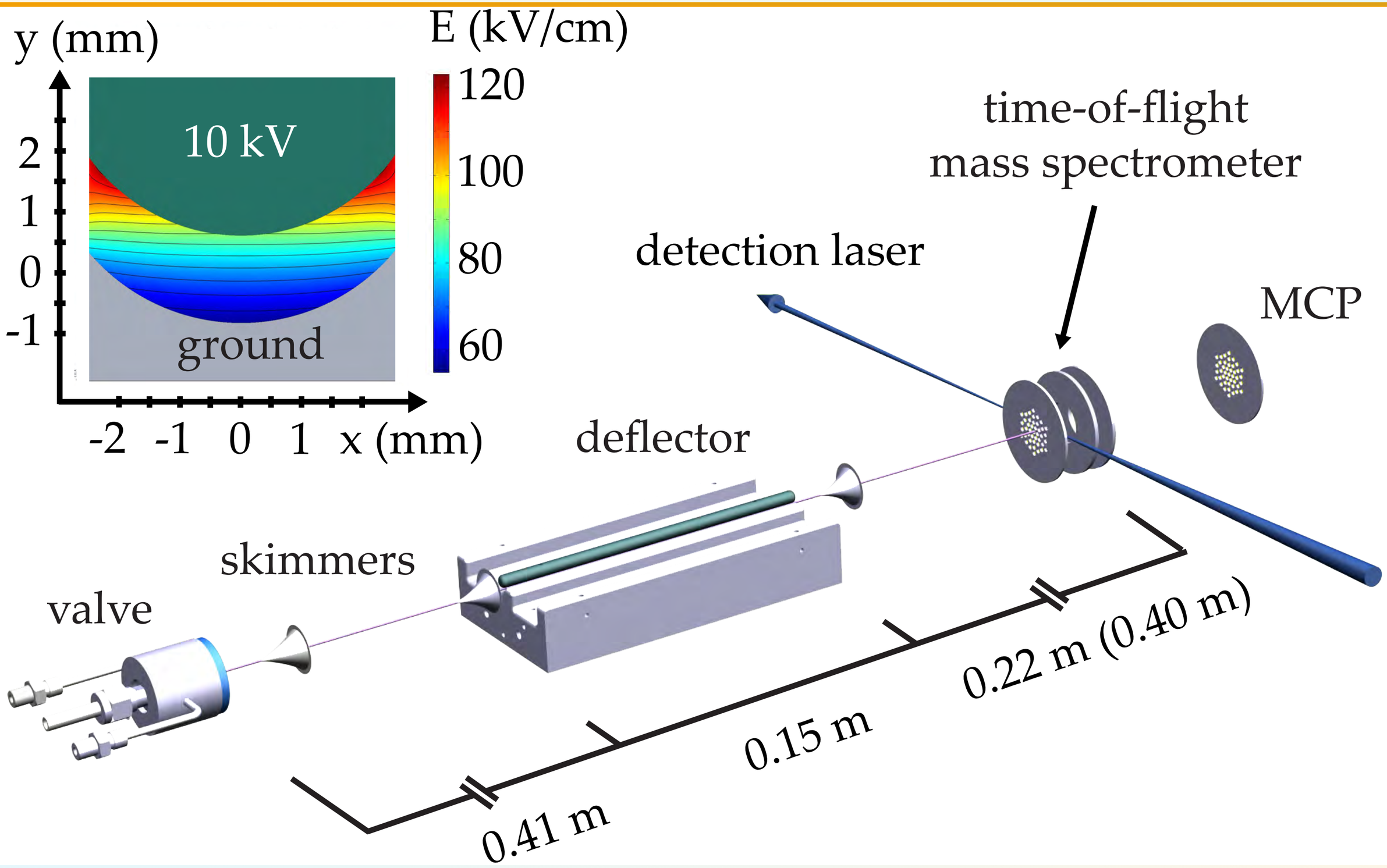
Electric manipulation of the motion of neutral molecules
– separating species according to m/μ –



Filsinger, Erlekam, von Helden, JK, Meijer, *Phys. Rev. Lett.* ***100***, 133003 (2008)
Wohlfart, Graetz, Haak, Meijer, JK *Phys. Rev.* A **77**, 031404(R) (2008)
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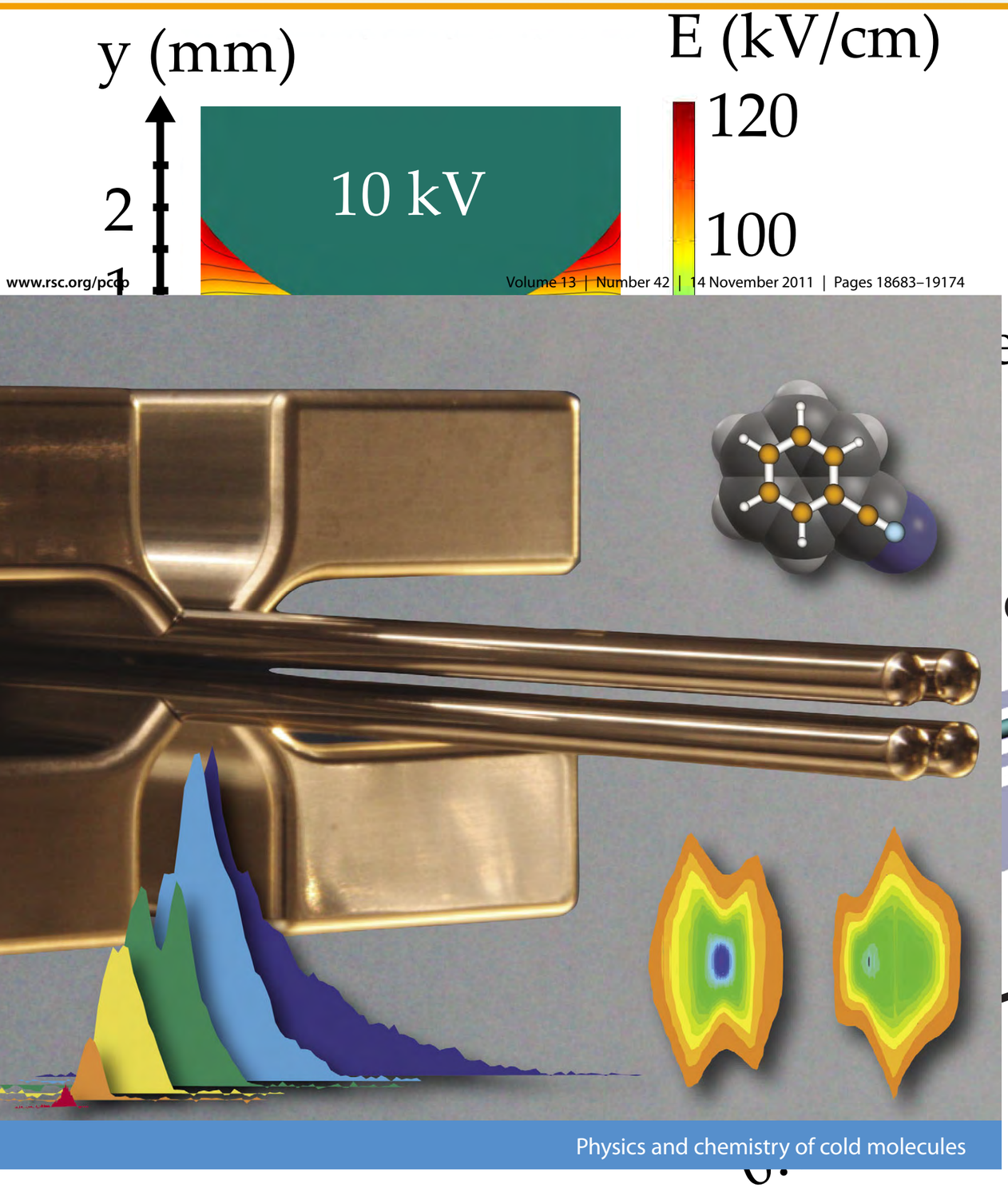

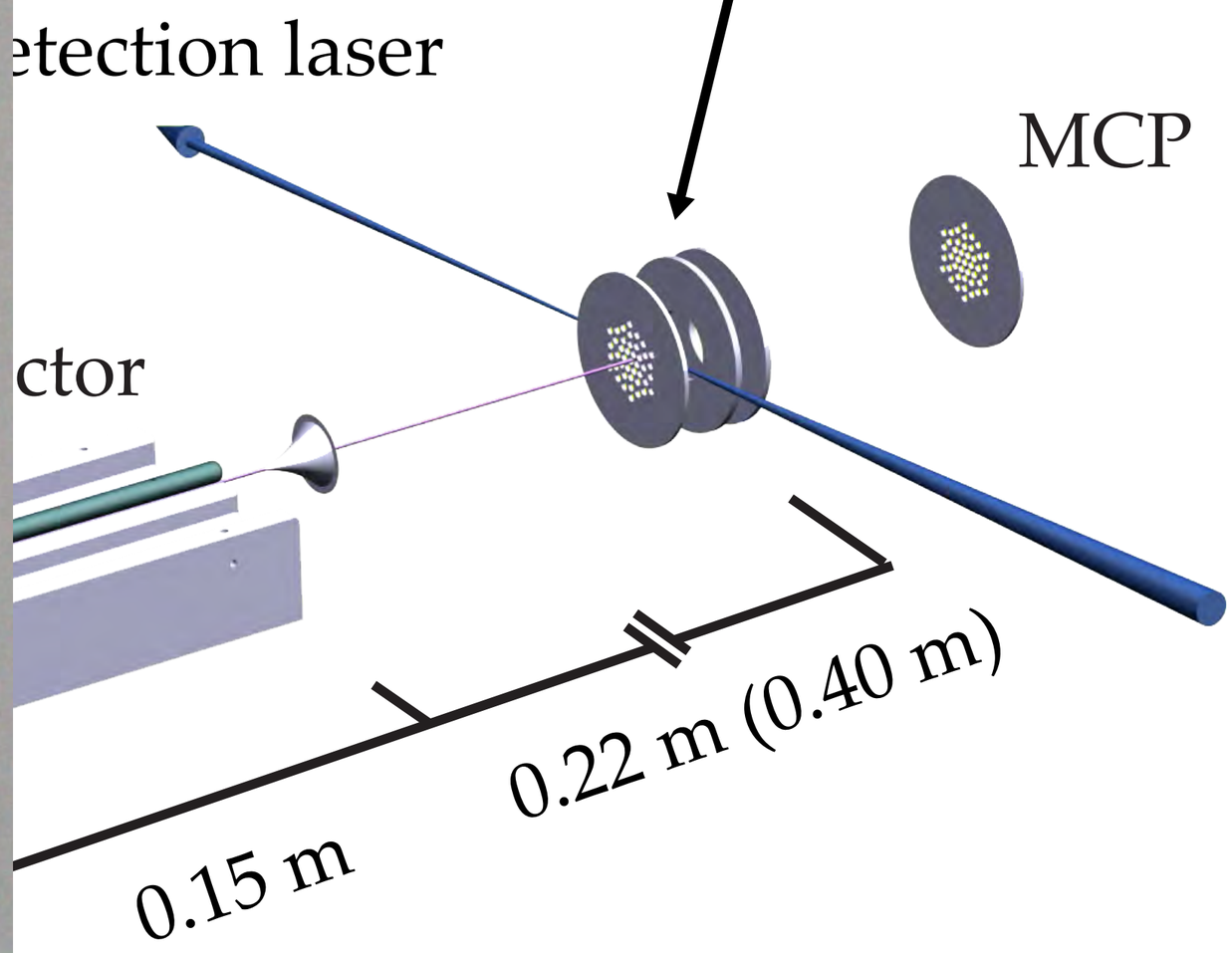

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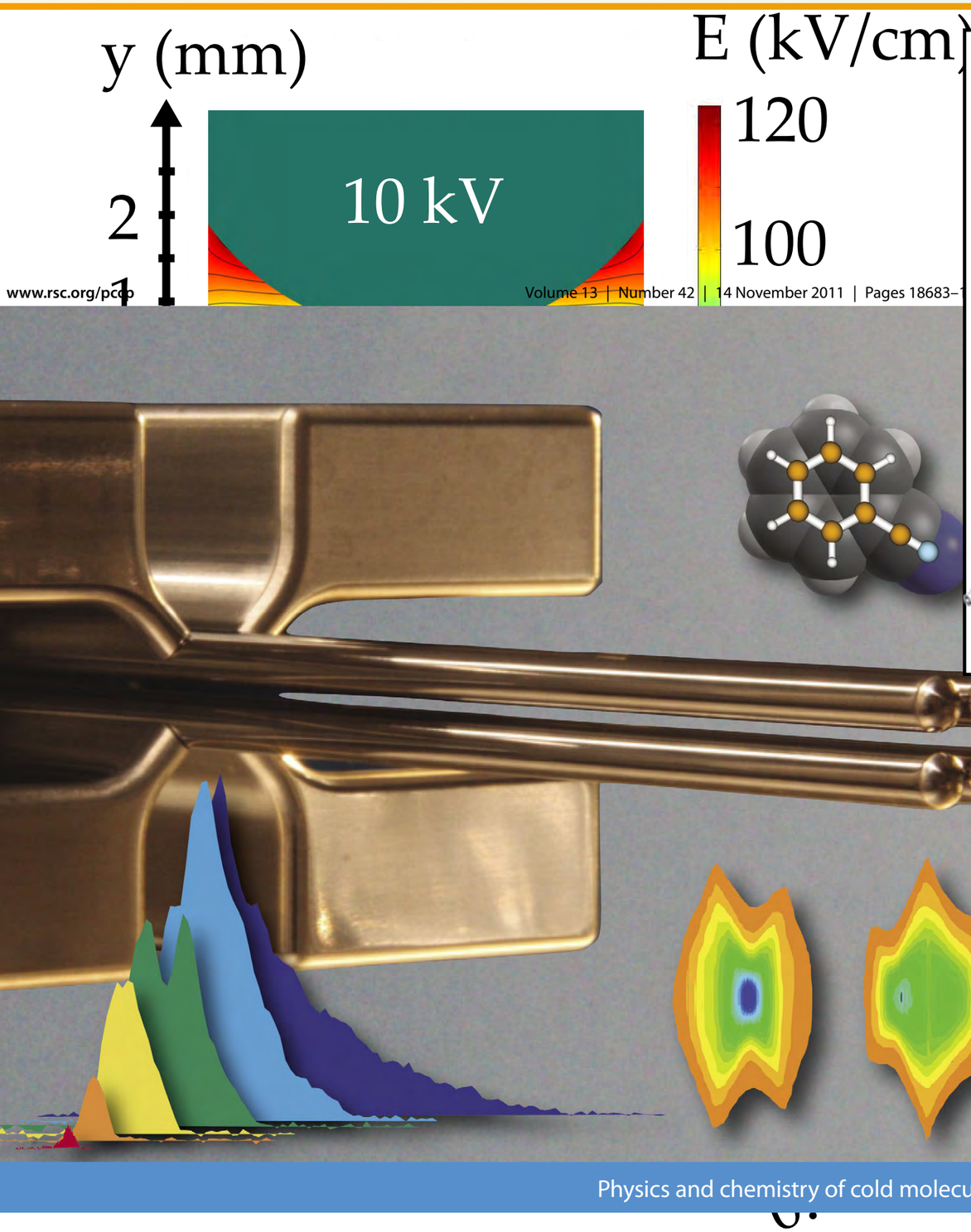

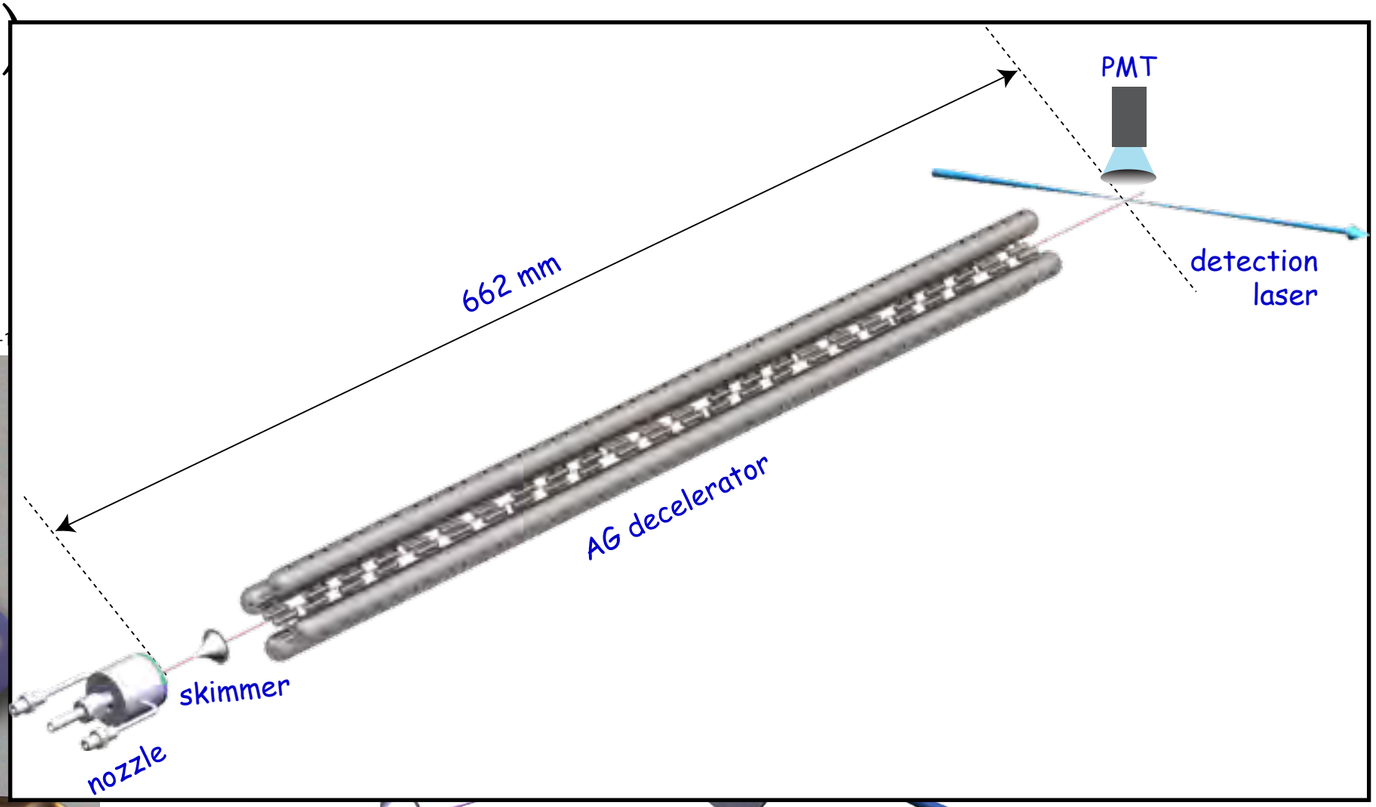

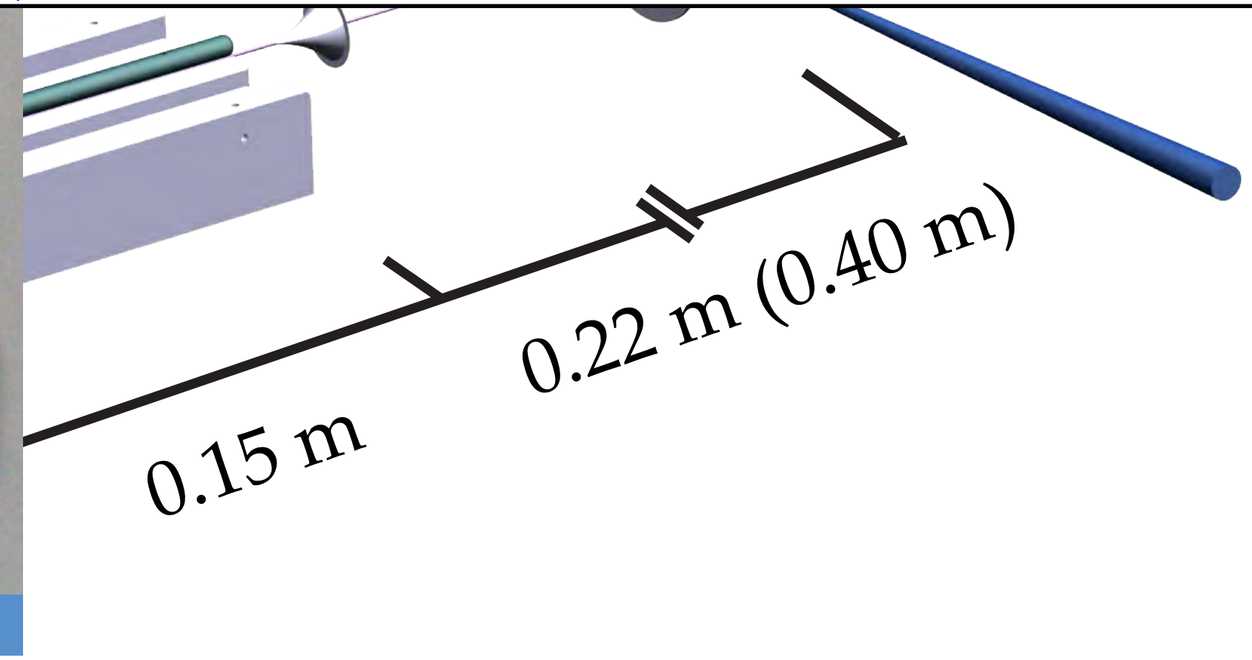

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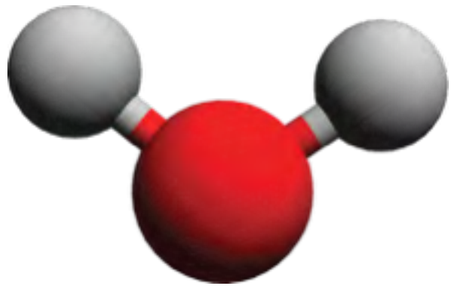
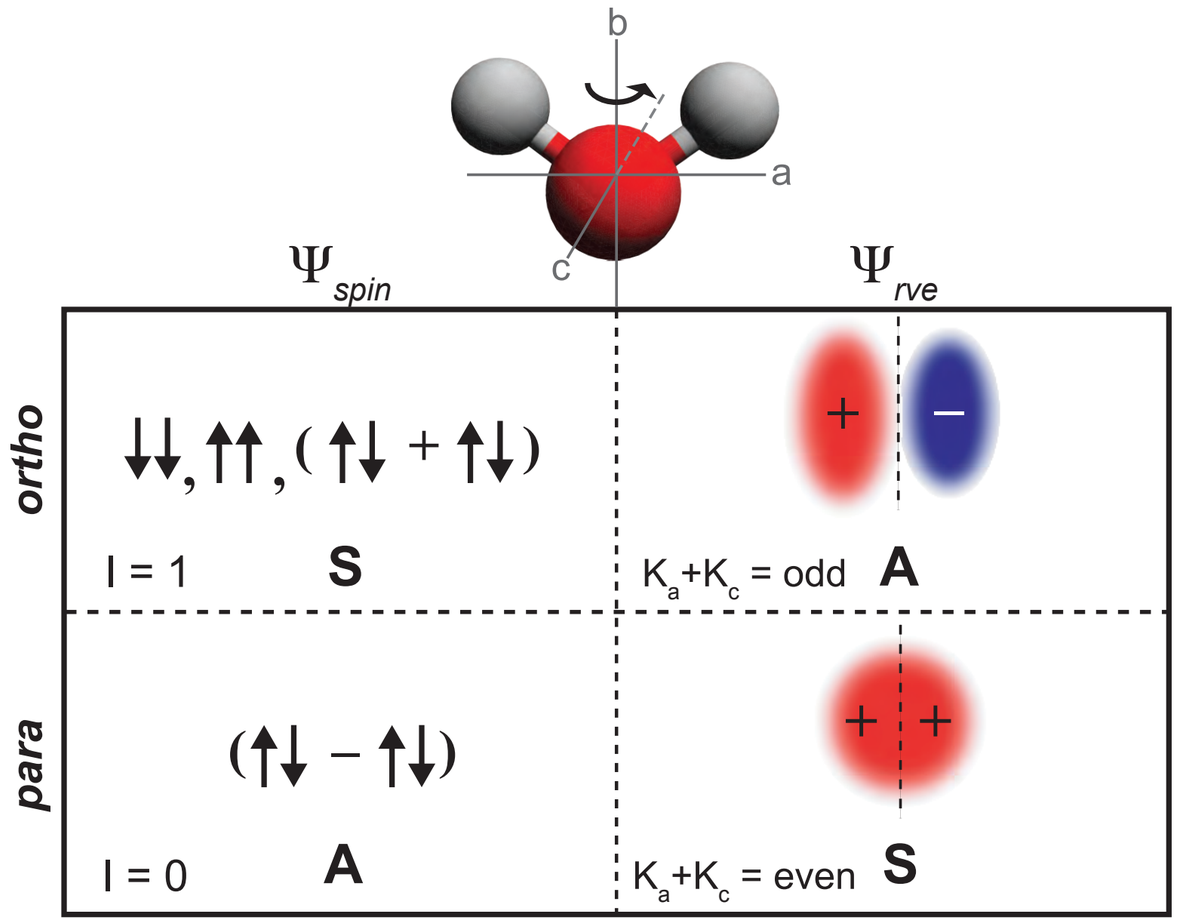
Nuclear-spin isomers of water (H_2O)

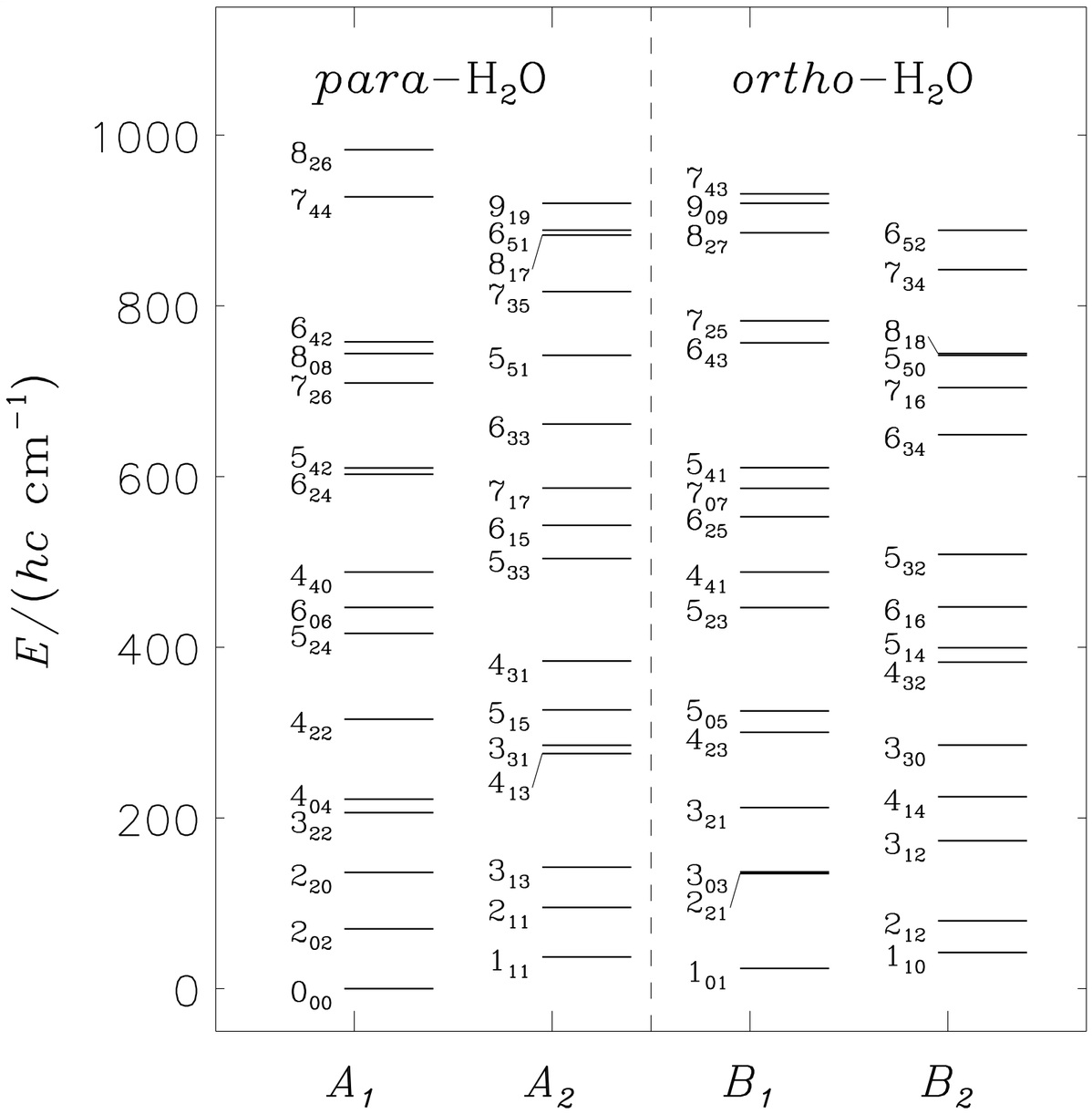
Structural details



$$(12)\Psi = -\Psi$$

$$\Gamma_{\Psi_{\rm tot}} = \Gamma_{\Psi_{\rm ns}} \otimes \Gamma_{\Psi_{\rm rve}}$$





Horke, Chang, Długołęcki, JK, *Angew. Chem. Int. Ed.* **53,** 11965 (2014, *VIP*)

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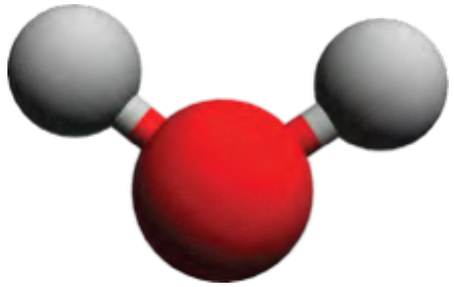

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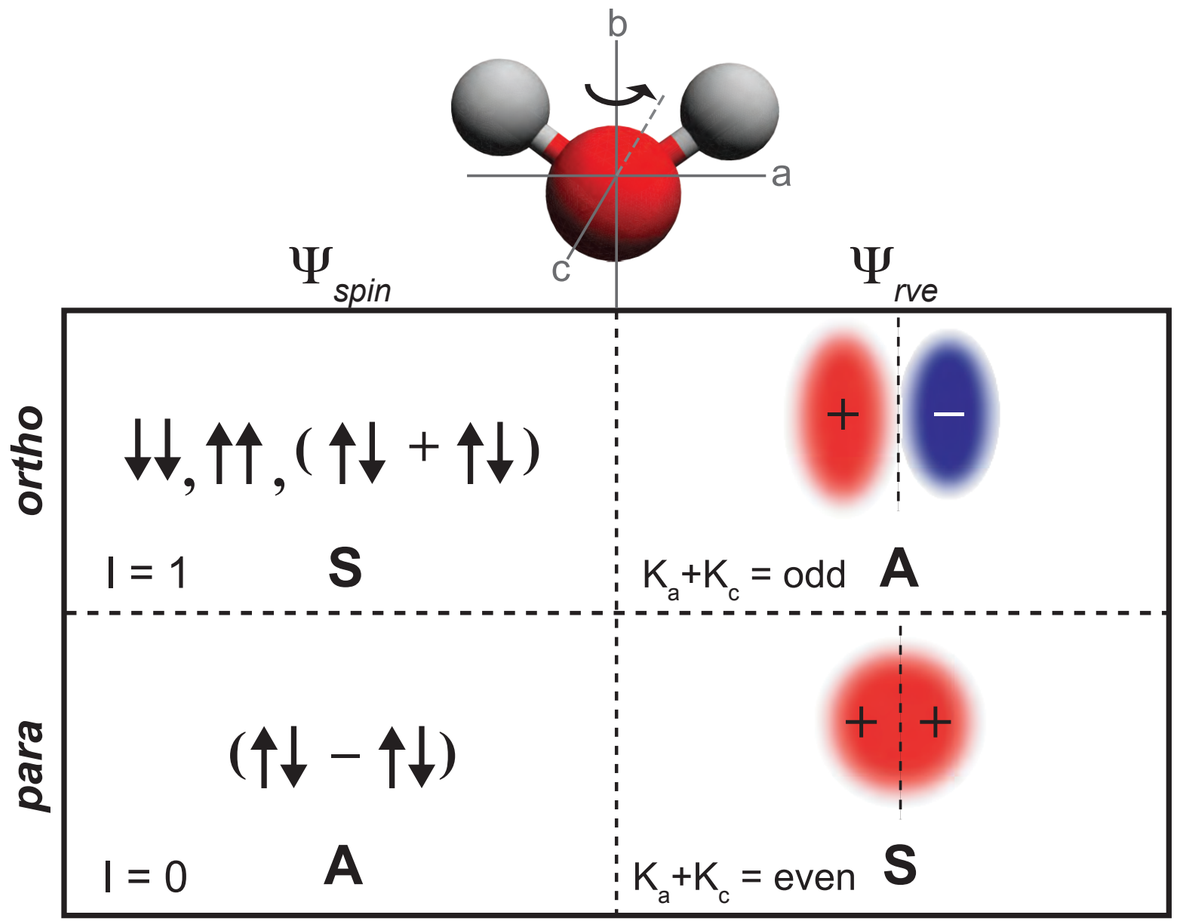
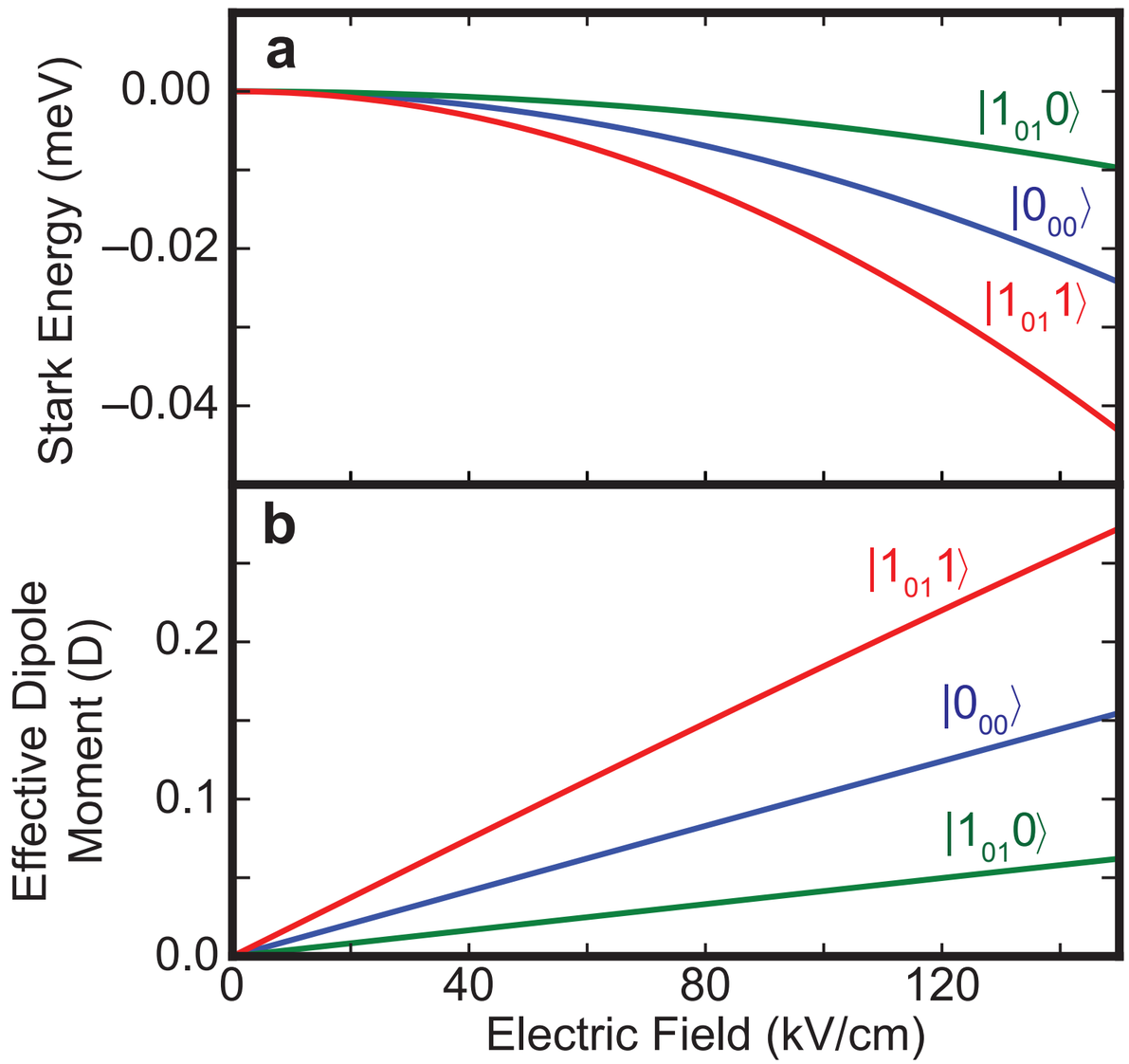
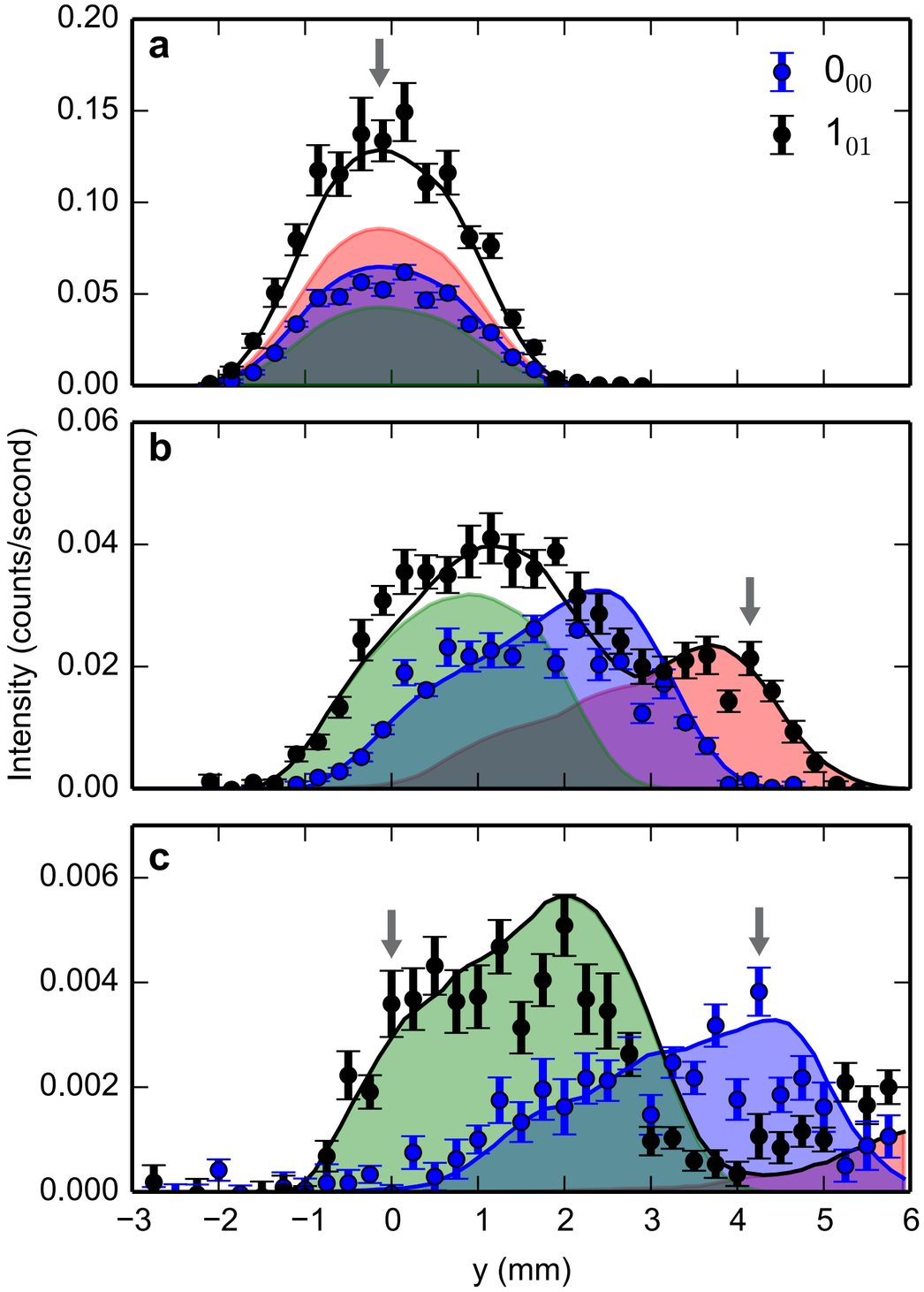
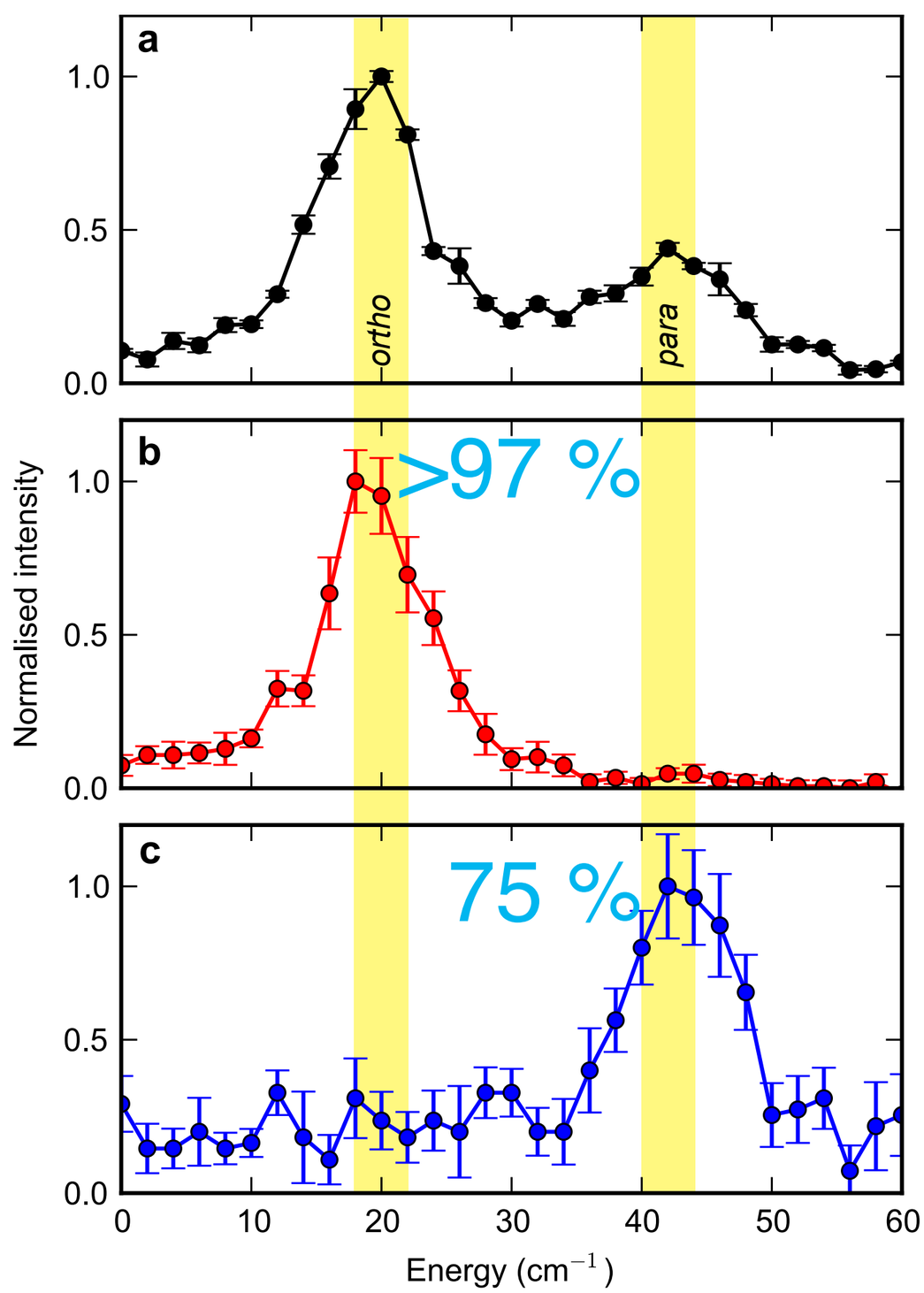




Horke, Chang, Długołęcki, JK, *Angew. Chem. Int. Ed.* **53,** 11965 (2014, *VIP*)

Separating para and ortho water





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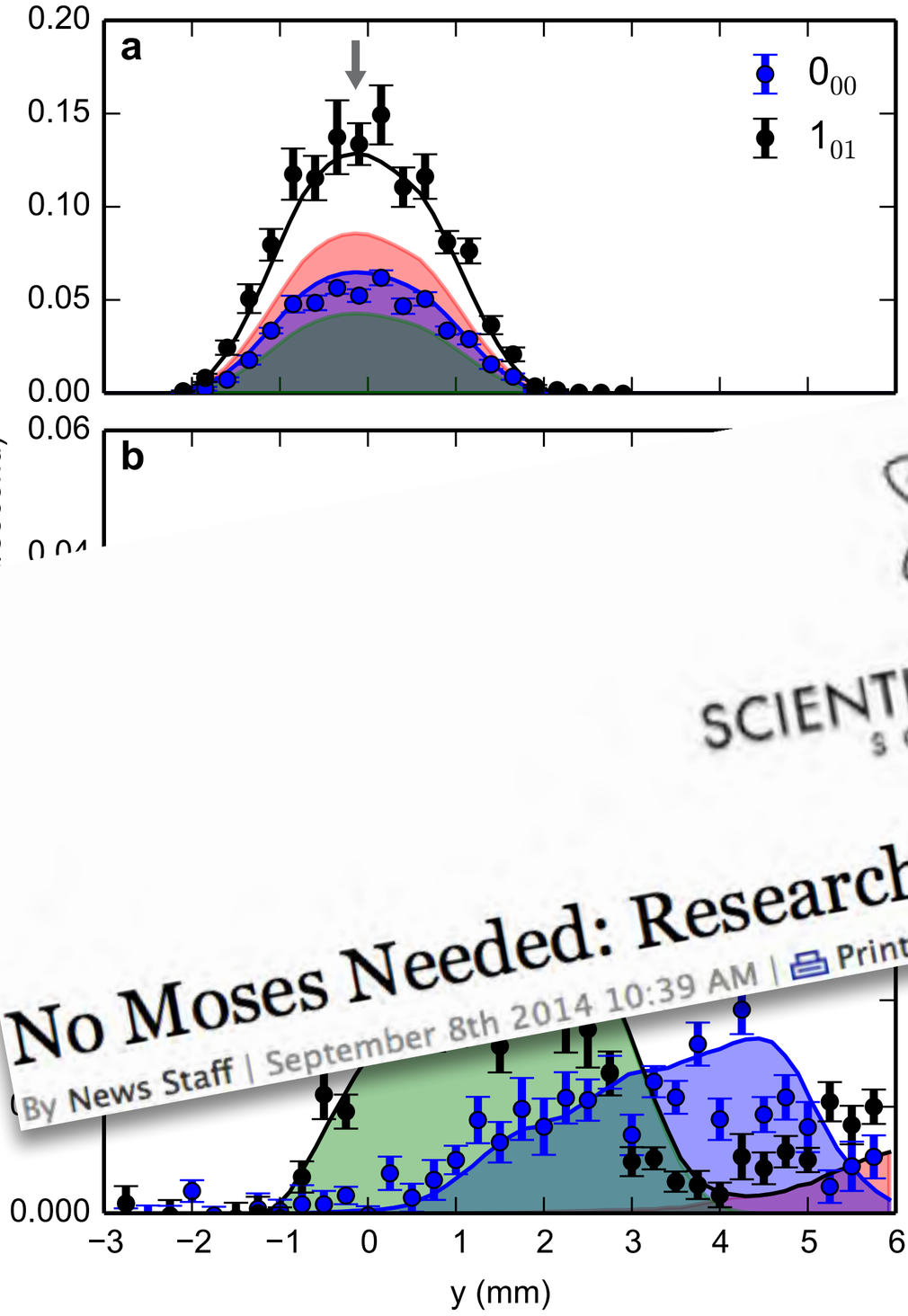

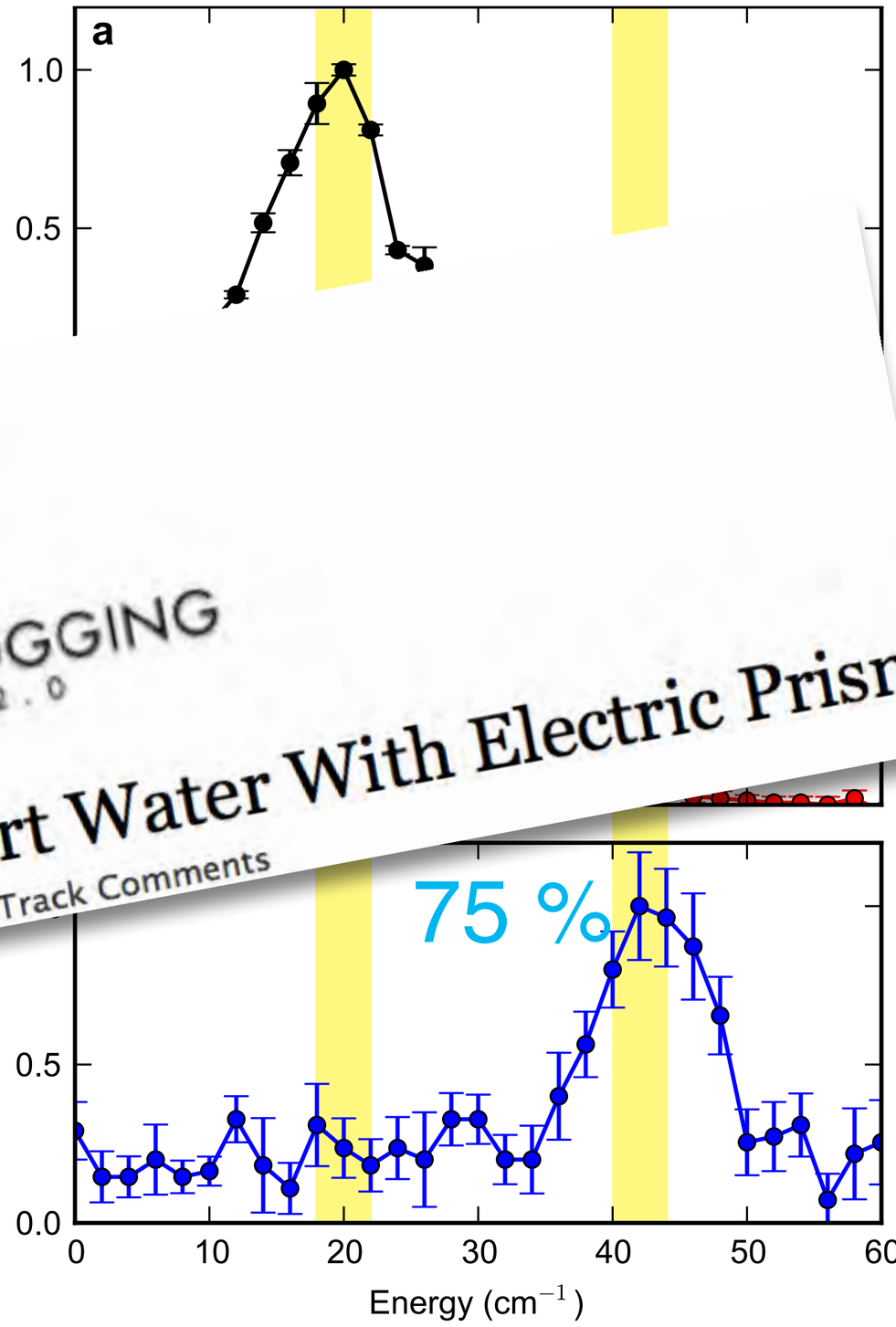

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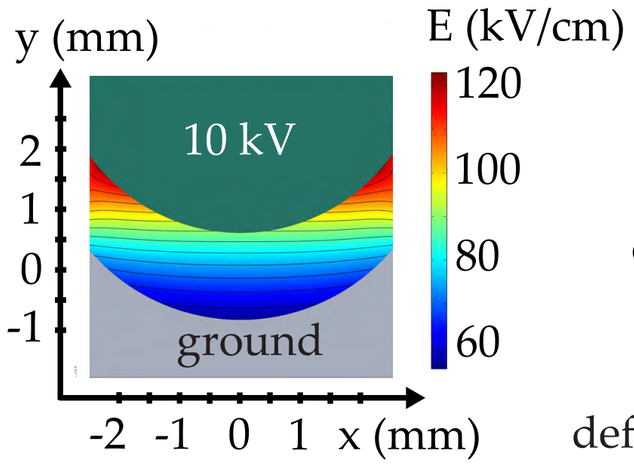
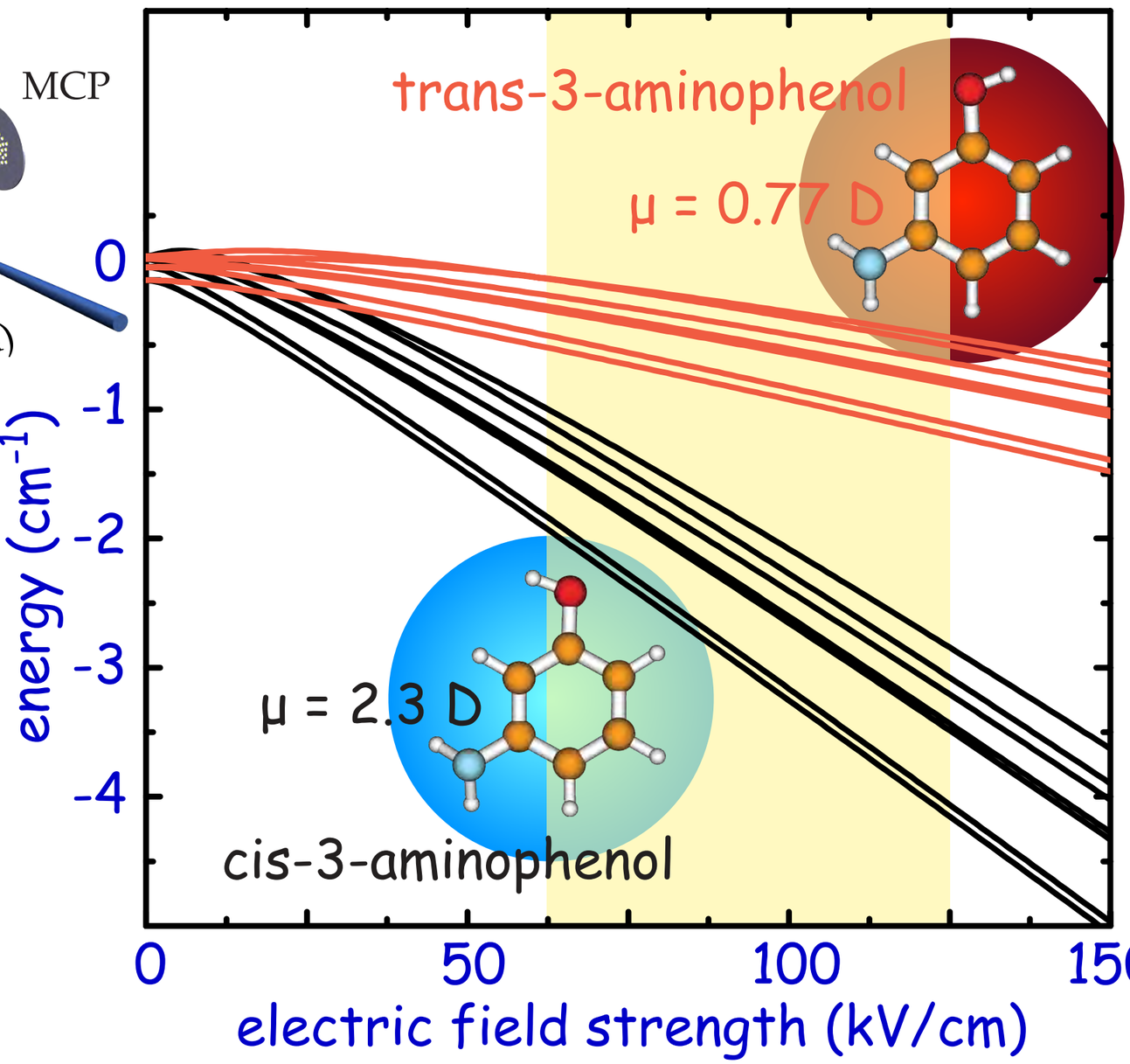
No Moses Needed: Researchers Part Water With Electric Prism

By News Staff | September 8th 2014 10:39 AM | Print | E-mail | Track Comments

Horke, Chang, Długołęcki, JK, *Angew. Chem. Int. Ed.* **53,** 11965 (2014, *VIP*)

Conformer selection with the m/μ deflector

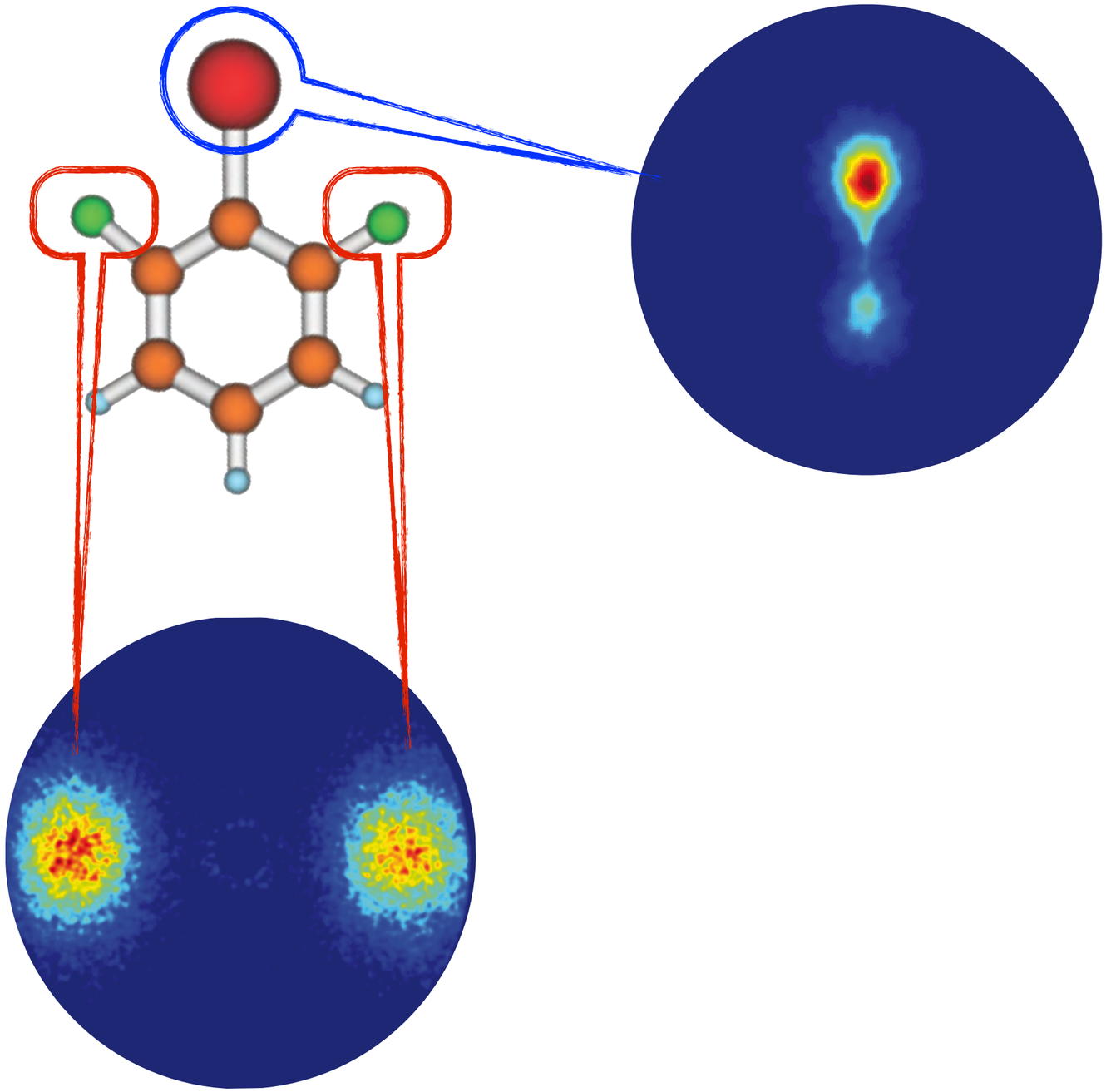




Filsinger, Erlekam, von Helden, JK, Meijer, *Phys. Rev. Lett.* ***100***, 133003 (2008)

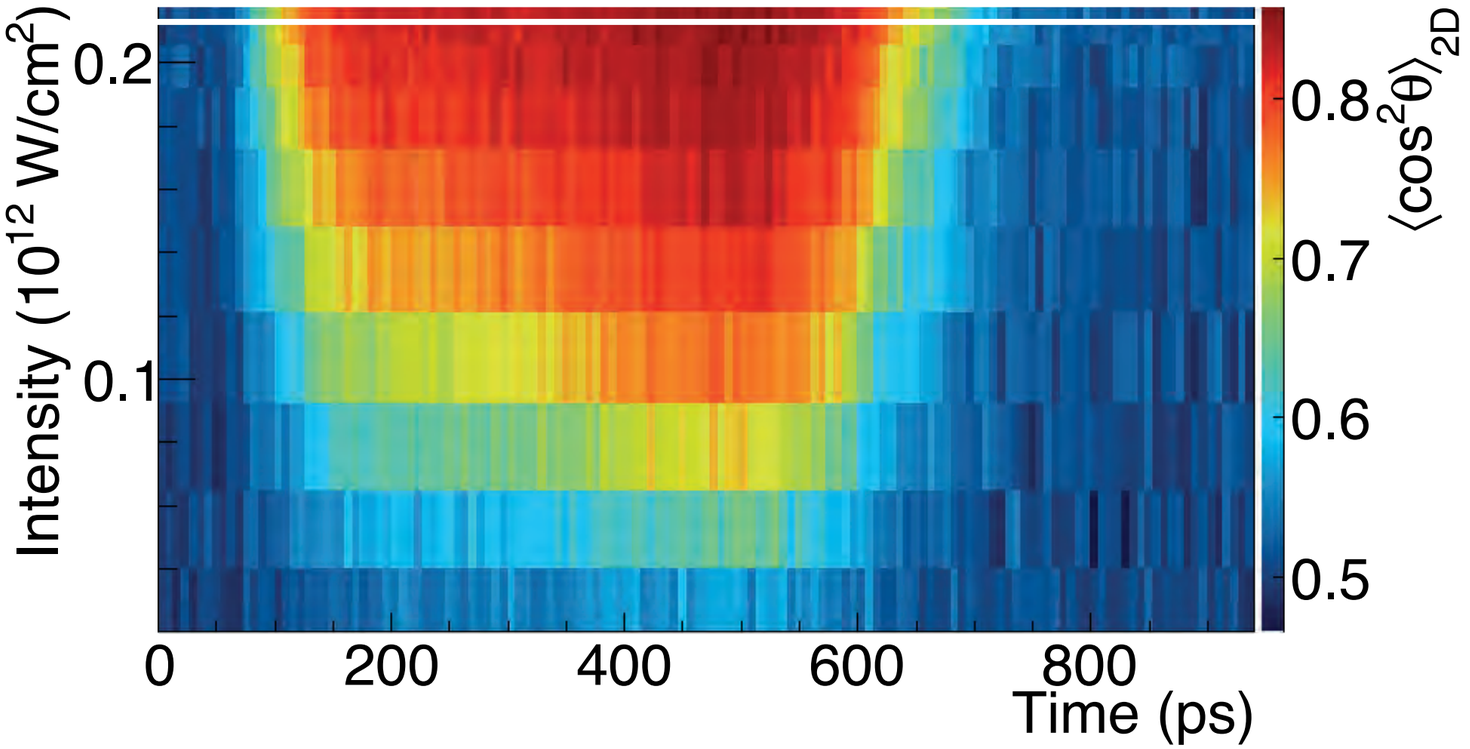
Filsinger, JK, Meijer, Hansen, Maurer, Nielsen, Holmegaard, Stapelfeldt, *Angew. Chem. Int. Ed.* **48**, 6900 (2009)

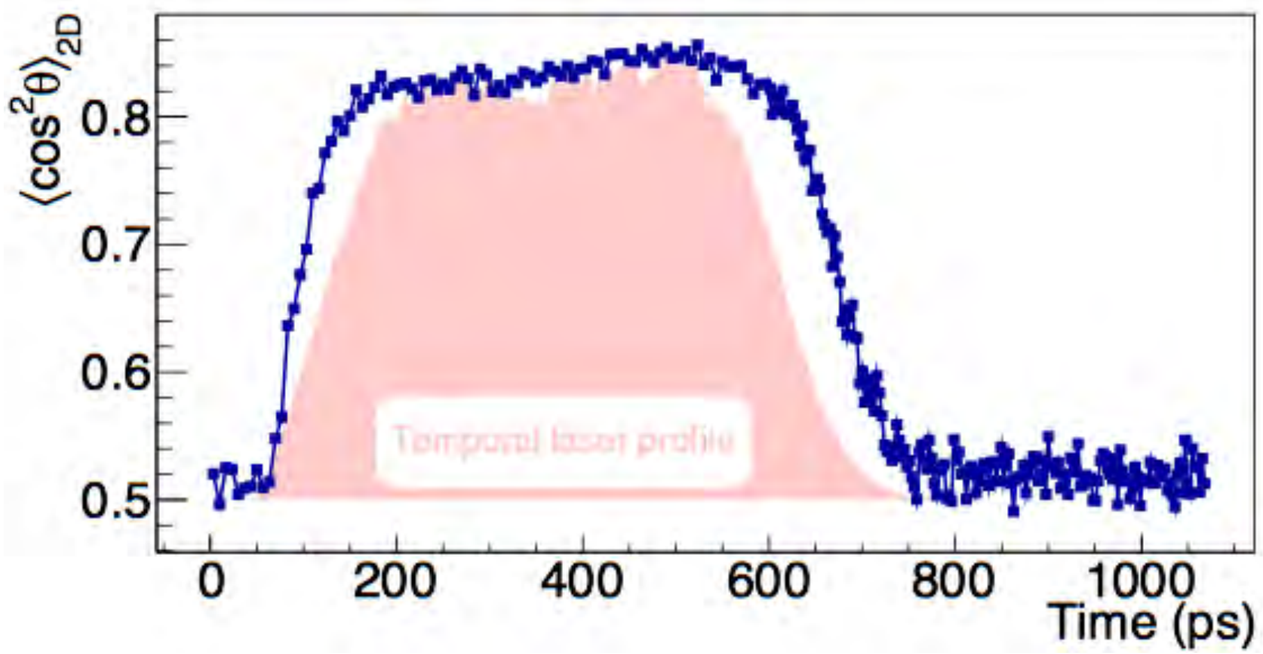
Fixing molecules in space
3D orientation

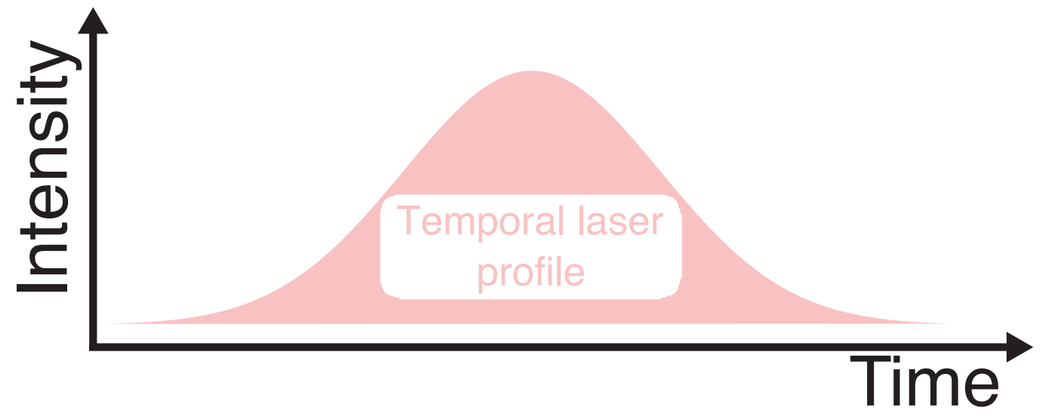


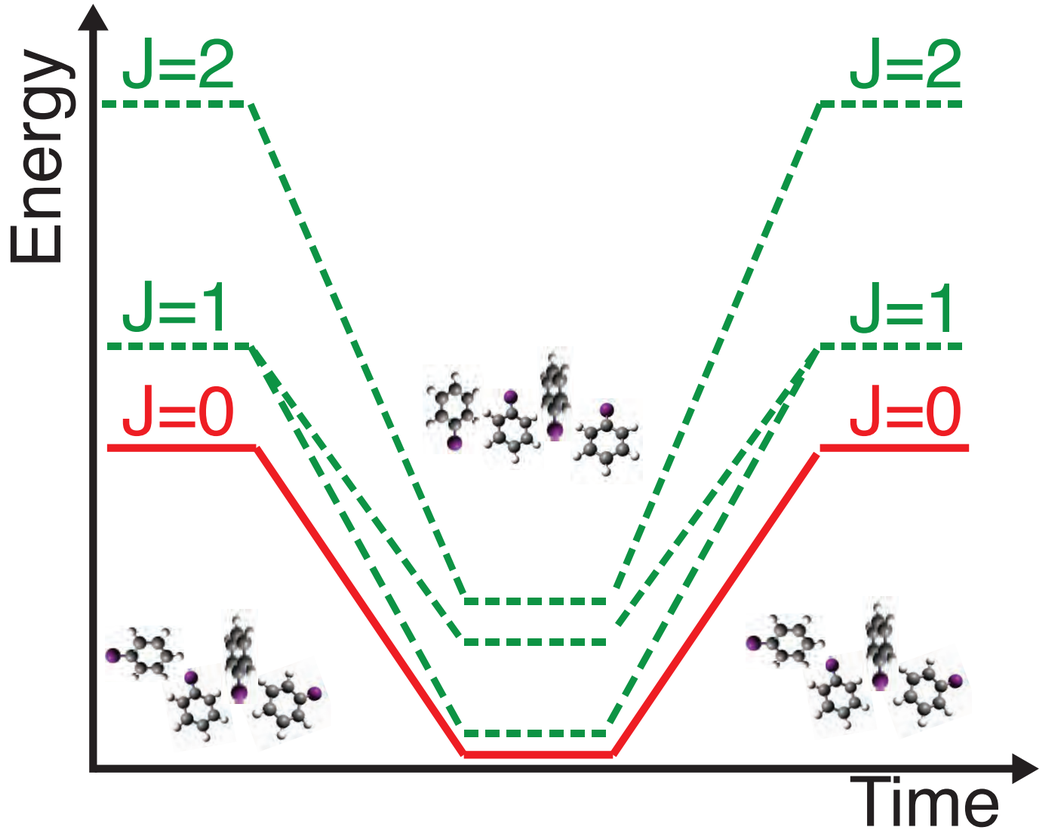
Holmegaard, Nielsen, Nevo, Stapelfeldt, Filsinger, JK, Meijer, *Phys. Rev. Lett.* **102**, 023001 (2009)
Nevo, Holmegaard, Nielsen, Hansen, Stapelfeldt, Filsinger, Meijer, JK, Phys. Chem. Chem. Phys. 11, 9912 (2009)

Scenarios of rotational dynamics in OCS (X, v=0, J=0)
Adiabatic alignment with a 485 ps pulse





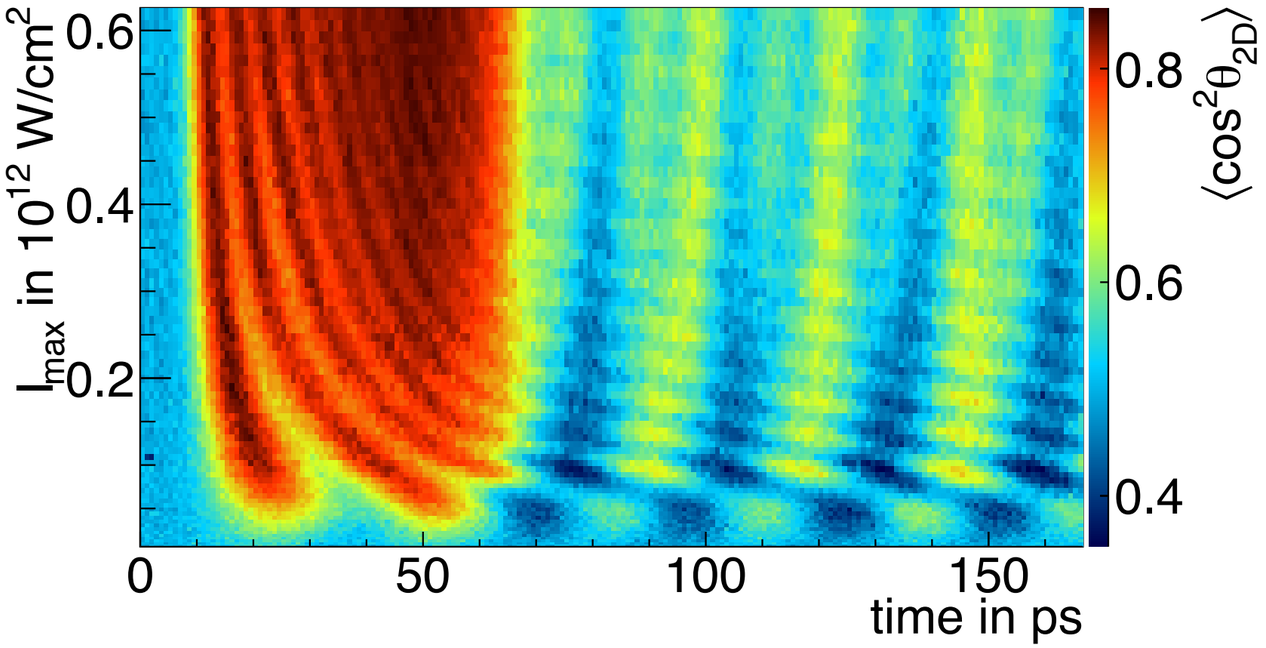




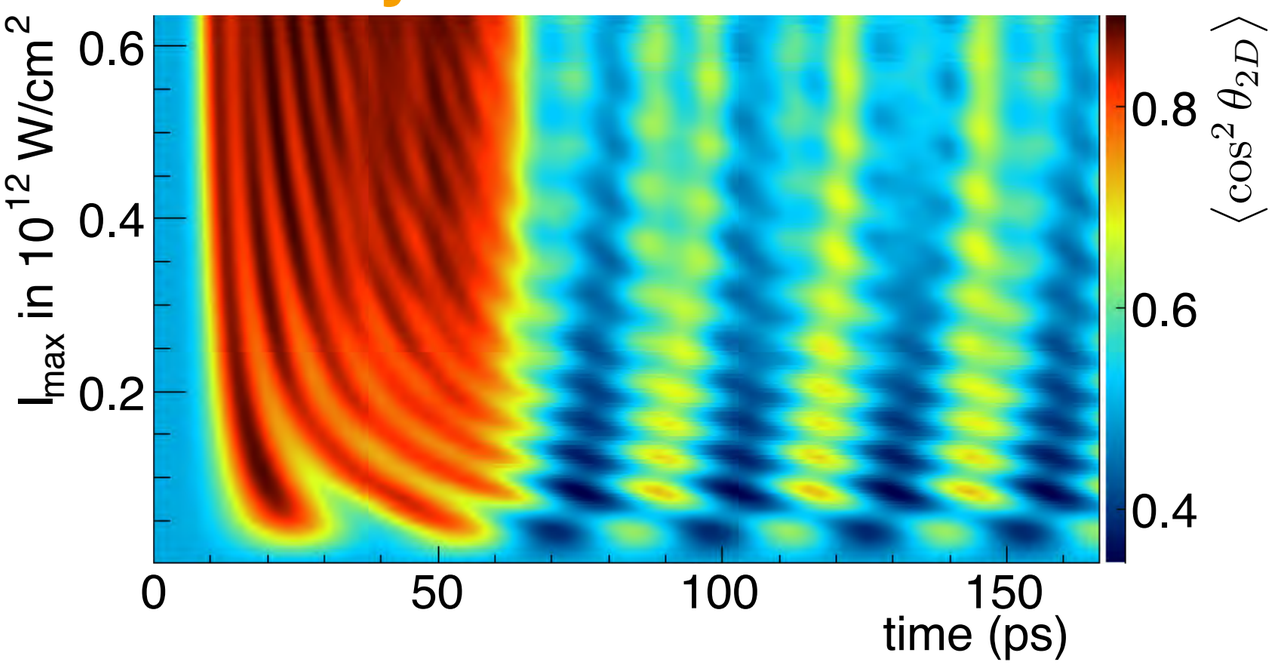
Trippel, Mullins, Müller, Kienitz, Omiste, Stapelfeldt, González Férez, JK , *Phys. Rev.* A **89**, 051401(R) (2014)

Scenarios of rotational dynamics in OCS (X, v=0, J=0)
Intermediate-case alignment with a 50 ps pulse

experiment



theory



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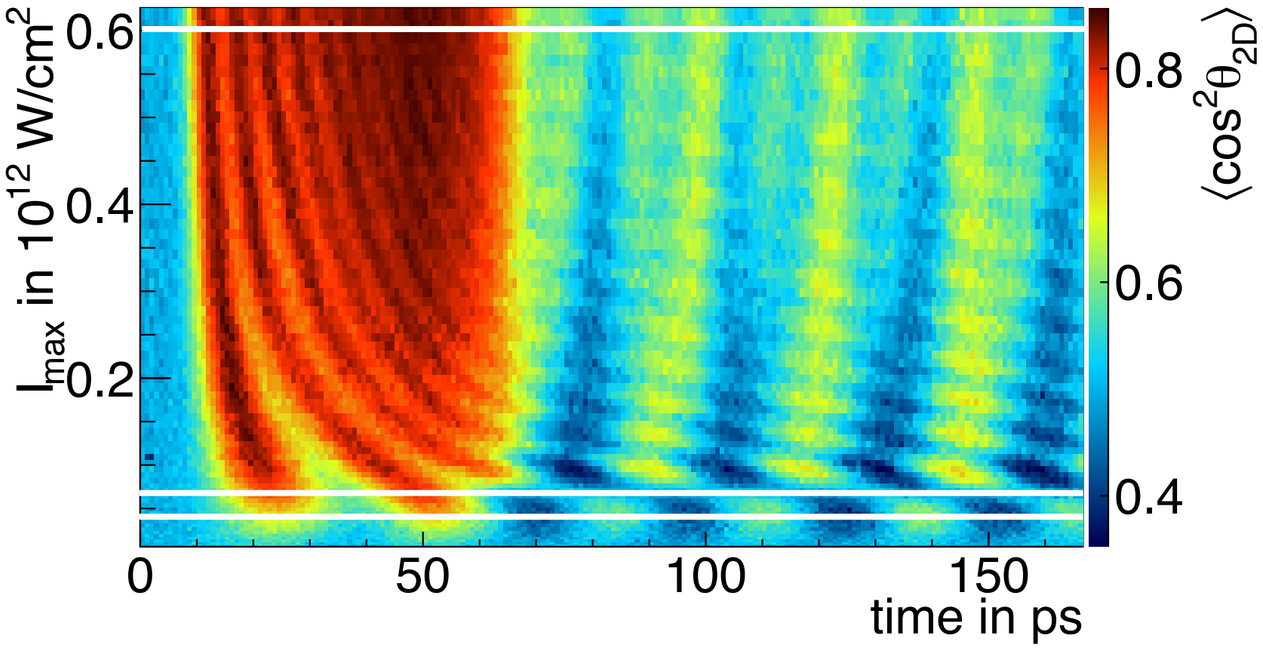
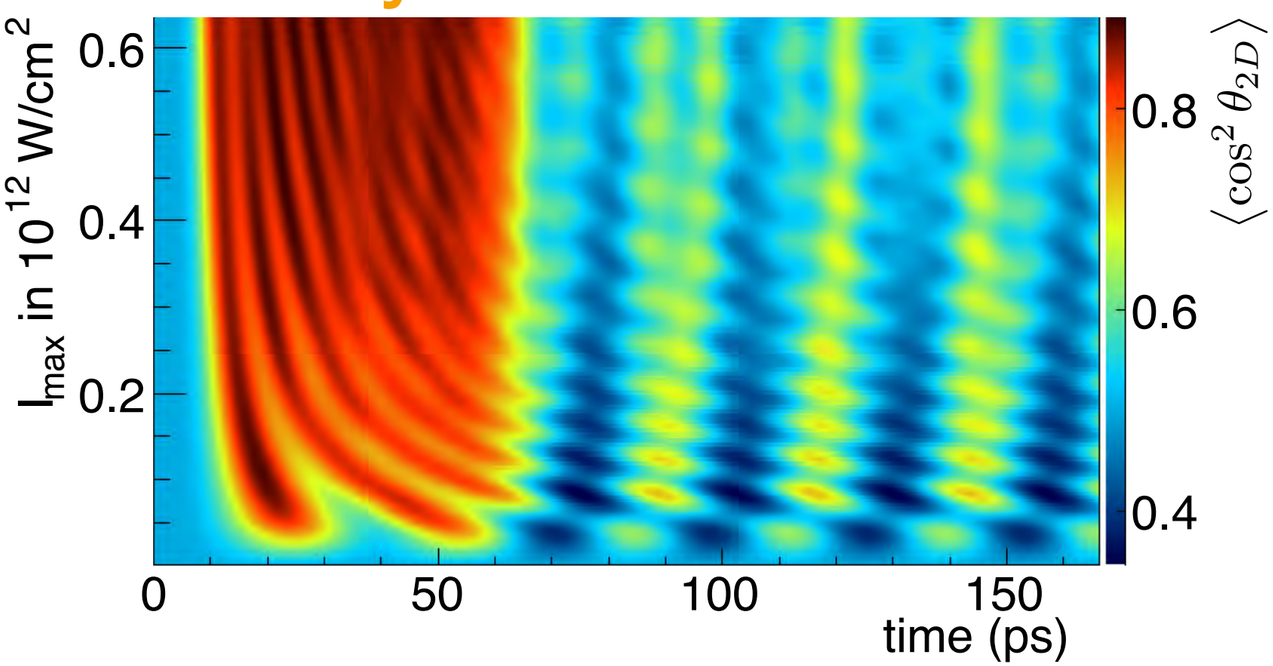
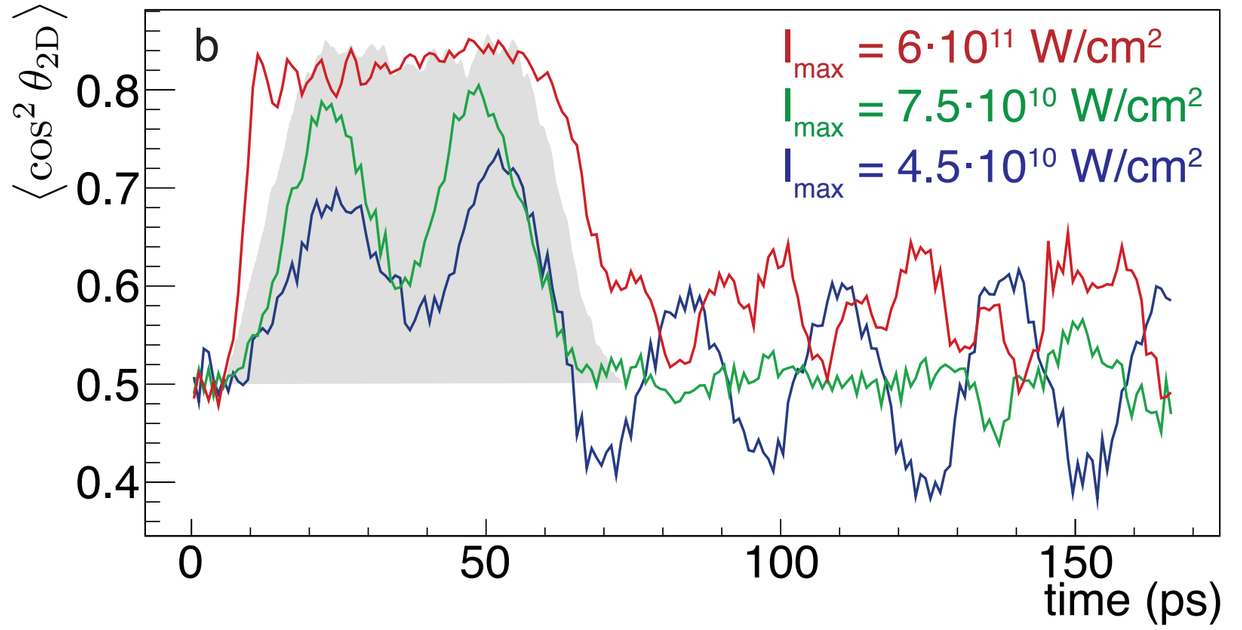


theory





A simple two state wave packet,
a working coherent control experiment
and a strongly-driven quantum pendulum

Trippel, Mullins, Müller, Kienitz, Omiste, Stapelfeldt, González Férez, JK , *Phys. Rev.* A **89**, 051401(R) (2014)

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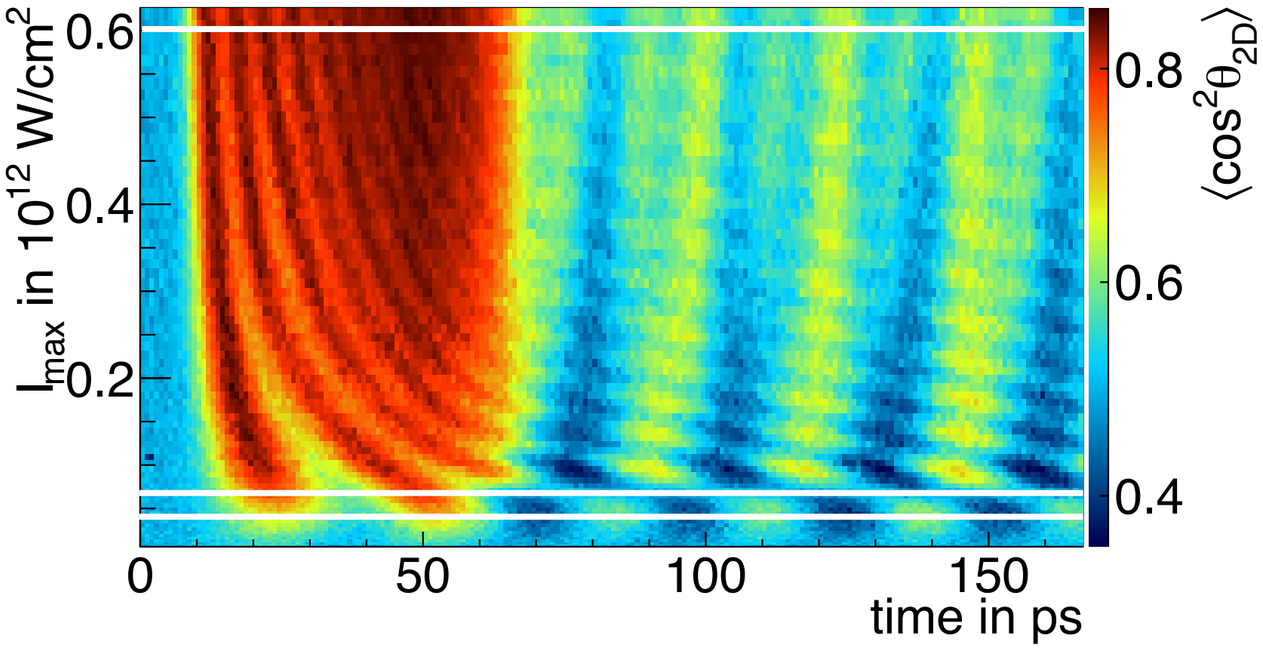

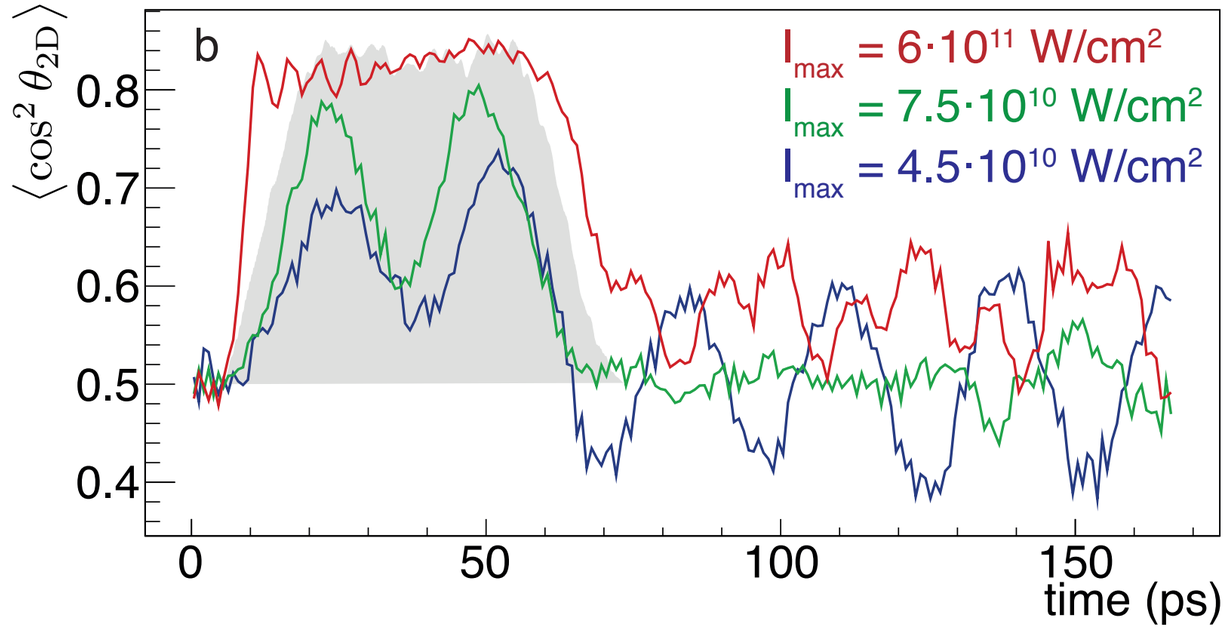

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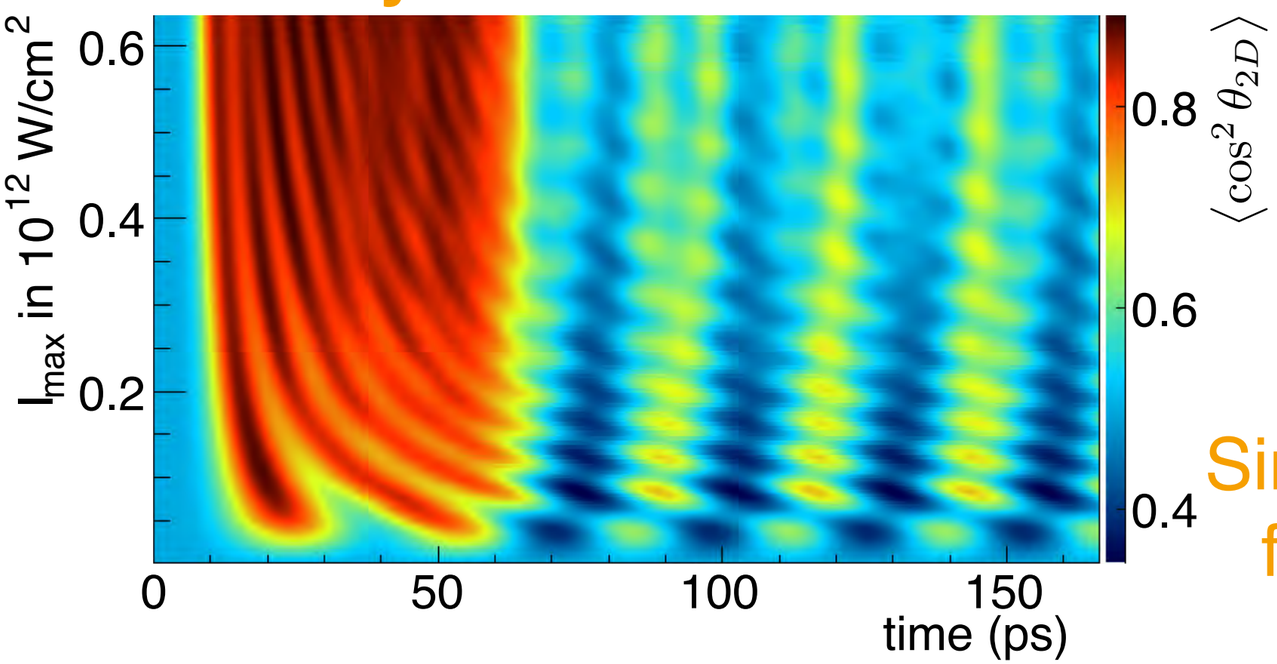

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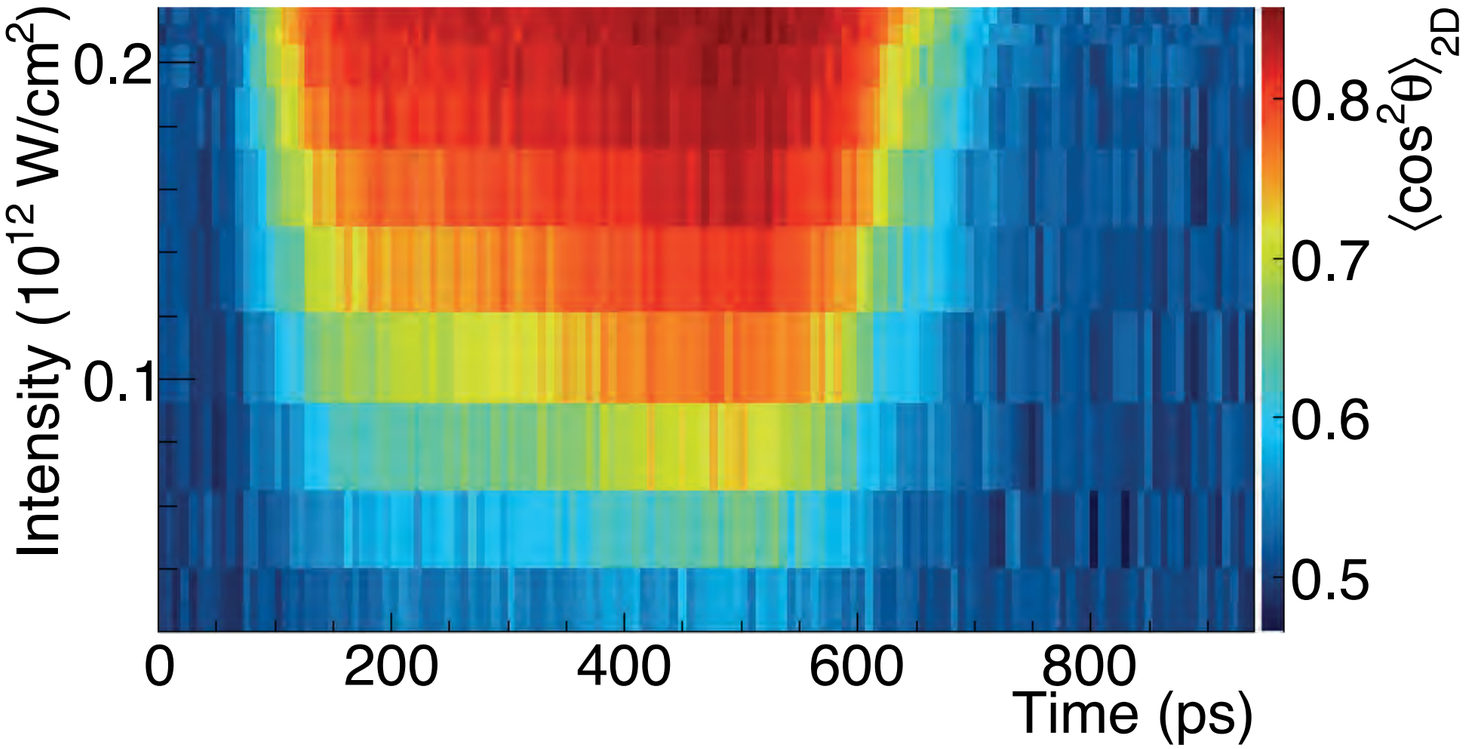
a working coherent control experiment
and a strongly-driven quantum pendulum

Achievable degree of Alignment
is comparable to adiabatic case!

Similar wave packets allow for very strong
field-free orientation (no time to show).

Trippel, Mullins, Müller, Kienitz, Omiste, Stapelfeldt, González Férez, JK , *Phys. Rev.* A **89**, 051401(R) (2014)

Scenarios of rotational dynamics in OCS (X, v=0, J=0)
Non-adiabatic *orientation* with a 500 ps pulse



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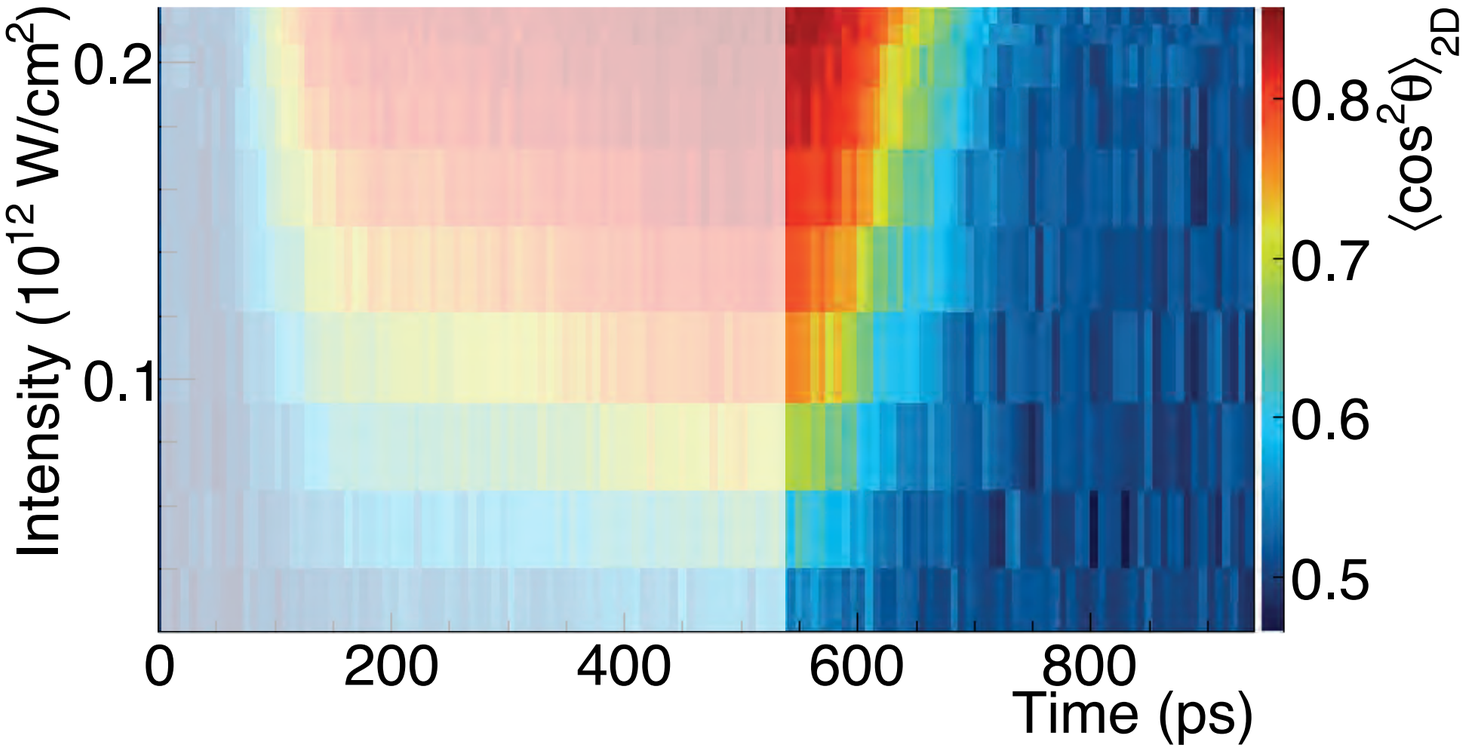

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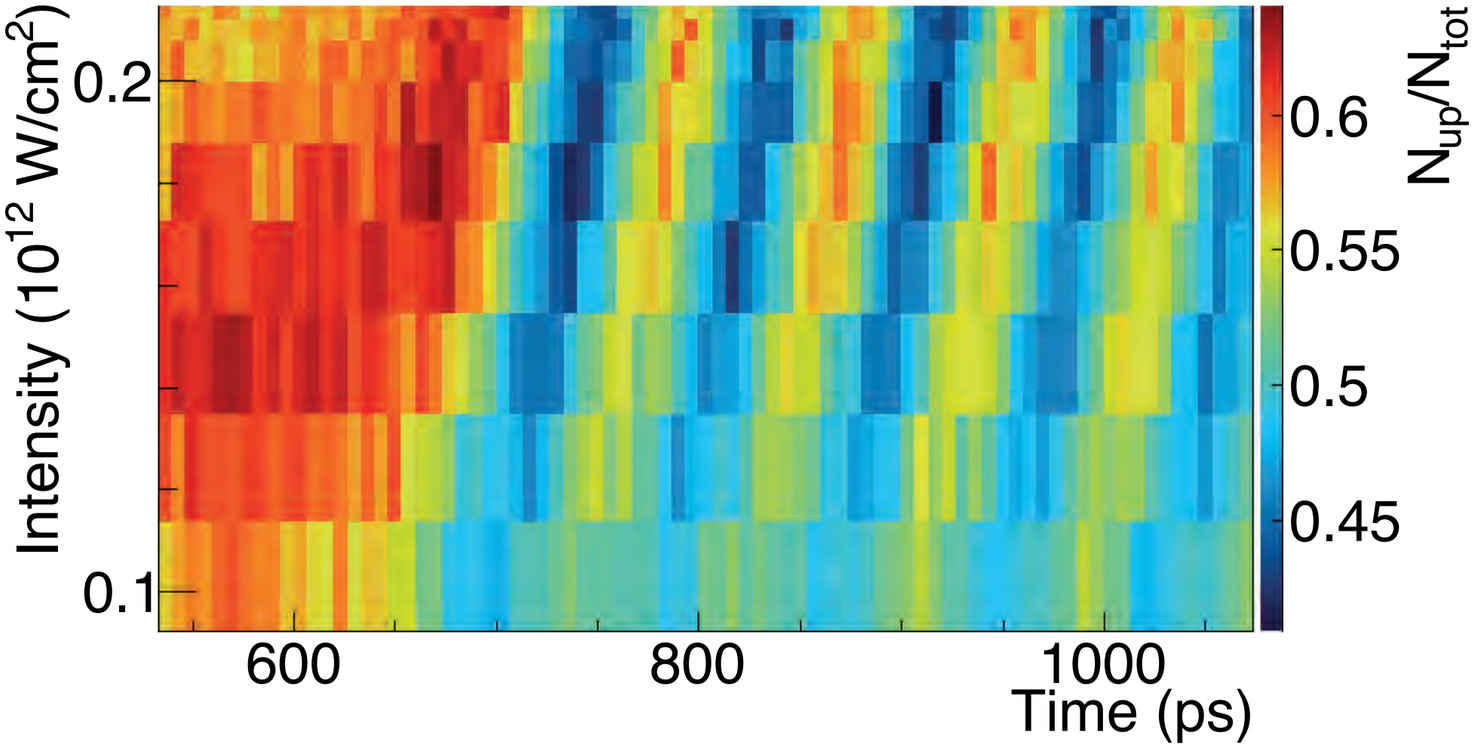

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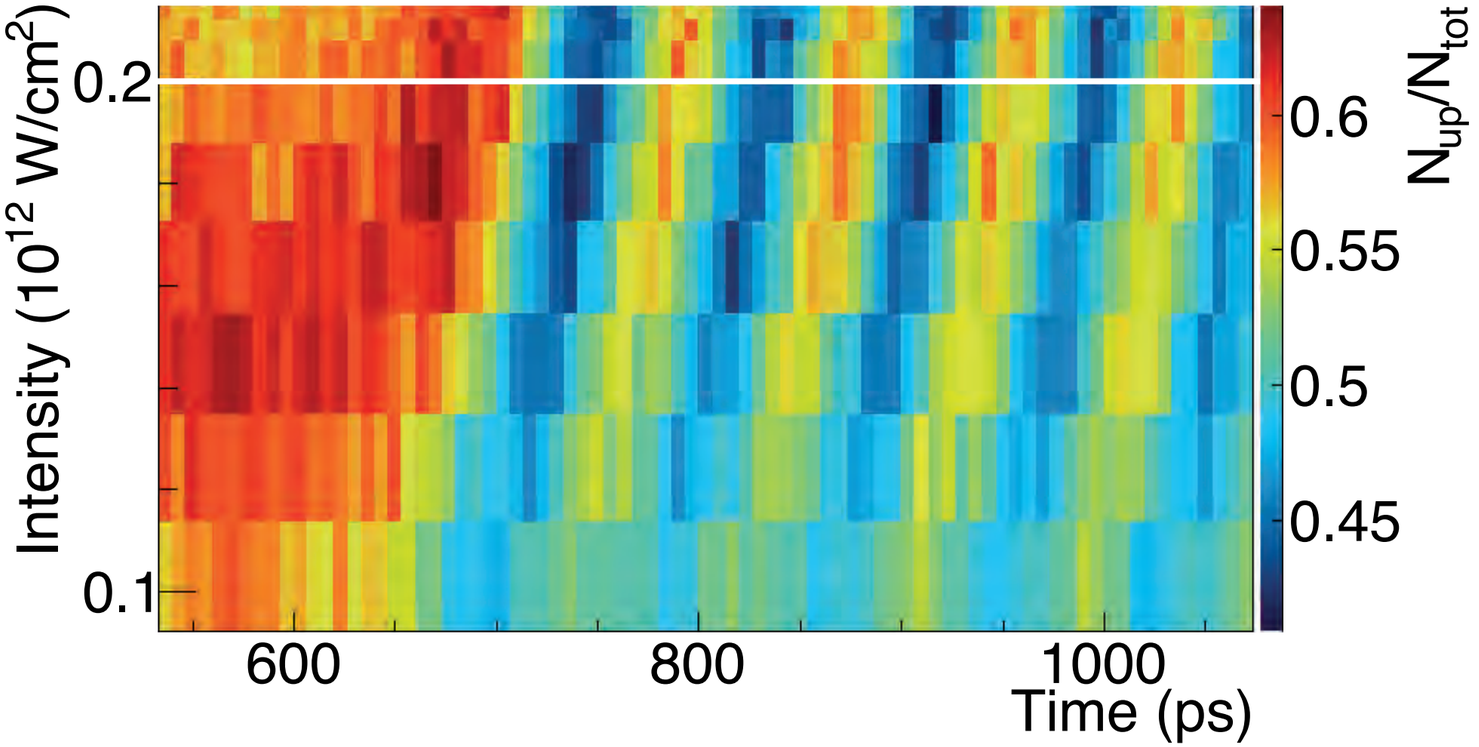

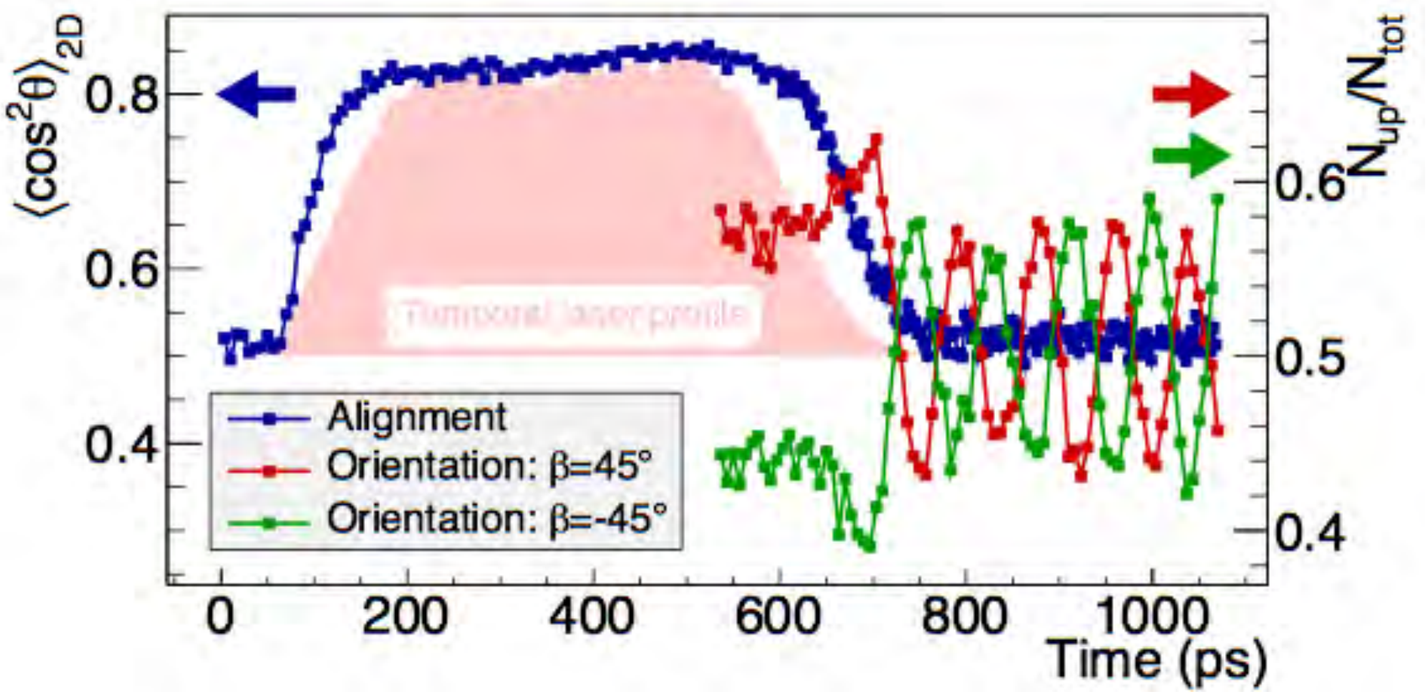

Trippel, Mullins, Müller, Kienitz, González Férez, JK, arXiv:1409.2836 [physics]

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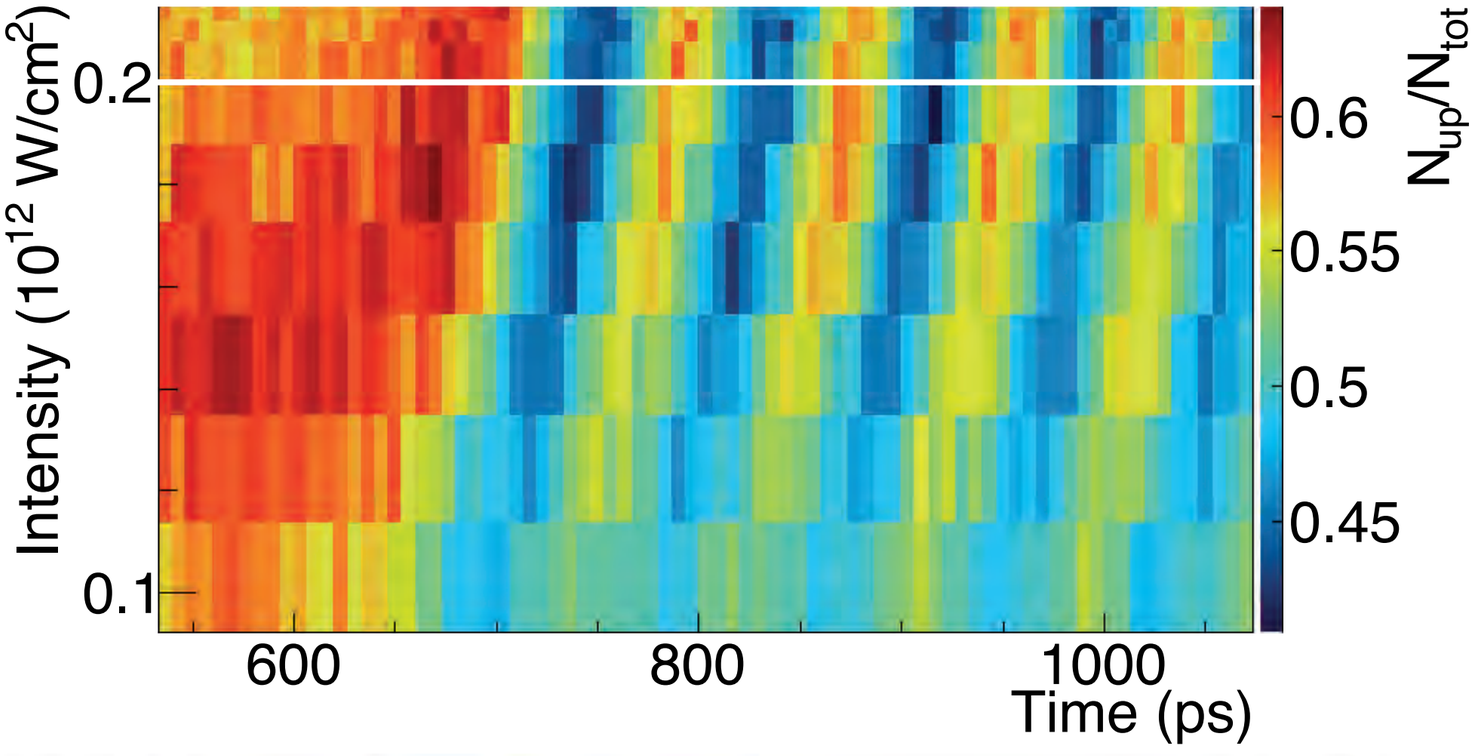
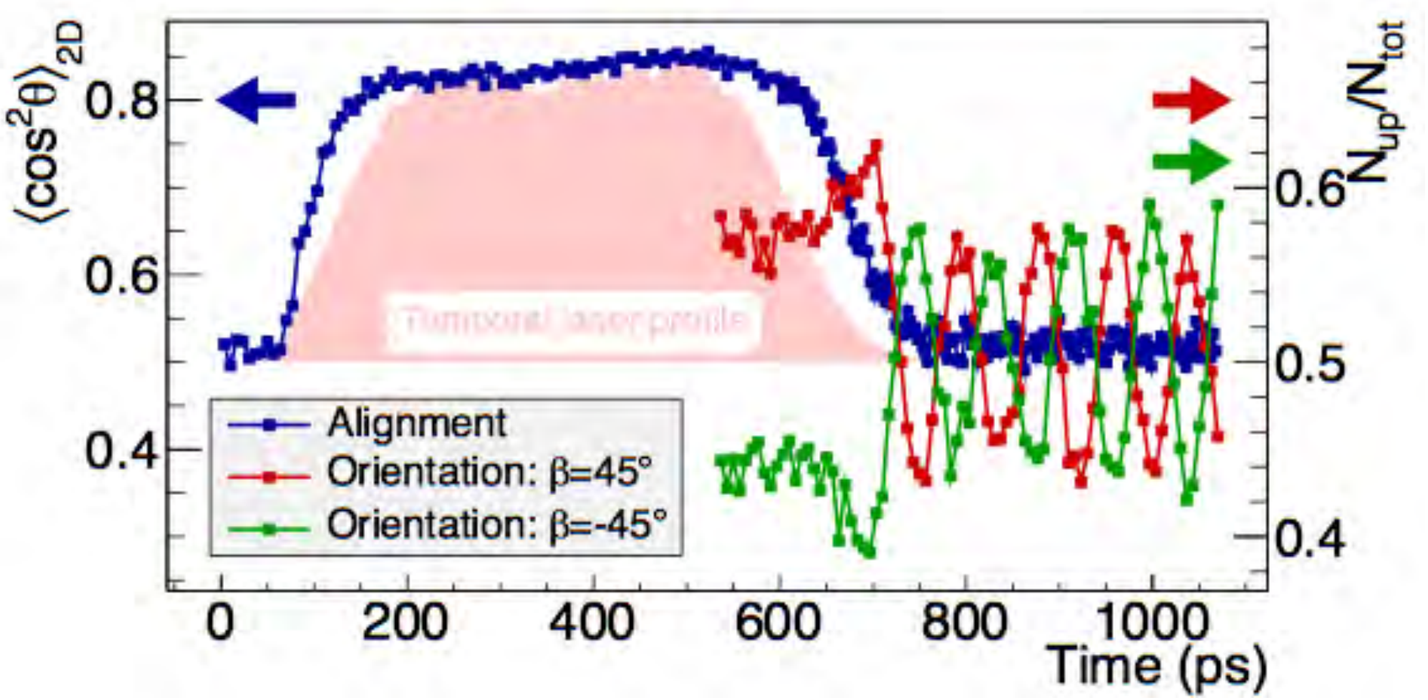
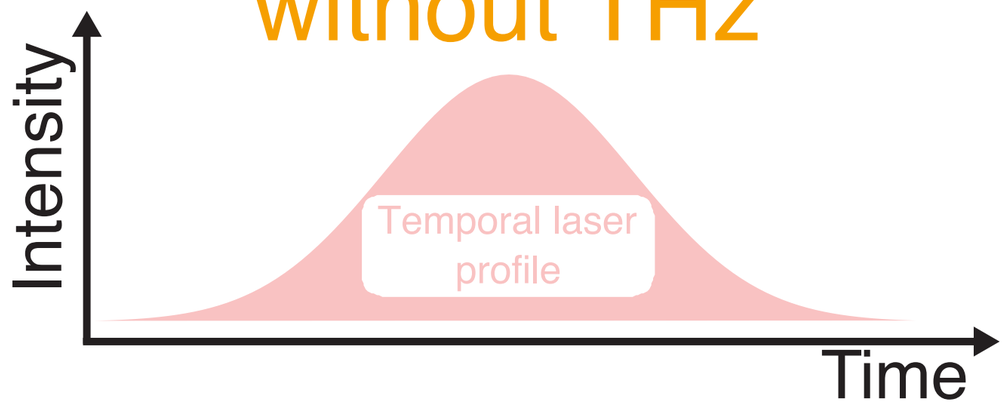
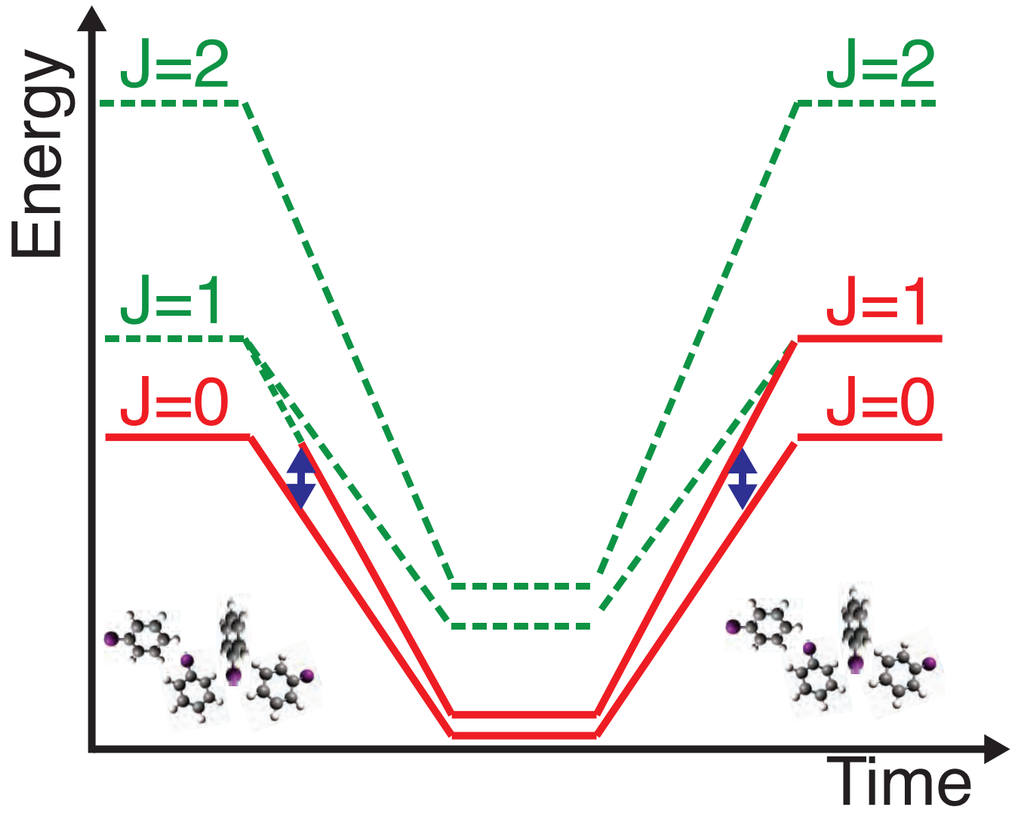




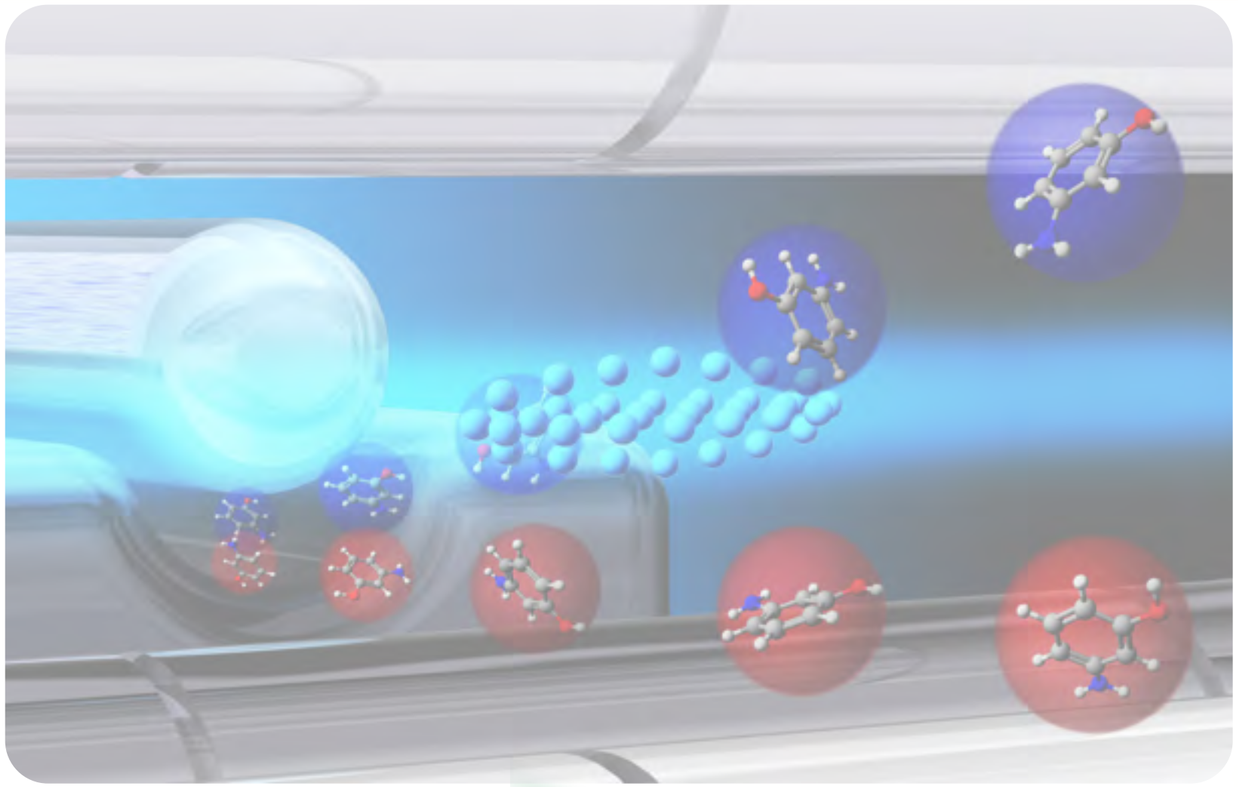




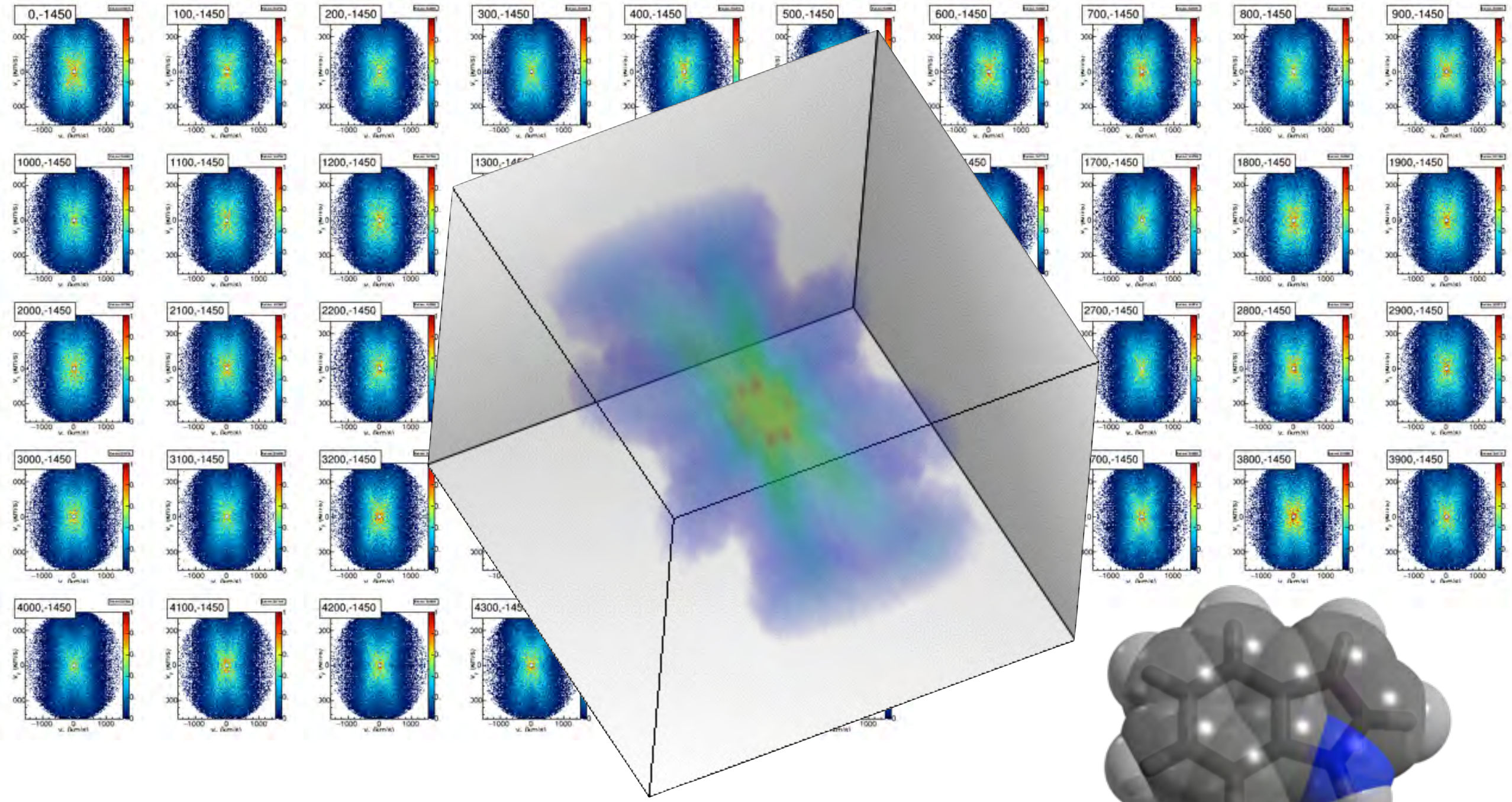
Field-free orientation – $\langle\cos\theta\rangle$=0.6

Trippel, Mullins, Müller, Kienitz, González Férez, JK, arXiv:1409.2836 [physics]

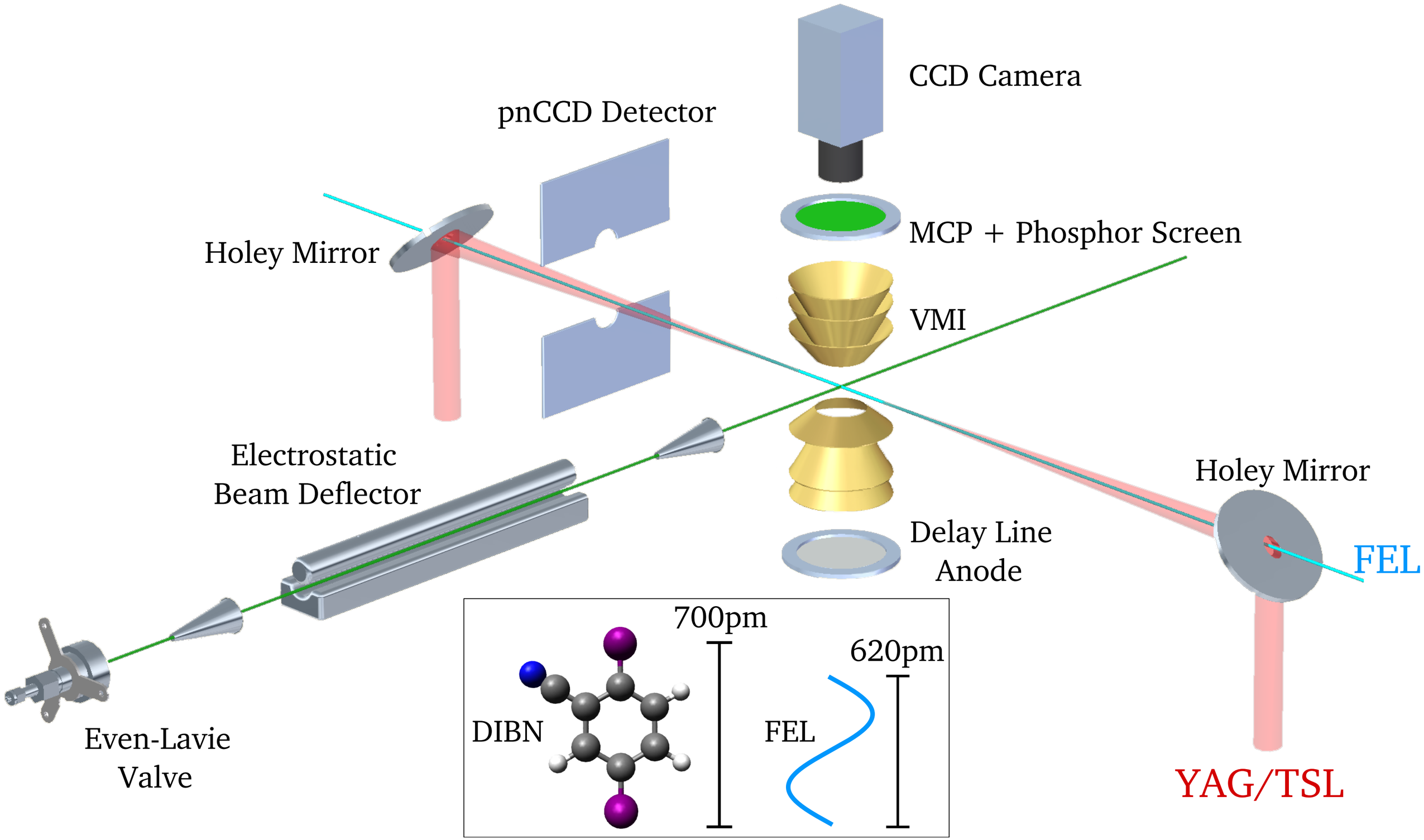
Imaging structural dynamics (nuclear and electronic)



MFPADs of molecular aggregates using a pure beam of indole-water

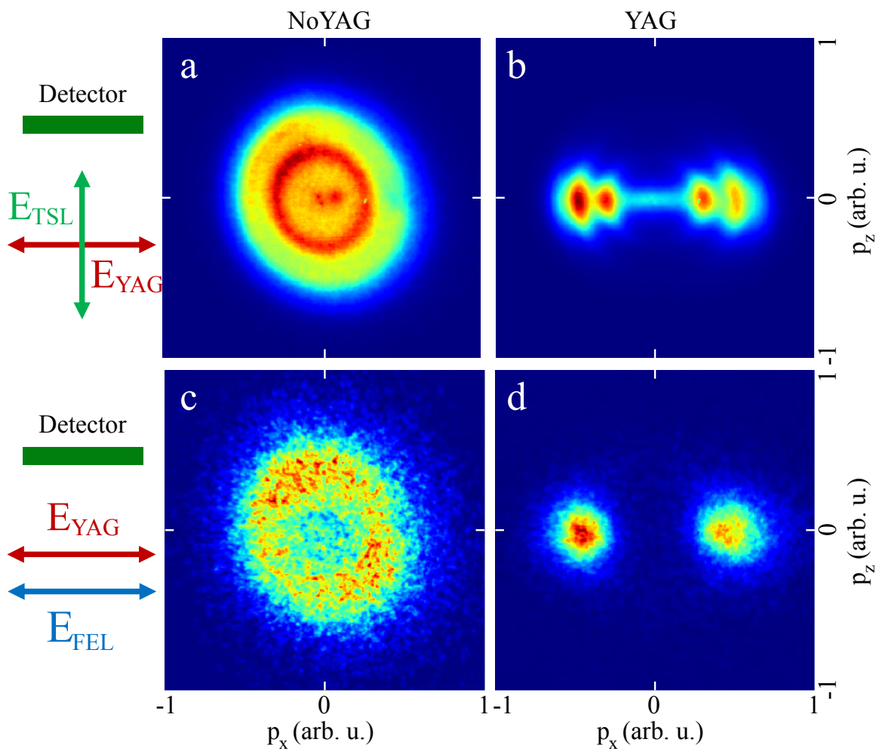


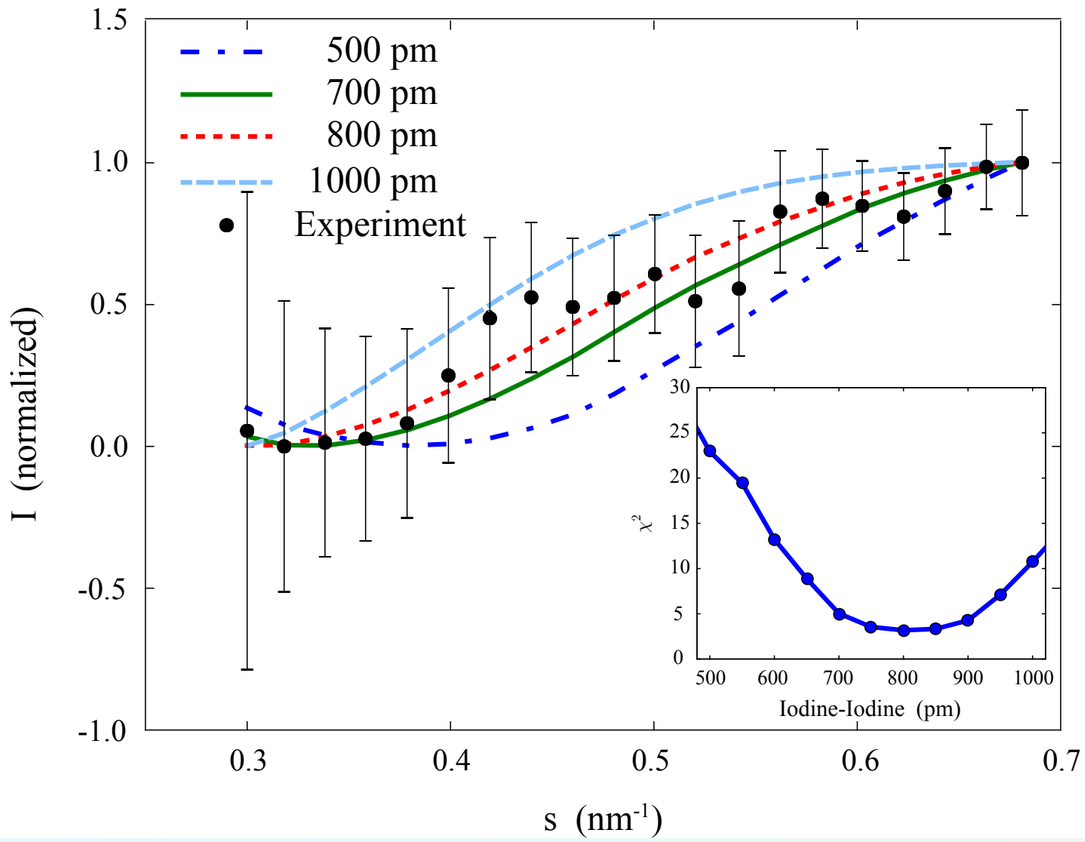
CFEL ASG Multi-Purpose Chamber (CAMP)
A traveling Free-Electron Laser endstation (now at FLASH)

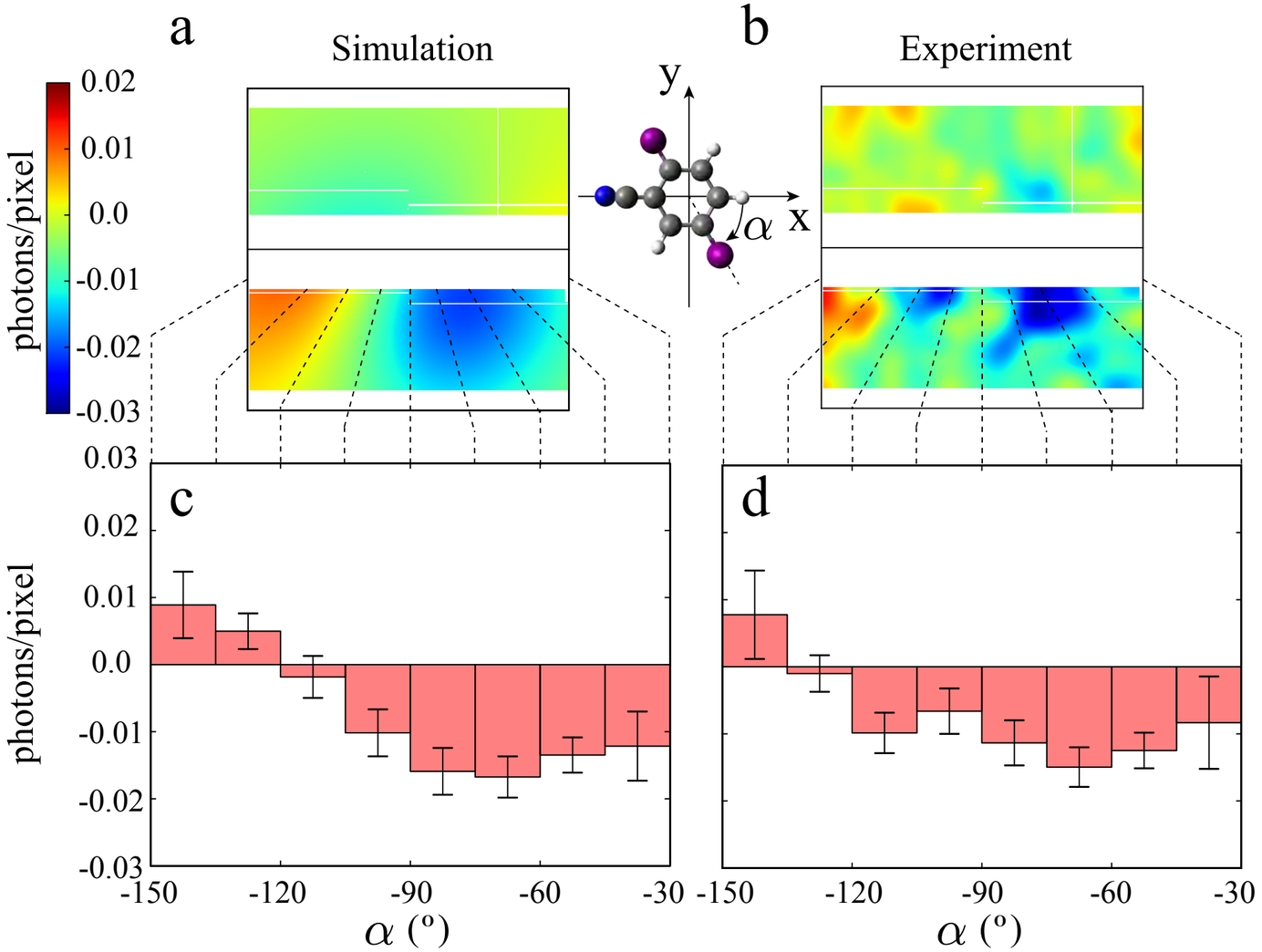


JK, Stern, et al (53 authors), *Phys. Rev. Lett.*, **112**, 083002 (2014)

Coherent (fs) *X-ray diffractive* imaging of 2,6-diiodobenzonitrile
Analysis of anisotropic part of molecular x-ray diffraction pattern





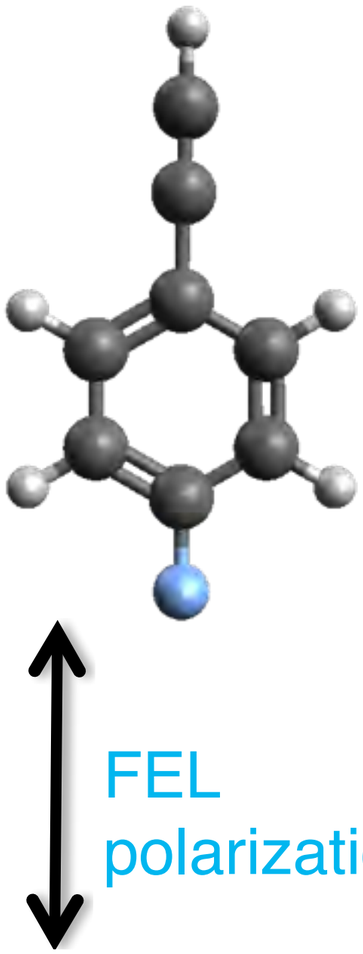


diffraction data yields
$\langle\cos^2\theta\rangle_{2D}$=0.8 (vs. 0.84)
r(I–I) ≈ 800 pm (vs. 700 pm)

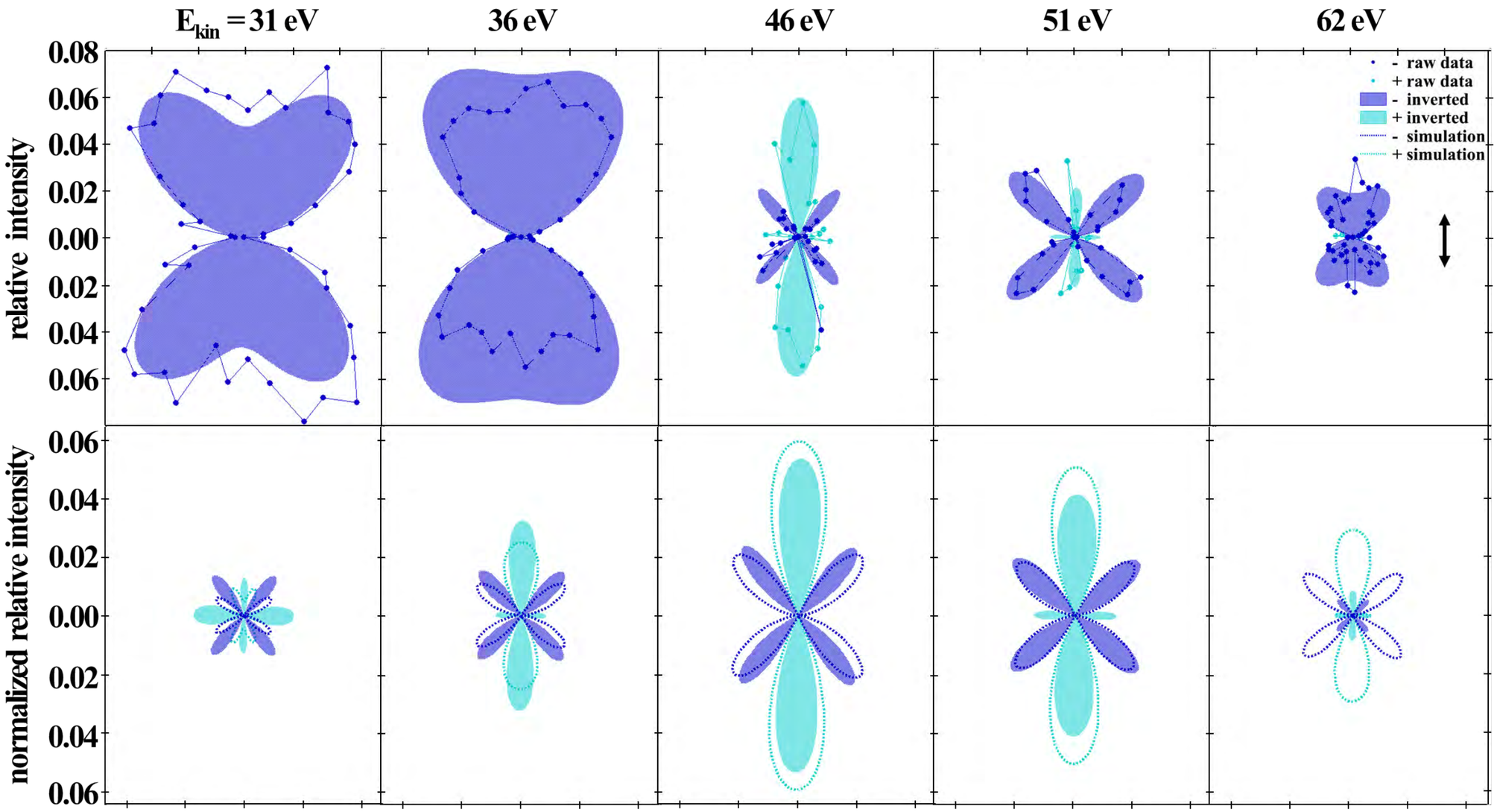
JK, Stern, et al (53 authors), *Phys. Rev. Lett.*, **112**, 083002 (2014)

Photoelectron diffraction of aligned molecules
F(1s) ionization of 1-ethynyl-4-fluorobenzene

detector



FEL polarization

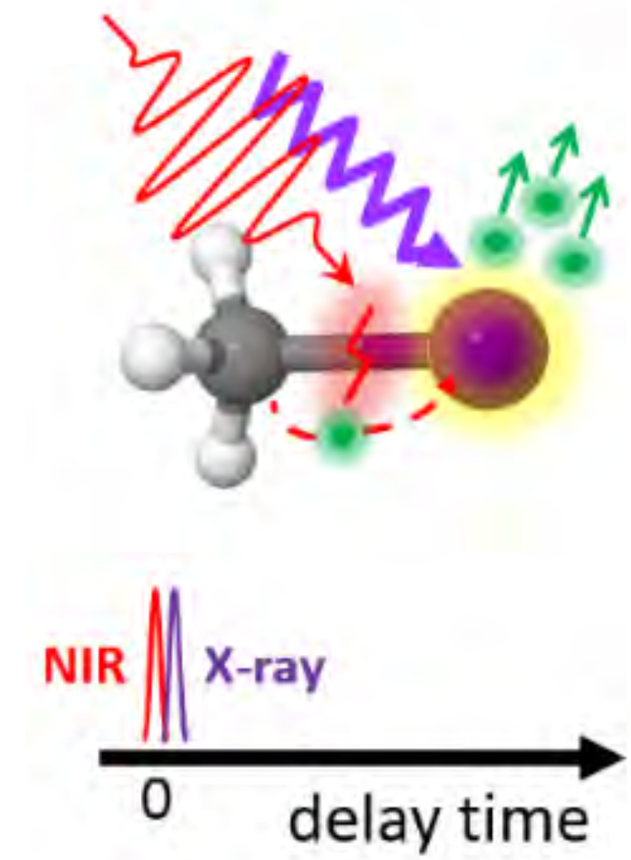


Photoelectron angular distribution difference between aligned and randomly oriented molecules as function of electron kinetic energy

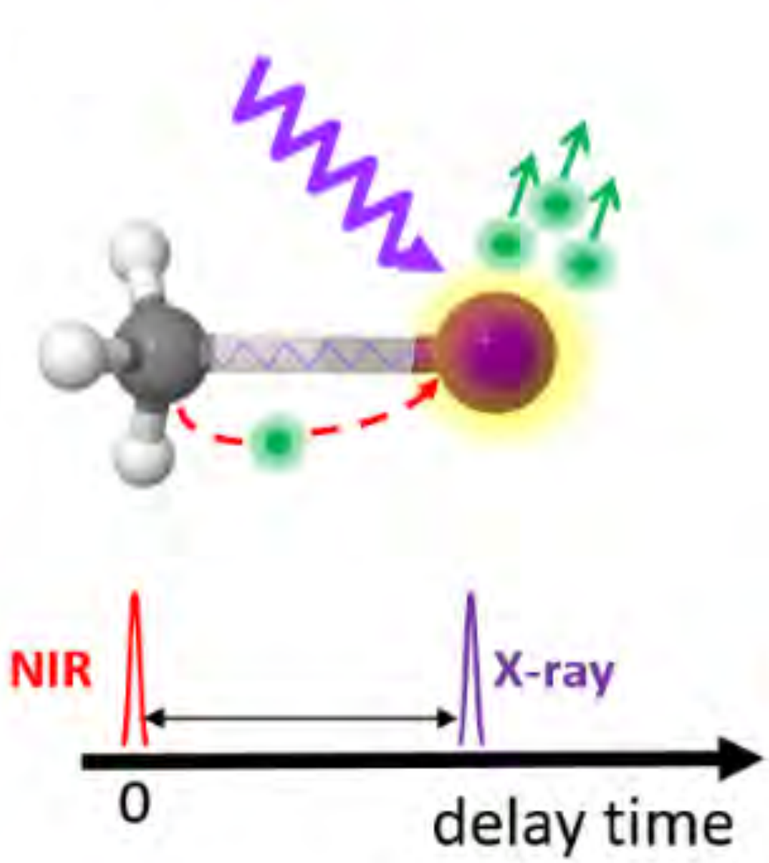
Boll, Rolles, et al (25 authors), *Phys. Rev.* A **88**, 061402(R) (2013)

Imaging *charge transfer* in iodomethane upon x-ray photoabsorption

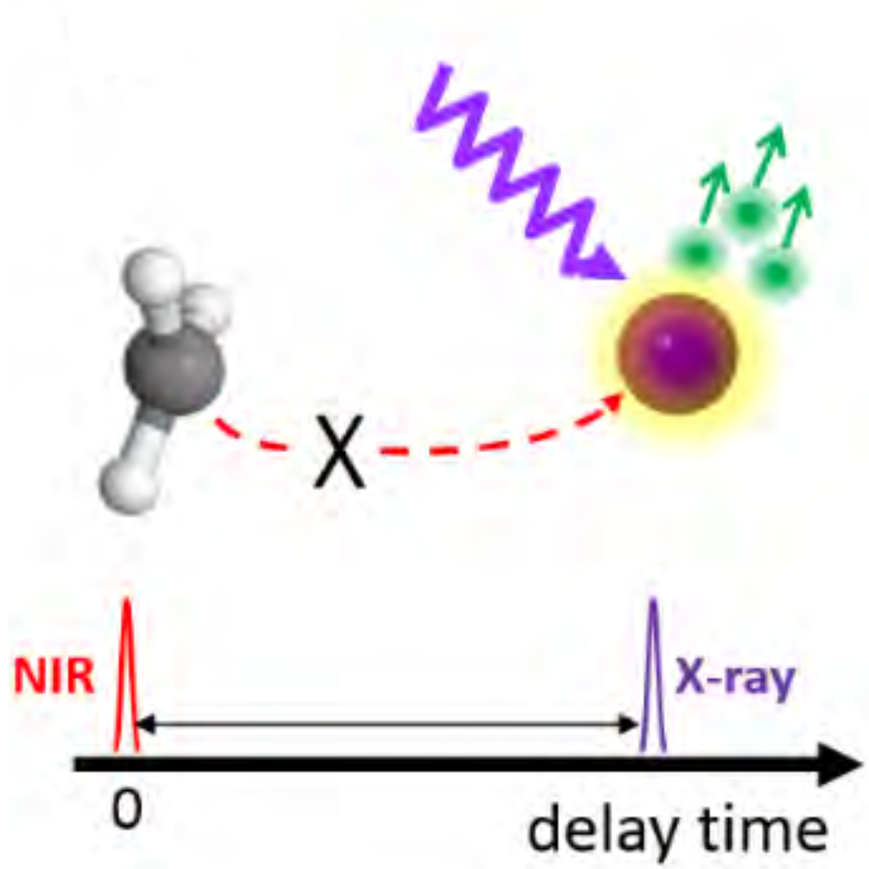
- **Break up the molecule**: strong-field ionization with a near-infrared (NIR) laser pulse
- **Knock out inner-shell electrons** from the iodine atom with the delayed x-ray pulse
- **Vary the delay** to tune the distance between the fragments



At small distances, the valence electrons can freely move within the molecule.



In the transition regime, the electrons exhibit a certain degree of localization.



At large separations, the probability of electron transfer becomes negligible.

Erk, et al (21 authors), *Science* **345**, 288 (2014)

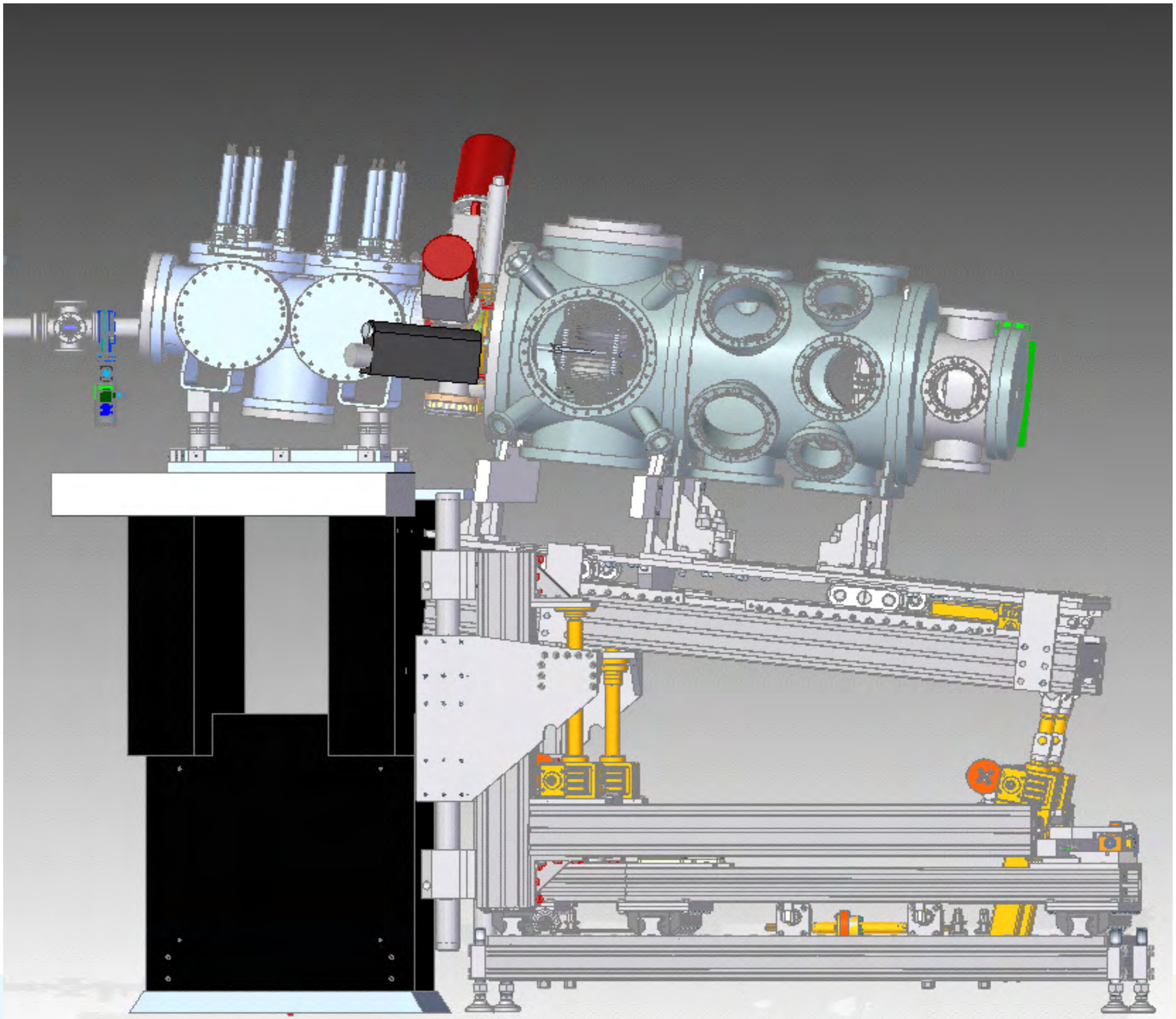
Light sources at DESY Photon Science

part II – experiments at free-electron lasers (FELs)
CFEL-ASG Multi-Purpose endstation

- CAMP @ FLASH – a BMBF supported program to convert CAMP into a (the first) permanent endstation at FLASH
- Installation, commissioning, and operation headed by Helmholtz Young Investigator Group (Daniel Rolles)
  - local coordination from summer 2015 by Benjamin Erk
  - MEDEA coordination by Daniel Rolles (and Jochen Küpper)

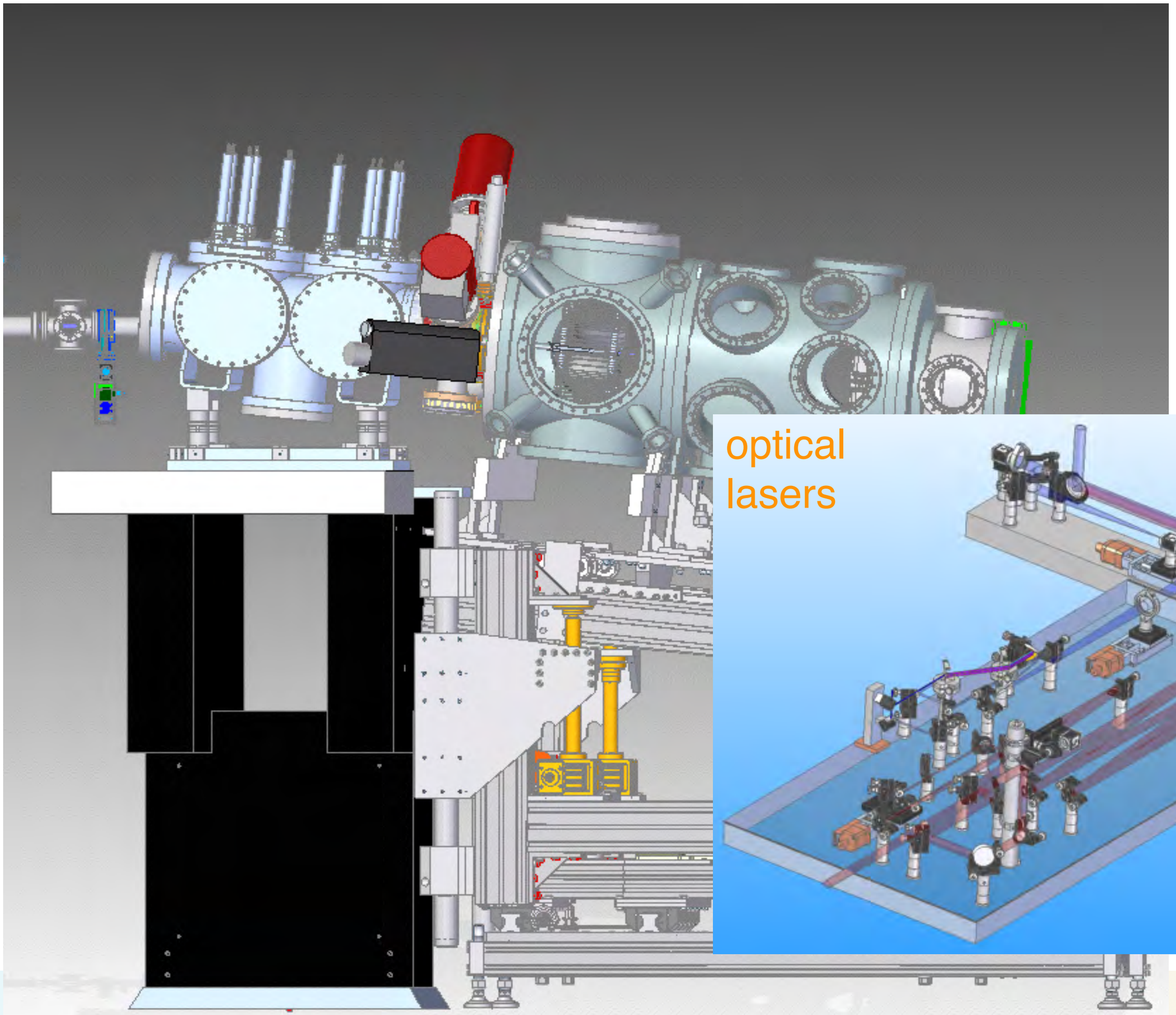
part II – experiments at free-electron lasers (FELs)
CFEL-ASG Multi-Purpose endstation

Assembly of CAMP@FLASH-BL1



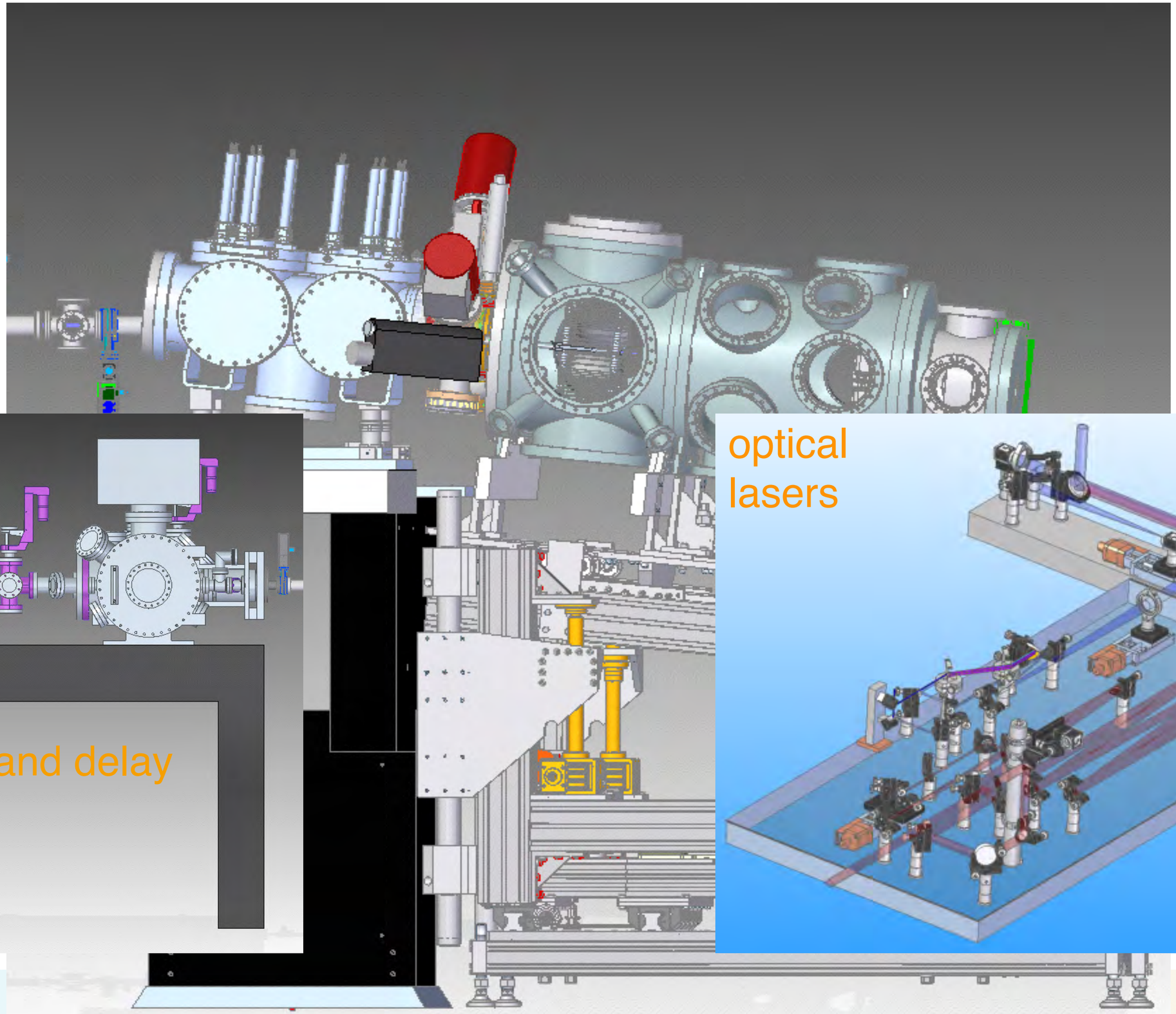
part II – experiments at free-electron lasers (FELs)
CFEL-ASG Multi-Purpose endstation

Assembly of CAMP@FLASH-BL1



part II – experiments at free-electron lasers (FELs)
CFEL-ASG Multi-Purpose endstation

Assembly of CAMP@FLASH-BL1



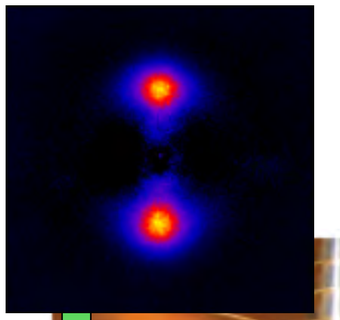
split and delay

optical lasers

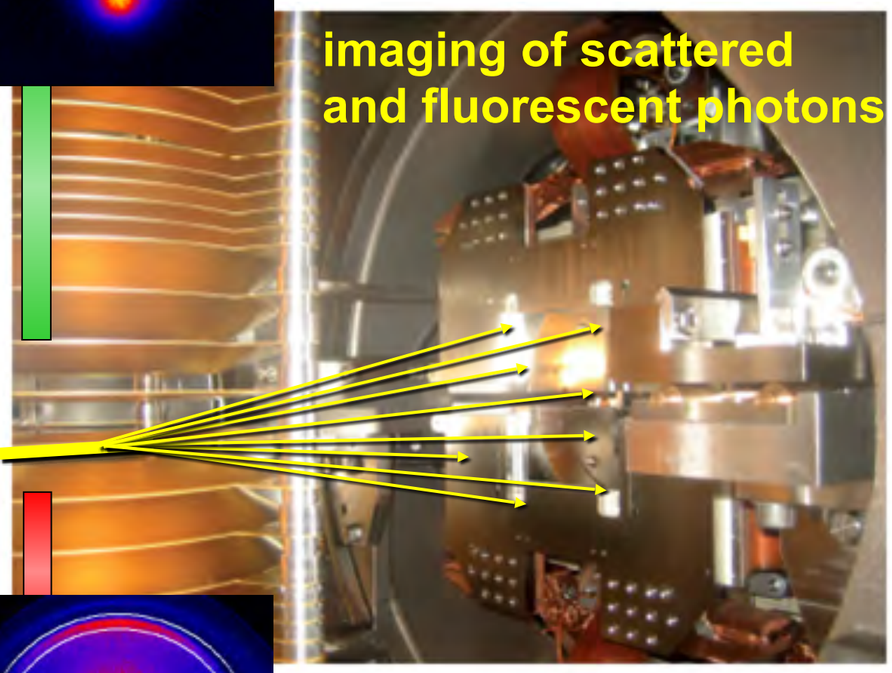
CAMP – experiments at free-electron lasers (FELs)
CFEL-ASG Multi-Purpose endstation

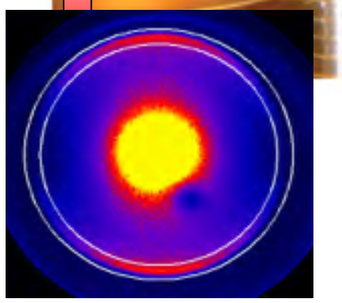
A variety of detectors available

electron and ion spectrometers
(REMI/COLTRIMS, VMI)



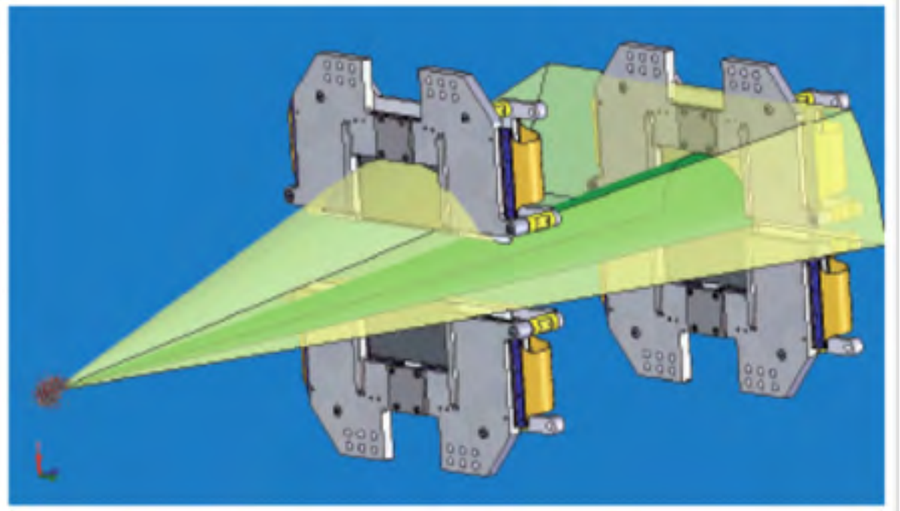
ion imaging

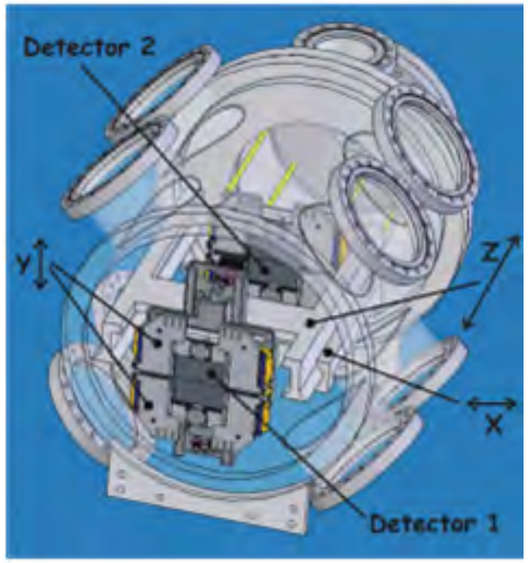




electron imaging

two planes of large-area pnCCD photon detectors





front pnCCD is
movable in-situ,
rear pnCCD has fixed
gap and preset position

Both charged-particle spectrometers can be operated with delay line detectors (coincidence mode) or MCP/phosphor screen detectors (covariance mode)

Summary

- Generation of well defined samples
  - separation of quantum states, structural isomers, cluster species
- Fixing molecules in space
  - one- and three-dimensional alignment and orientation
- Imaging of molecules
  - x-ray and electron diffraction, ion and electron momentum imaging

- CAMP @ FLASH
  - a permanent endstation at FLASH for AMO/imaging experiments

- ESR DESY: Attosecond dynamics in conformer-selected amino acids
- ESR training/secondments
  - “sample preparation” – cold intense beams, species selection, alignment and orientation concepts
  - (imaging) experiments with complex molecules

Example video: http://desy.cfel.de/cid/cmi/outreach/jove_video

Acknowledgments
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Fenglin Wang
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JOACHIM HERZ STIFTUNG

Alexander von Humboldt Stiftung/Foundation

Bundesministerium für Bildung und Forschung

DFG

CUI THE HAMBURG CENTER FOR ULTRAFAST IMAGING

erc European Research Council
Established by the European Commission

DESY

HELMHOLTZ ASSOCIATION

We are looking for motivated colleagues – please see http://desy.cfel.de/cid/cmi/opportunities

Acknowledgments
CAMP @ FLASH

Daniel Rolles[1,2,12], Benjamin Erk[1,2], Cédric Bomme[1], Evgeny Savelyev[1], Jonathan Correa[1], Jan P. Müller[3], Angad Swiderski[1], Rolf Treusch[1], Rebecca Boll[1,2,4], Barbara Keitel[1], Elke Plönjes[1], Günter Brenner[1], Siarhei Dziarzhytski[1], Marion Kuhlmann[1], Stefan Düsterer[1], Kai Tiedtke[1], Heinz Graafsma[1], Thomas Tilp[5], Lars Gumprecht[5], Henry Chapman[5], Mario Sauppe[2], Daniela Rupp[2], Thomas Zeschke[6], Frank Siebert[6], Robert Hartmann[7], Lothar Strüder[7], Günter Hauser[8], Simone Techert[1,9], Ilme Schlichting[10], Stefan Eisebitt[3], Joachim Ullrich[2,4,11], Robert Moshammer[2,4], Thomas Möller[3]

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10. Max-Planck-Institut für medizinische Forschung, Heidelberg, Germany
11. Physikalisch-Technische Bundesanstalt, Braunschweig, Germany
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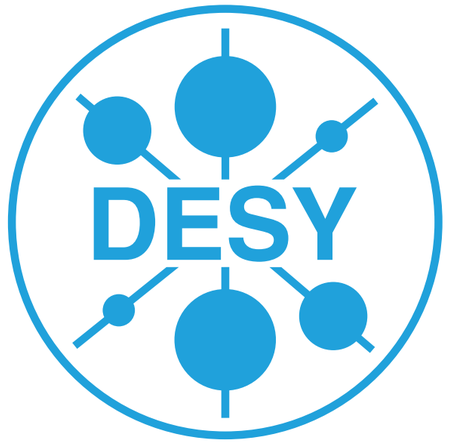

Acknowledgments
Collaborators

Center for Free-Electron Laser Science
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Joe Robinson, Ryan Coffee, Alan Fry, Bill White

We are looking for motivated colleagues – please see http://desy.cfel.de/cid/cmi/opportunities

Announcements

We are looking for motivated colleagues, please see http://desy.cfel.de/cid/cmi/opportunities

The Hamburg Conference on Femtochemistry
Femto XII, Hamburg, DE, 12.–17. July 2015

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SCIENCE
Controlled Molecule Imaging