

Photoemission spectroscopy - A versatile tool for investigations of the electronic structure of different materials

Friedrich Roth

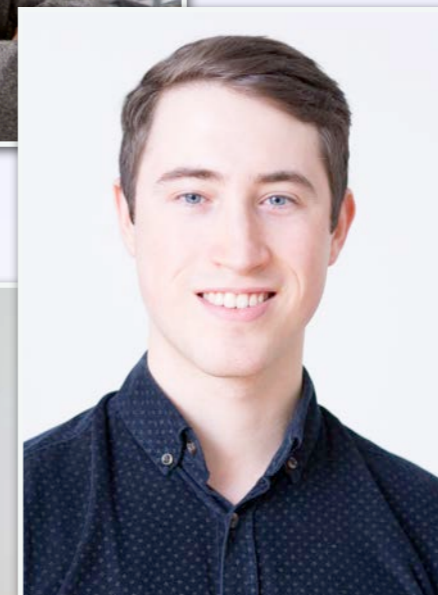
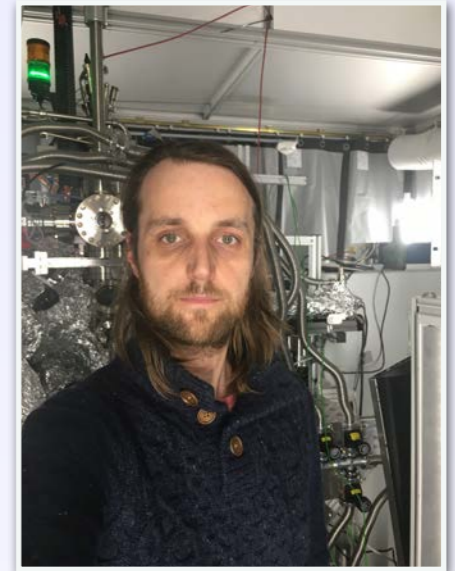
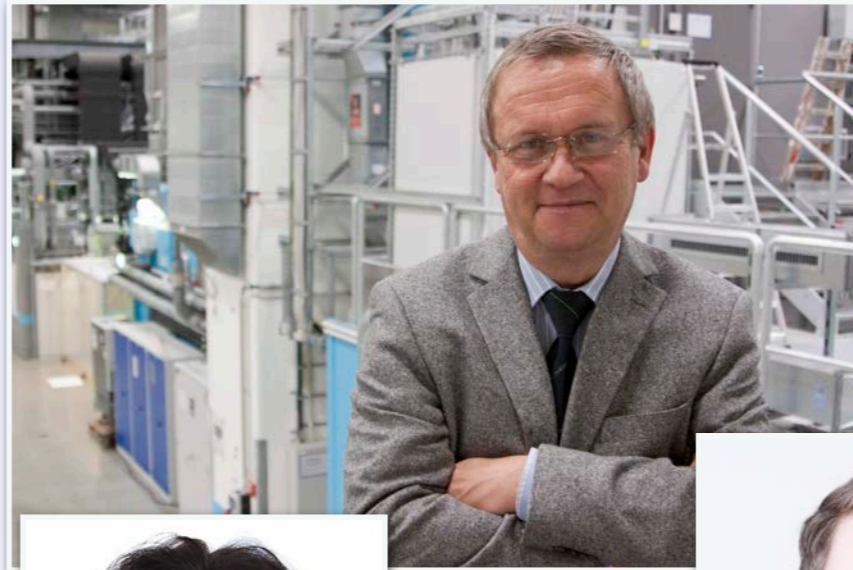
Workshop

Sachsen-DESY Cooperation Center



Team

- Serguei Molodtsov
- Friedrich Roth
- Dmitrii Potorochin
- Marieke Zickner
- Ekaterina Tikhodeeva 
- Mikhail Mishchenko 
- Nikhil Biju Joseph



- Wolfgang Eberhardt



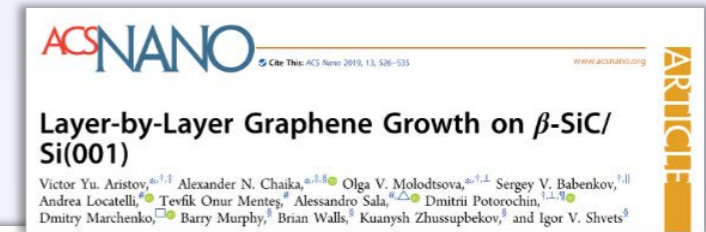
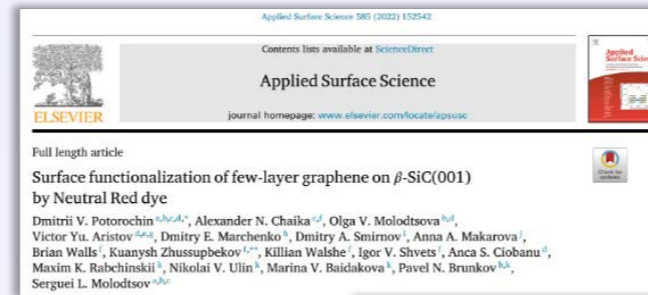


Research possibilities - previous work at PETRA



Saxony-DESY collaboration @ Petra III

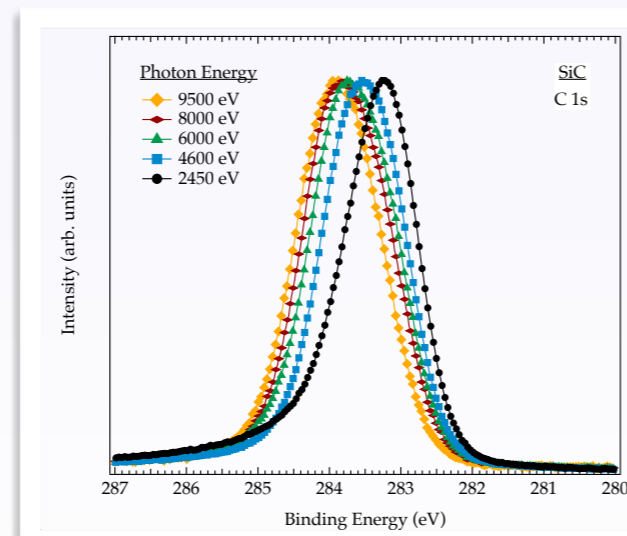
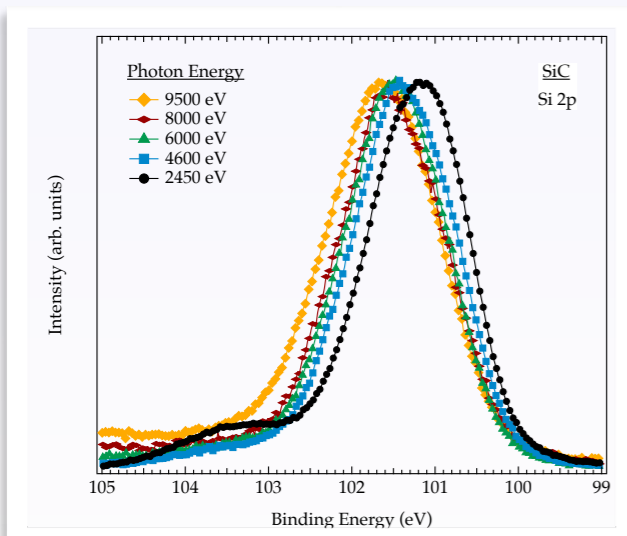
- Dynamic-XPS Argus endstation @ P04 Beamline



Olga Molodtsova & Victor Aristov



- HAXPES @ P22 Beamline — Christoph Schlueter
Andrei Gloskovskii

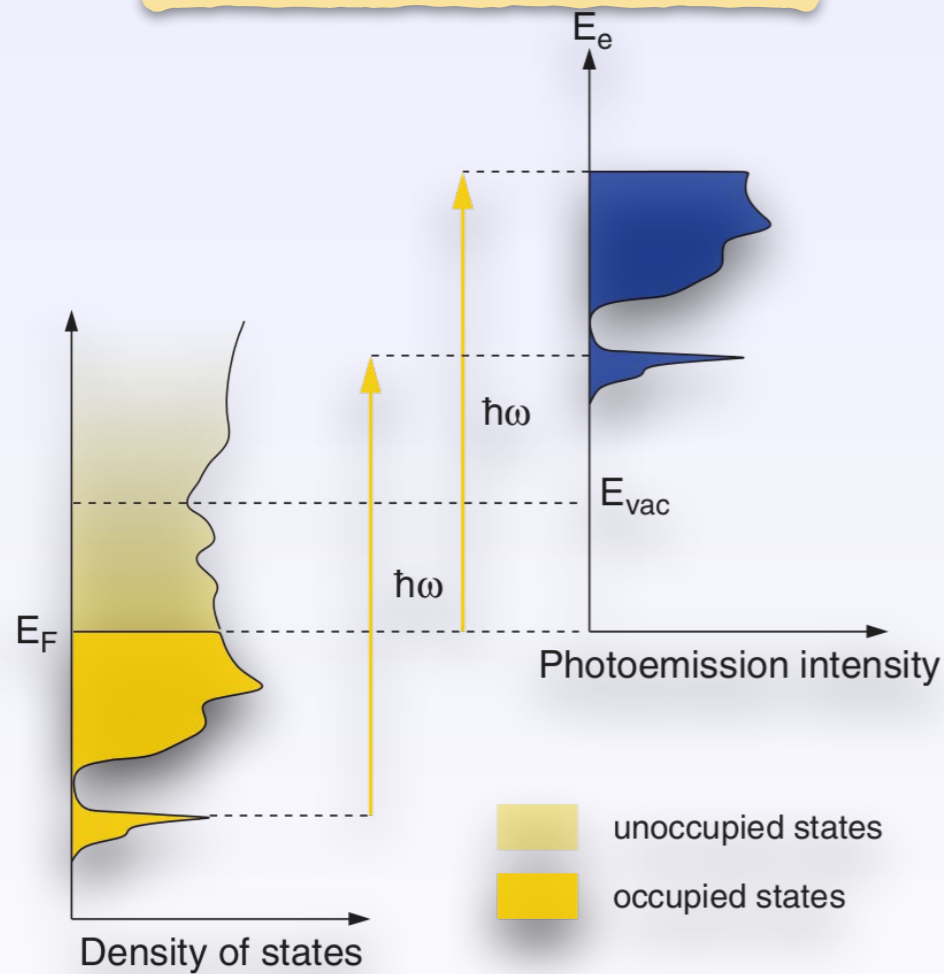


FR et al., in preparation



Photoelectron Spectroscopy (PES)

PES energy scheme



$$E_{kin} = \hbar\omega - E_b - \Phi_W$$

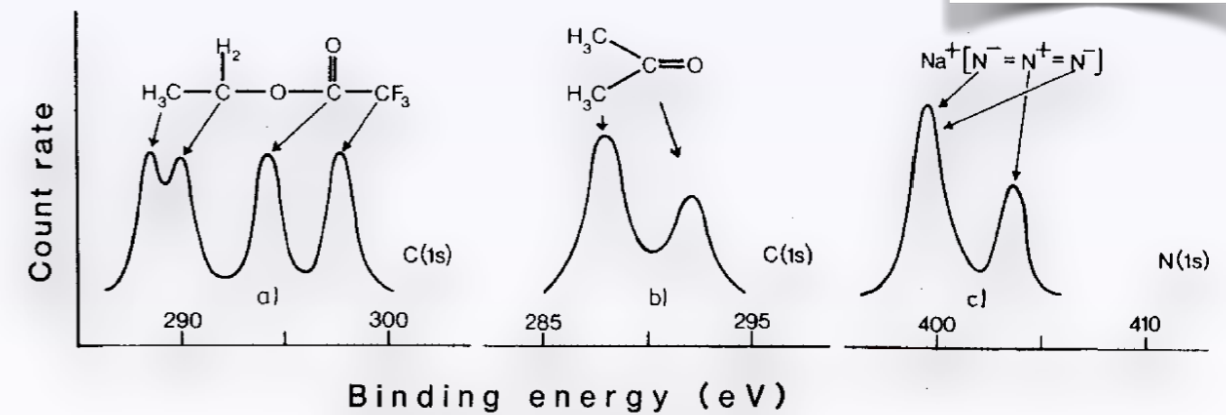
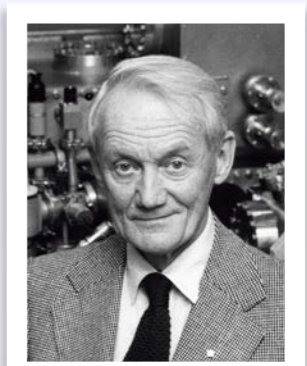
From: P. Willmott, *An Introduction to Synchrotron Radiation*, Wiley (2011)

XPS or ESCA

Probing the local chemical and physical environment

Fingerprint of sample

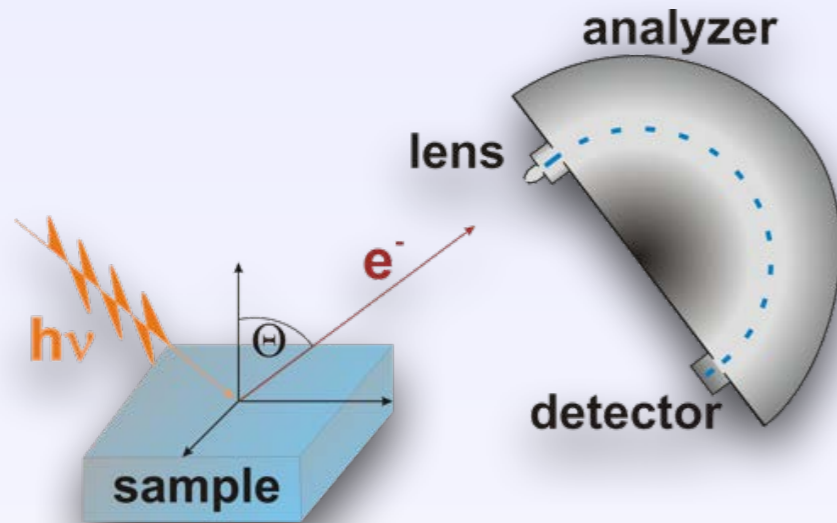
→ **chemical shifts**



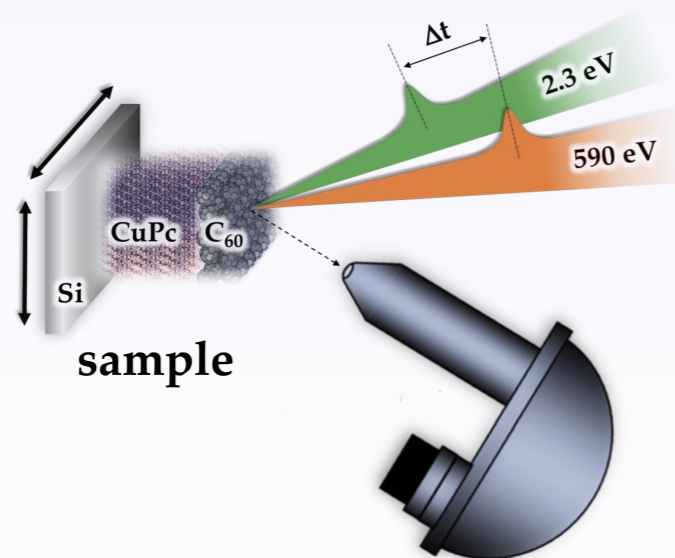
S. Hüfner, *Photoelectron Spectroscopy*. Springer-Verlag, 2010 (3rd ed.). Chapter 2.

Spectroscopy of Ultrafast Electron Dynamics

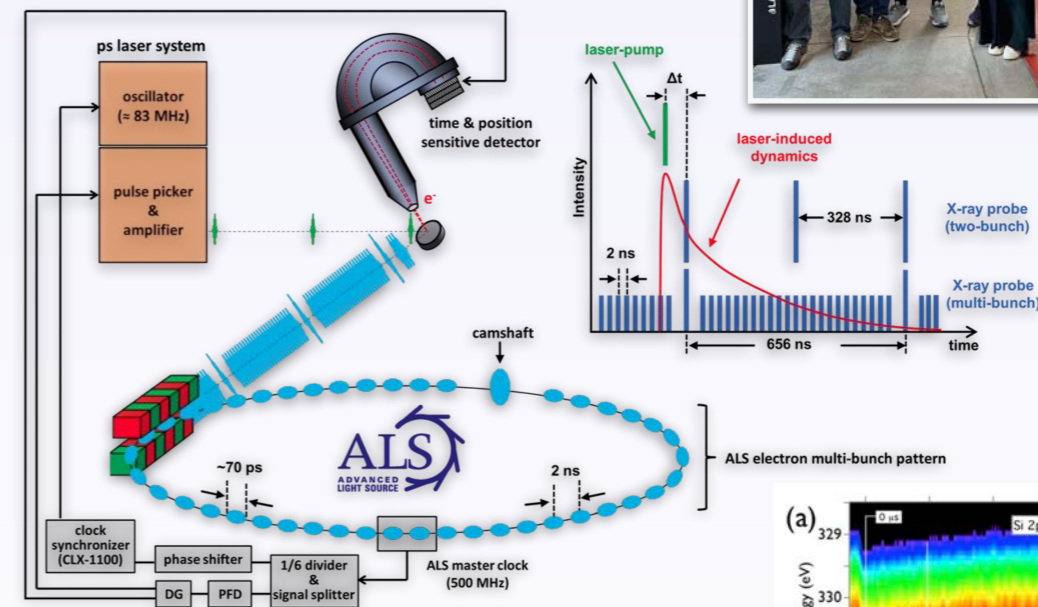
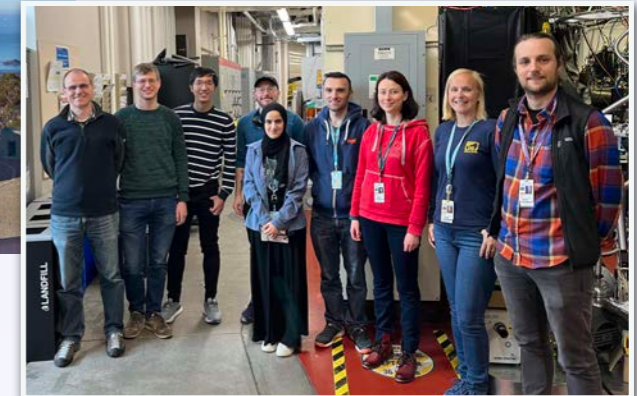
static PES



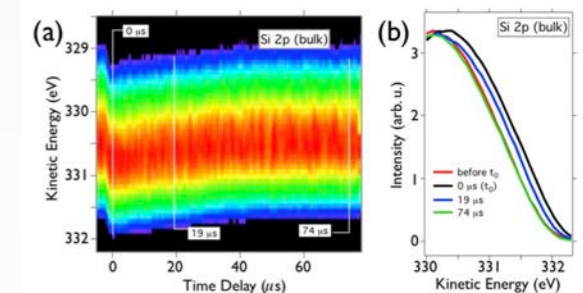
time-resolved PES



Time-resolved XPS

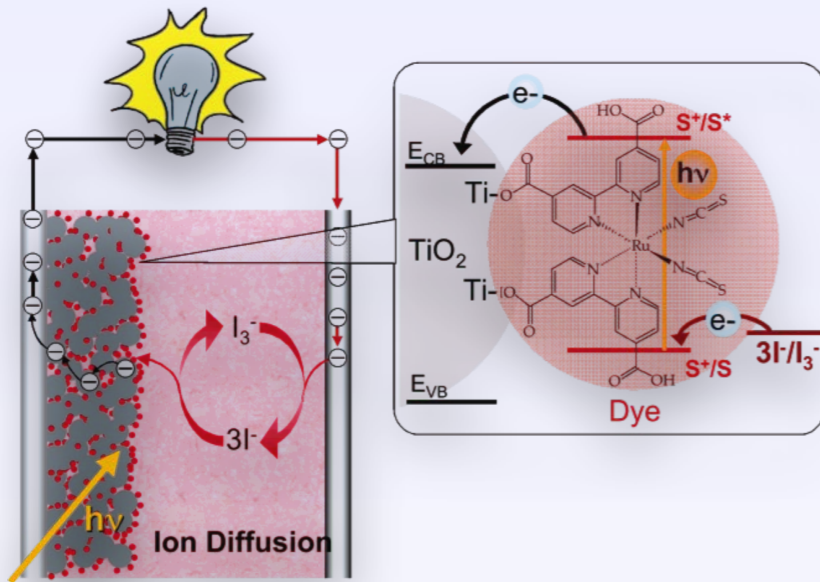


A. Shavorskiy et al., RSI 85, 093102 (2014)
 S. Neppl et al., *J. Electron. Spectrosc. Relat. Phenom.* 200, 64 (2015)



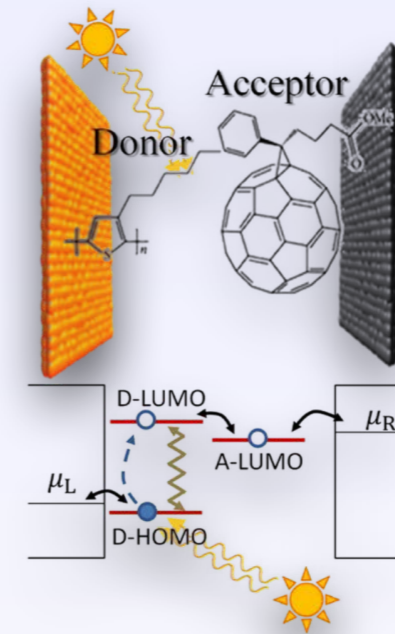
Why tr-XPS - Current research challenges

Charge Transfer at Molecule-Semiconductor Interfaces



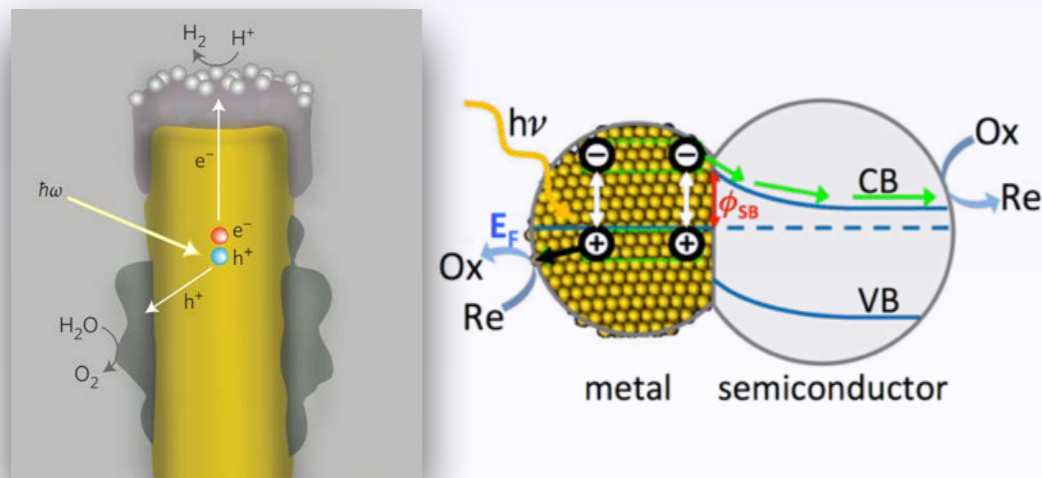
M. Grätzel, *Inorg. Chem.* **44**, 6841 (2005)

Charge Migration in Organic Semiconductors



S. Ajisaka et al., *Sci. Rep.* **5**, 8312 (2015)

Plasmon Enabled Photochemistry



S. Mubeen et al, *Nature Nanotech* **8**, 247-251 (2013)

Charge transfer (CT) processes are the basis for many fields of fundamental research and technology



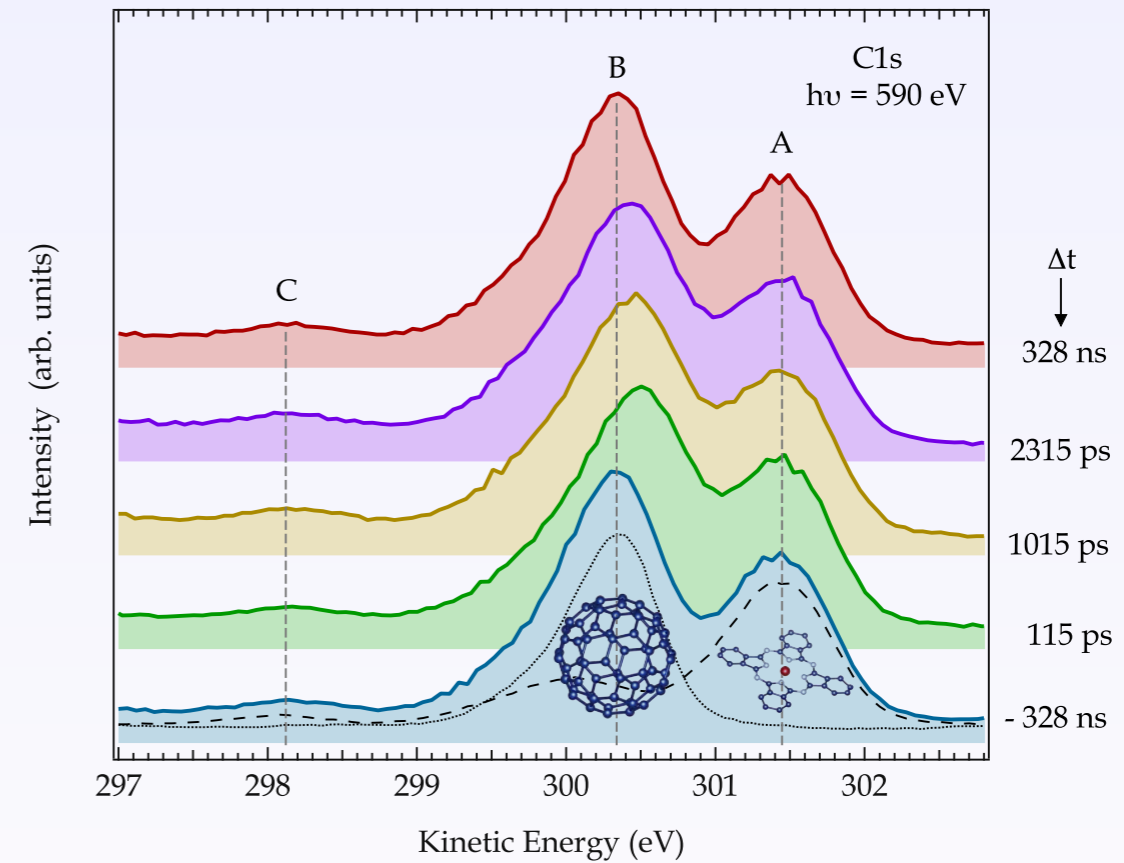
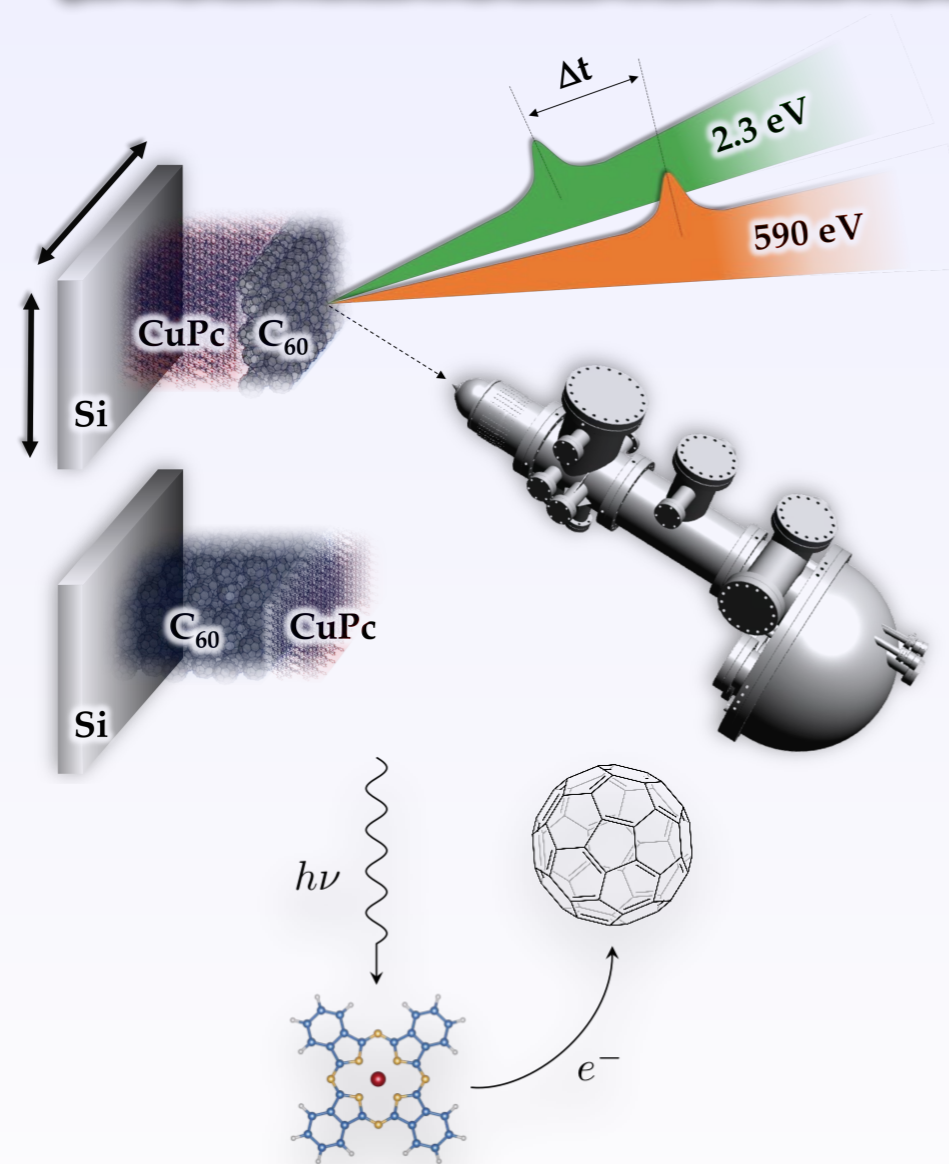
Functional interfaces

Ultrafast processes (fs ... ns time scale)

Results of the tr-XPS measurements



Charge Transfer Dynamics in Organic Donor-Acceptor Blends



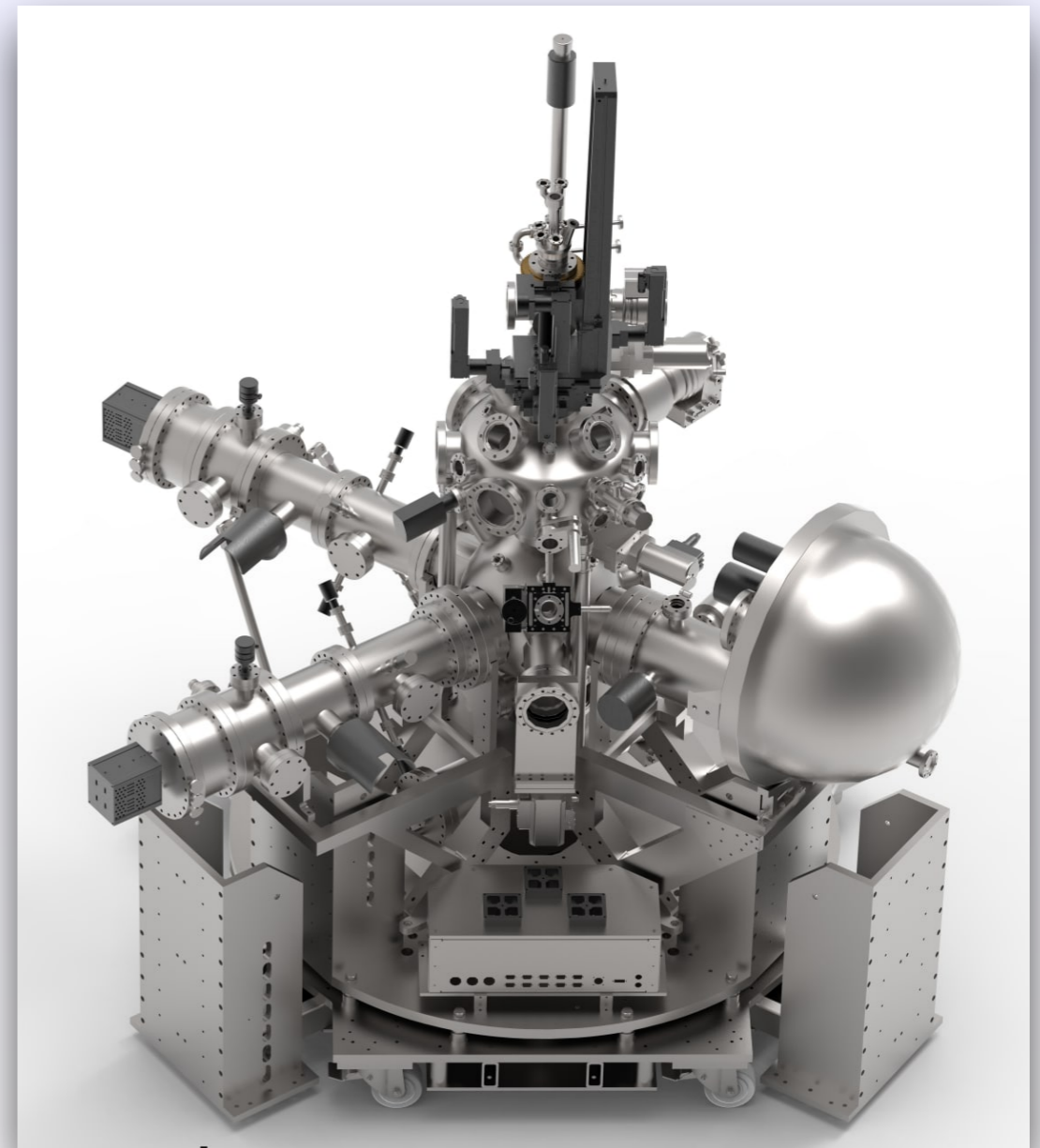
T. Arion, FR et al. *Appl. Phys. Lett.*, **106**, 121602 (2015)

FR et al. *Phys. Rev. B*, **99**, 020303(R) (2019)

Methodes of choice II - tr-XPS @ FLASH



FLASH.
Free-Electron Laser FLASH



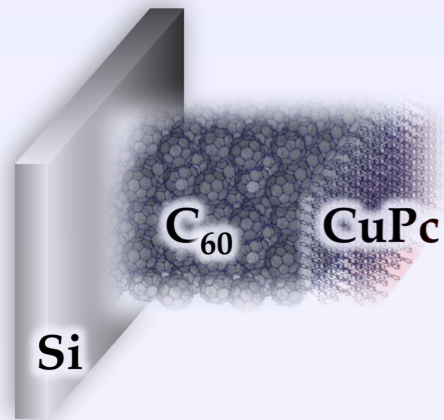
Courtesy of S. Gieschen & H. Meyer

Results of the tr-XPS measurements

FLASH.
Free-Electron Laser FLASH



Sub-picosecond tr-XPS @ FLASH

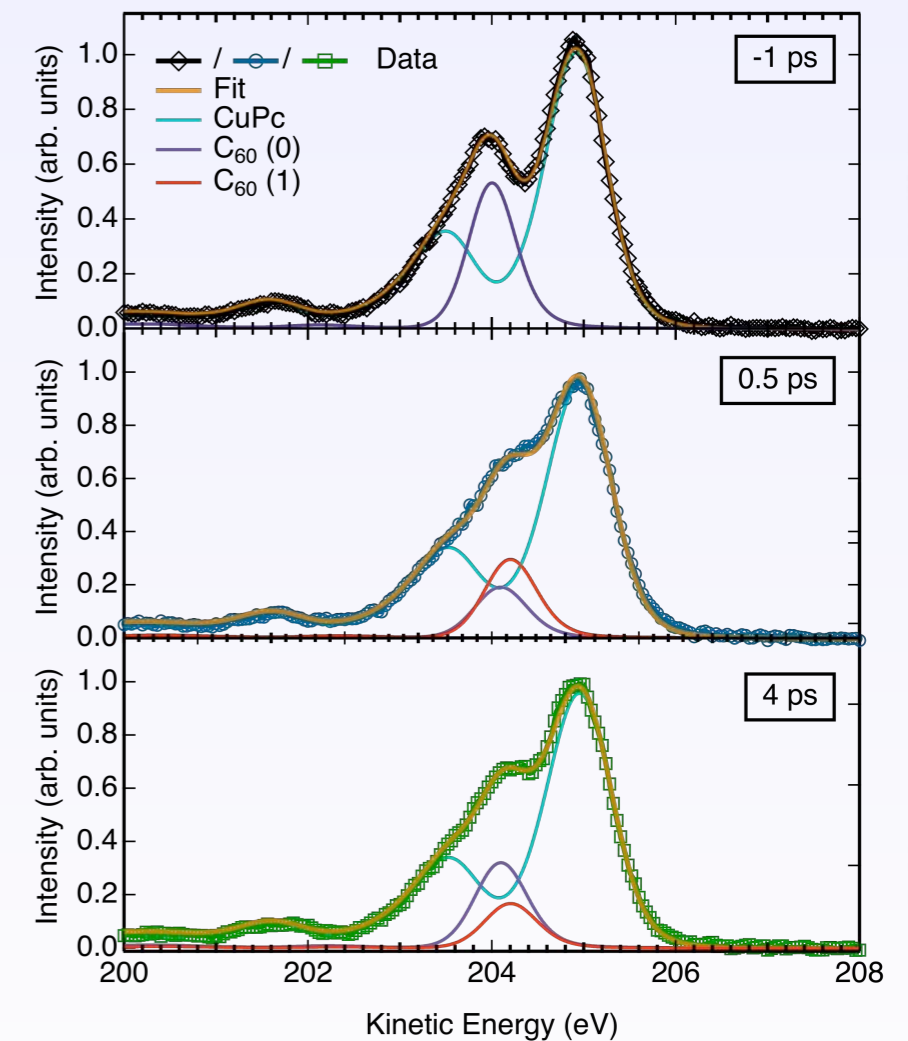
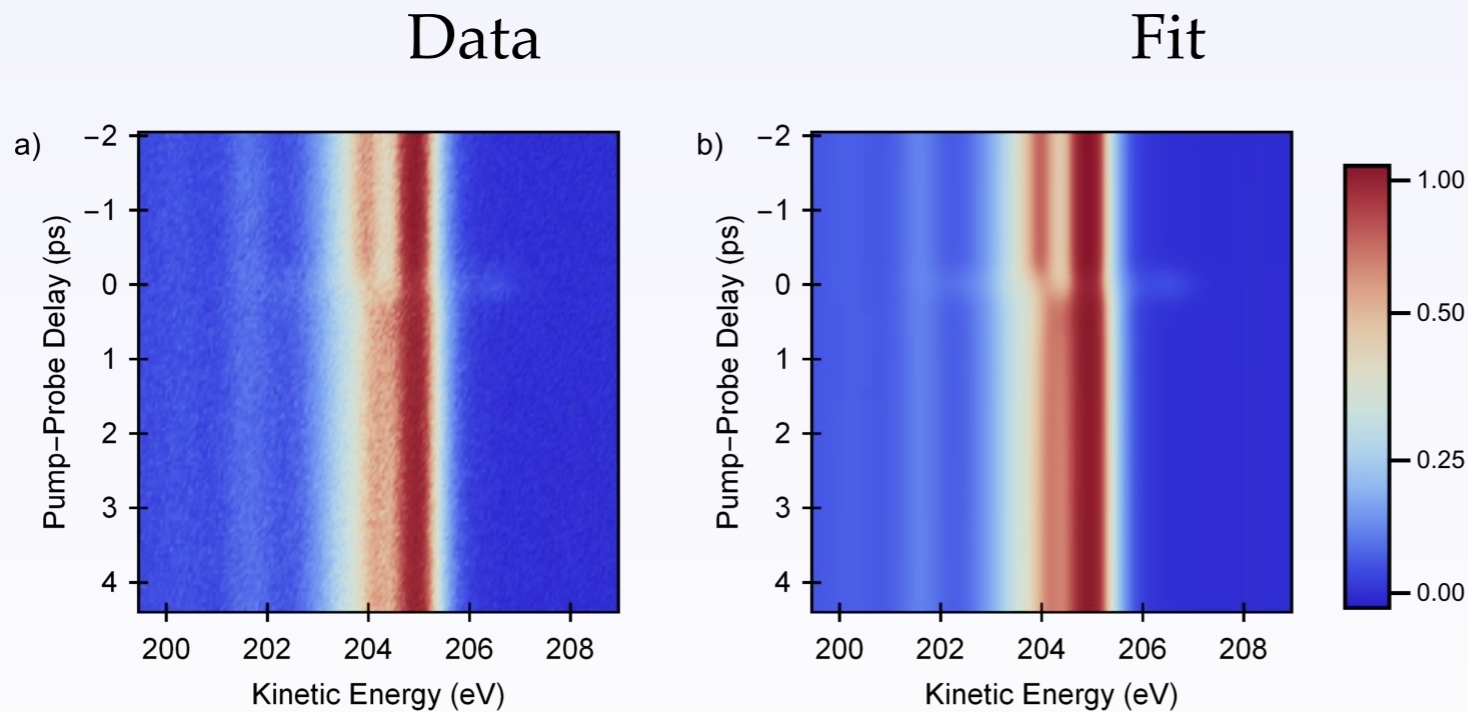


Pump: 775 nm, 100 fs

Probe: 3rd Harmonic @ 7.4 nm

→ $h\nu = 500$ eV

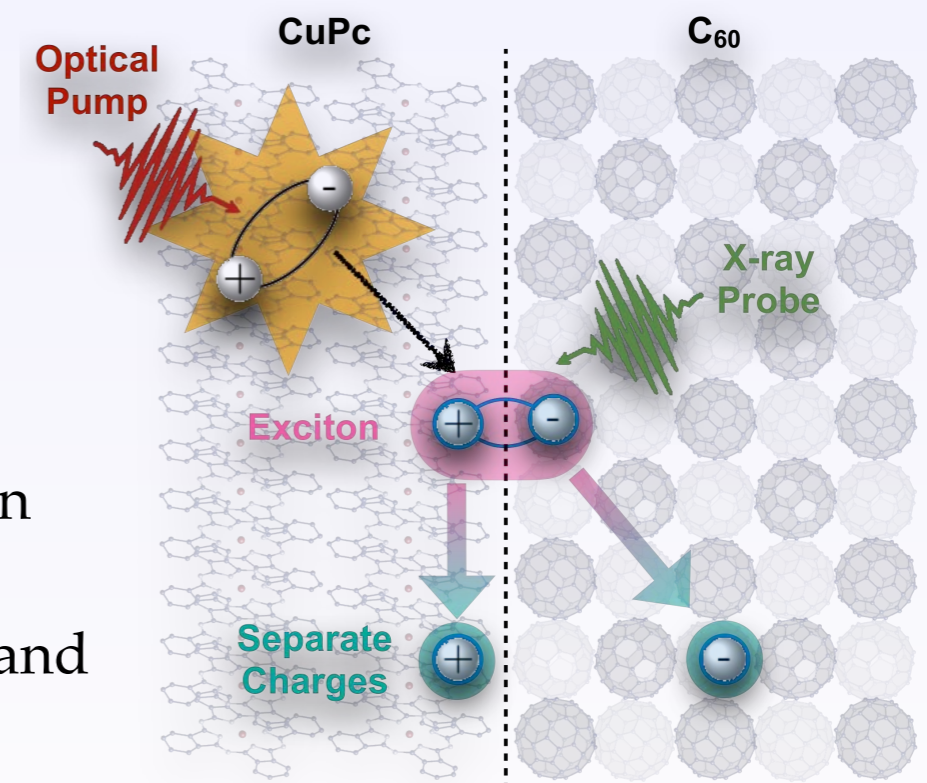
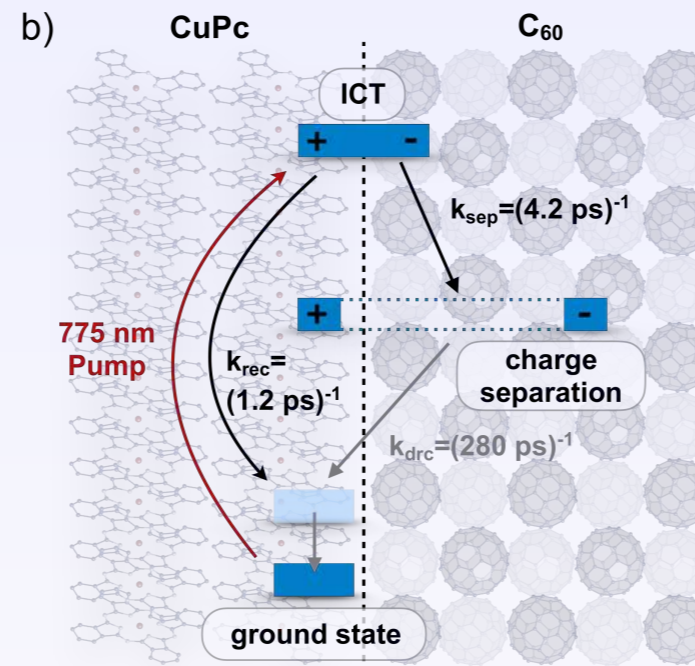
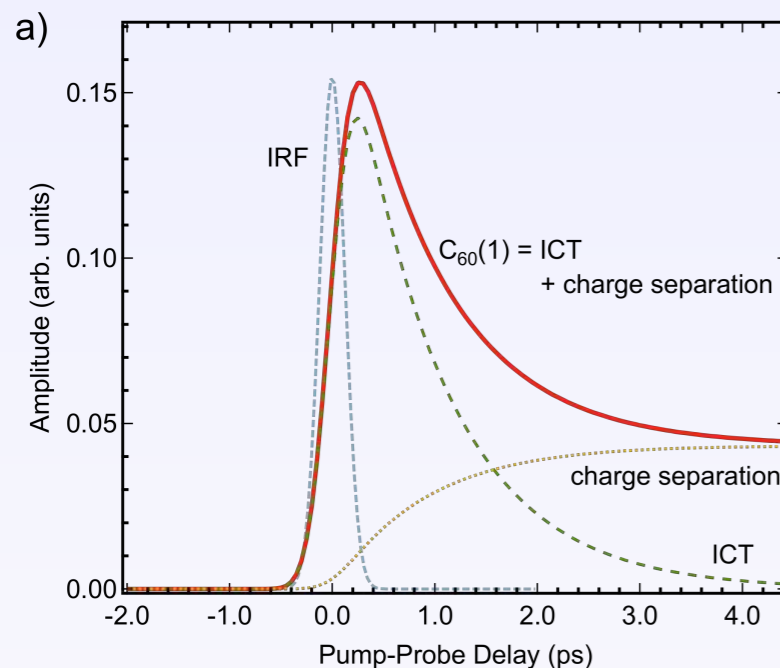
Selected spectra



FR et al. *Nat. Commun.*, **12**, 1196 (2021)

Results of the tr-XPS measurements

Sub-picosecond tr-XPS @ FLASH



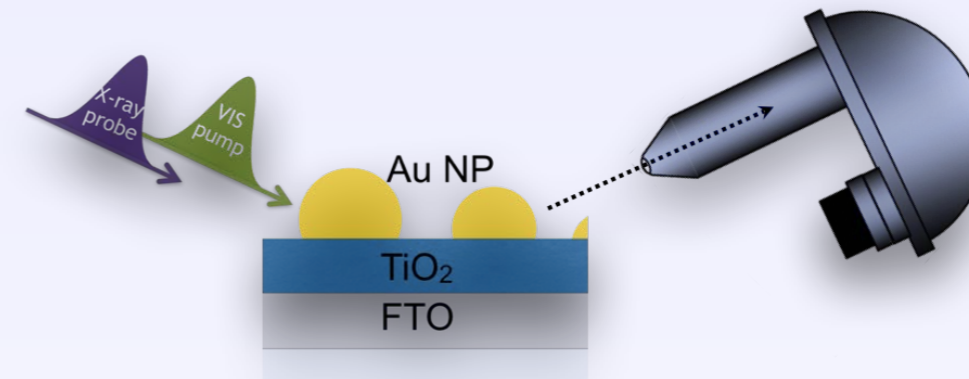
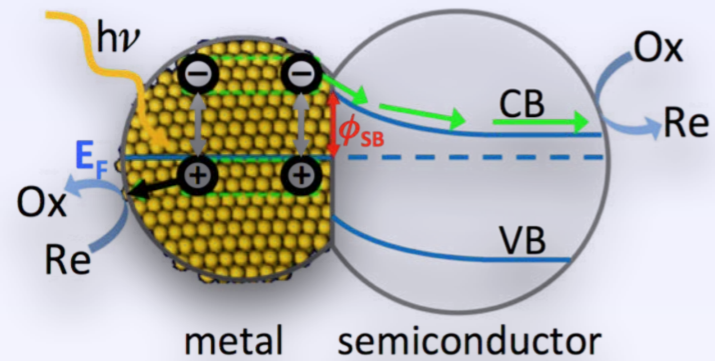
- previously unobserved channel for exciton dissociation into mobile charge carriers is identified
- first direct, real-time characterization of the timescale and efficiency of charge generation

FR et al. *Nat. Commun.*, **12**, 1196 (2021)

Results of the tr-XPS measurements

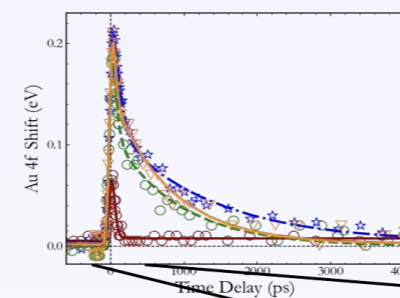


Nanoplasmonics-Enabled Charge Generation

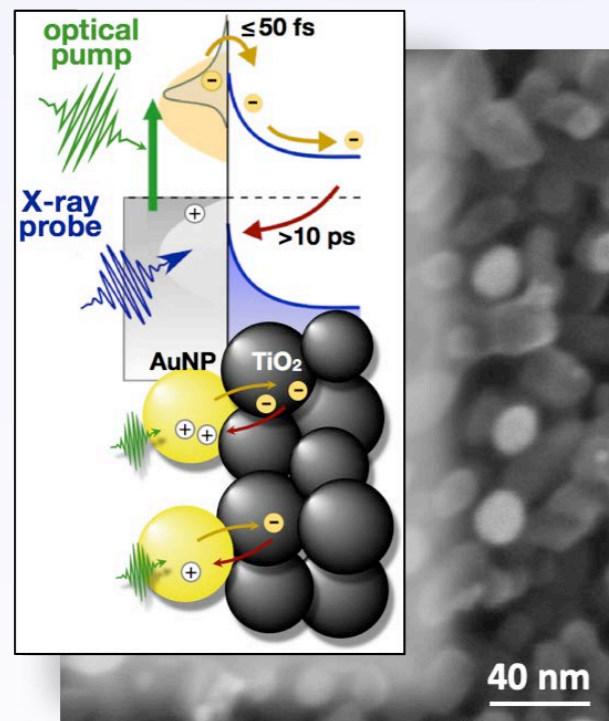


Preliminary Experimental Results

H₂O Pressure Dependent Photoinduced Au4f Shift

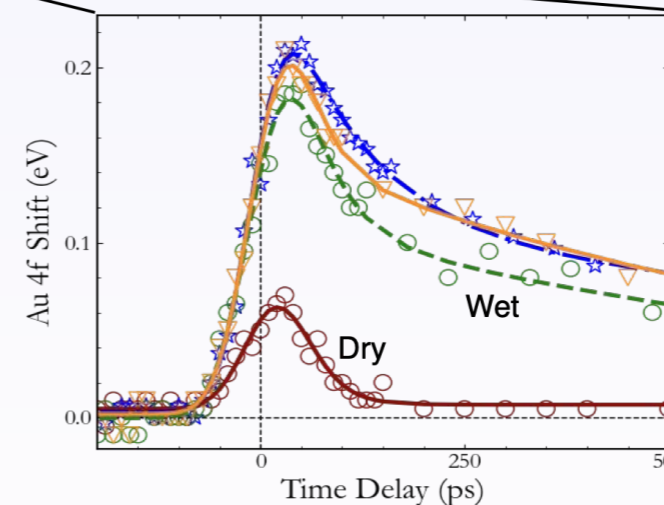


Reactants and catalyst must be studied together to understand interfacial electron dynamics driving photocatalysis!



H₂O Pressure

- <math><10^{-4}</math> mTorr
- ☆ 60 mTorr
- 100 mTorr
- ▽ 200 mTorr



Future



Berlin Joint Lab for Electrochemical Interfaces

BEIChem



HZB Helmholtz Zentrum Berlin

M. Borgward et al., J. Phys. Chem. Lett. 11, 5476 (2020)

Results of the tr-XPS measurements II



Photo-catalytically reactive ternary quantum dot sensitized TiO₂

The Nobel Prize in Chemistry 2023

The Royal Swedish Academy of Sciences has decided to award the Nobel Prize in Chemistry 2023 to

Moungi G. Bawendi

Massachusetts Institute of Technology (MIT),
Cambridge, MA, USA

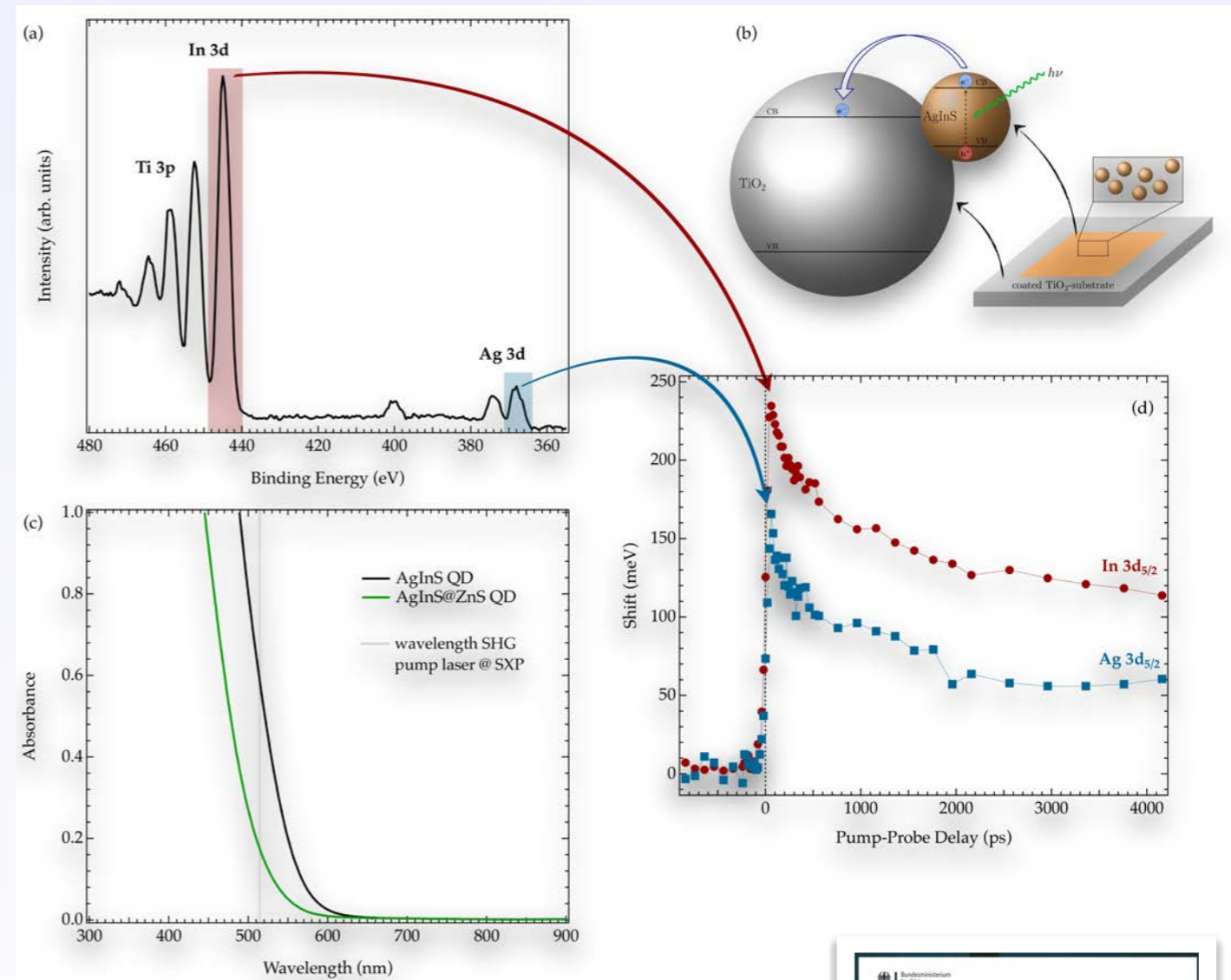
Louis E. Brus

Columbia University, New York, NY, USA

Aleksey Yekimov

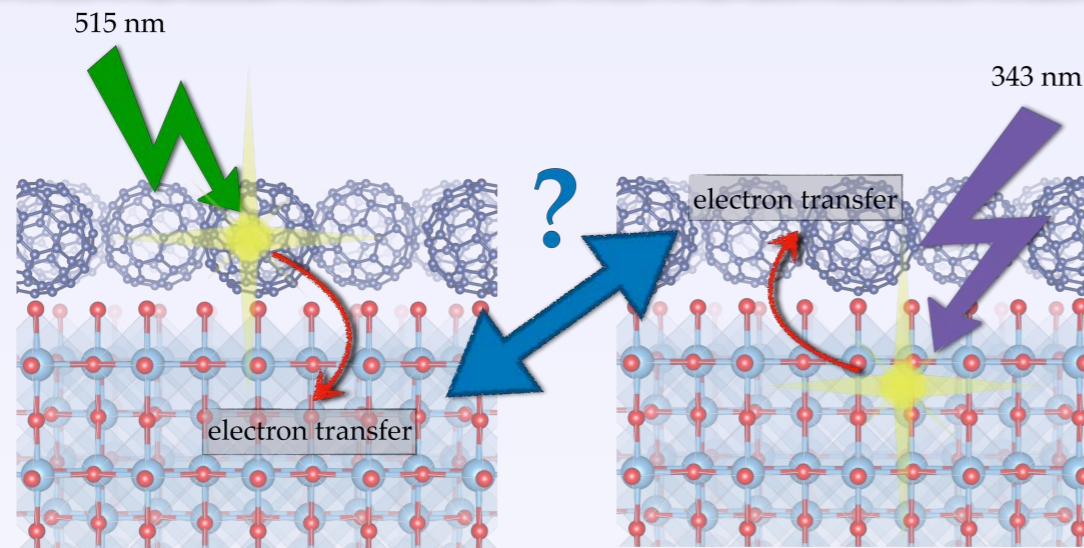
Nanocrystals Technology Inc., New York,
NY, USA

"for the discovery and synthesis of quantum dots"

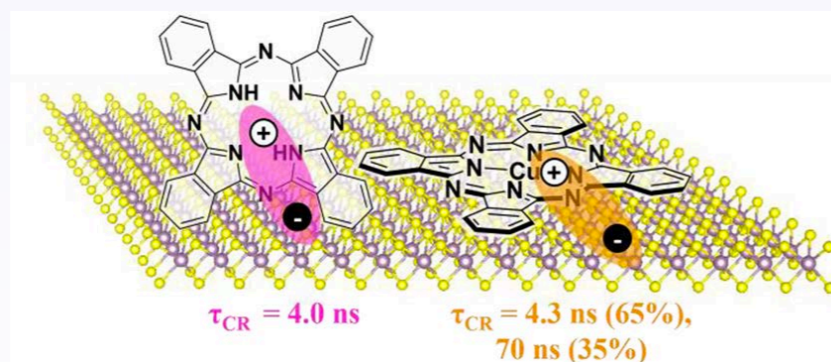


Science Case (selection)

Charge Transfer at Molecule-SC interface

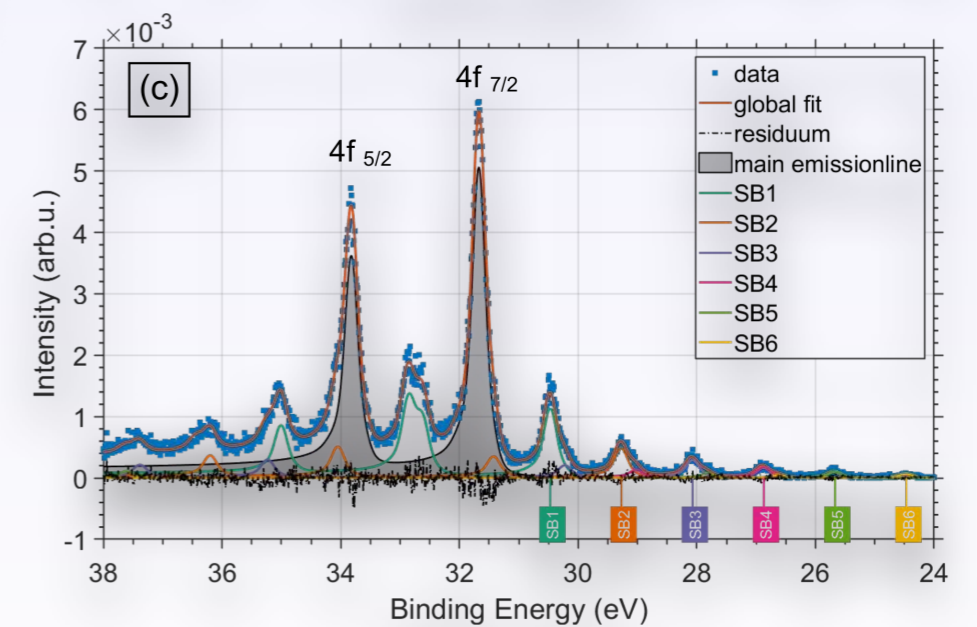
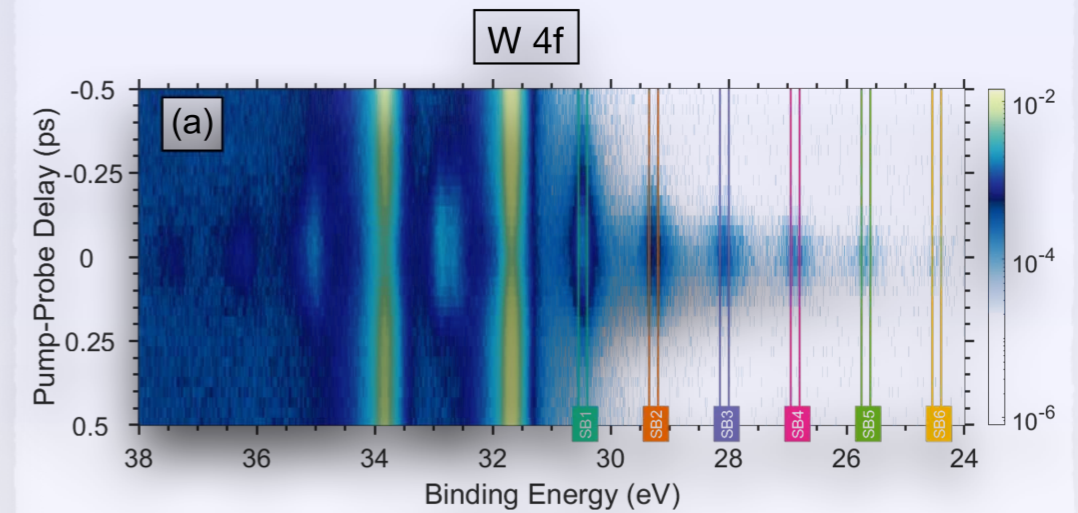


TMDC / Organic interfaces



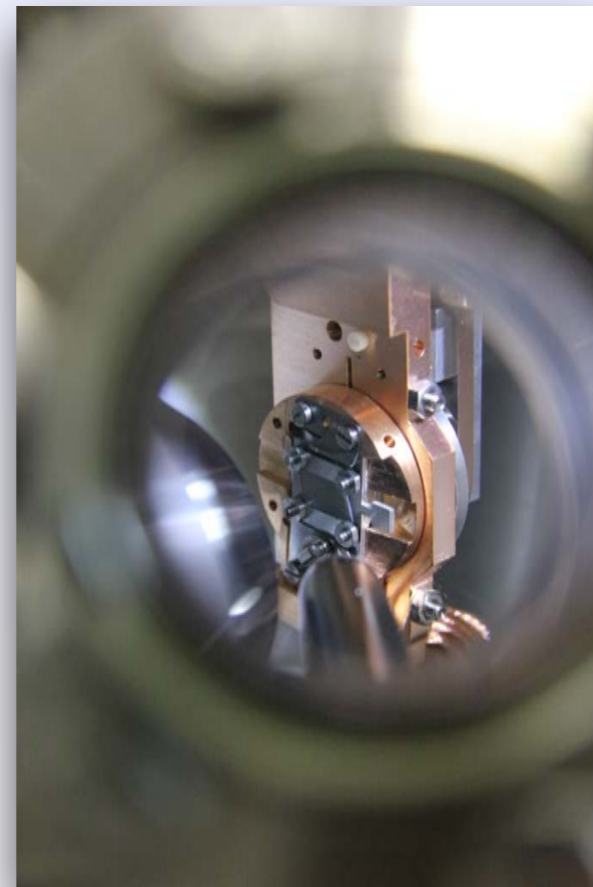
S. Padgaonkar et al., *J. Phys. Chem C* **123**, 13337 (2019)

LAPE

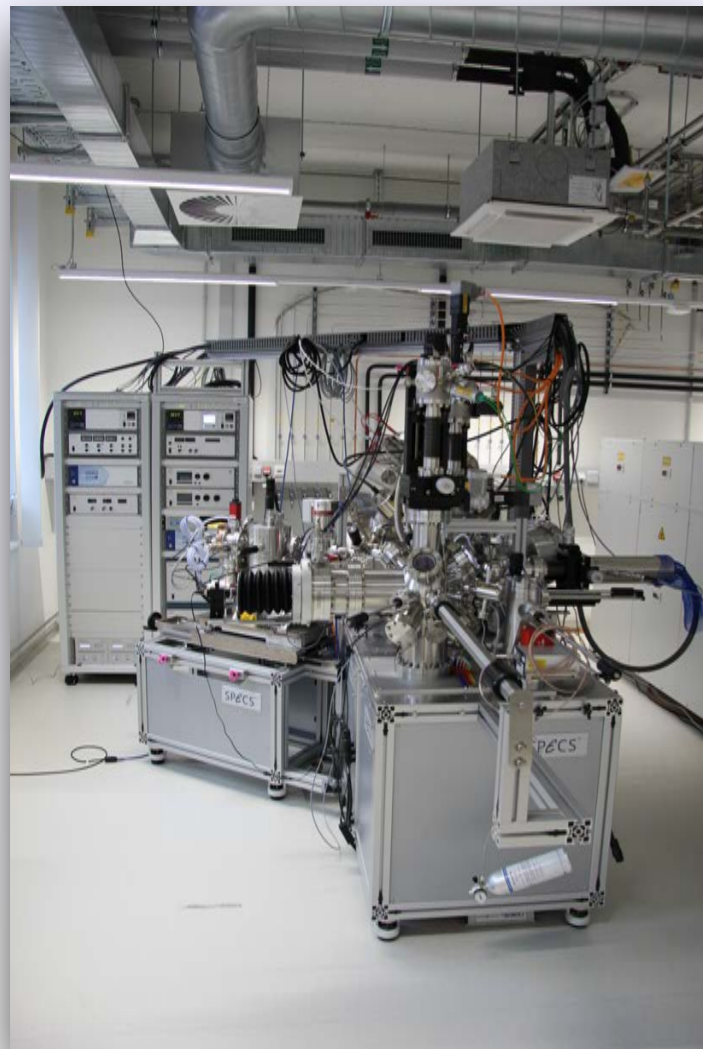
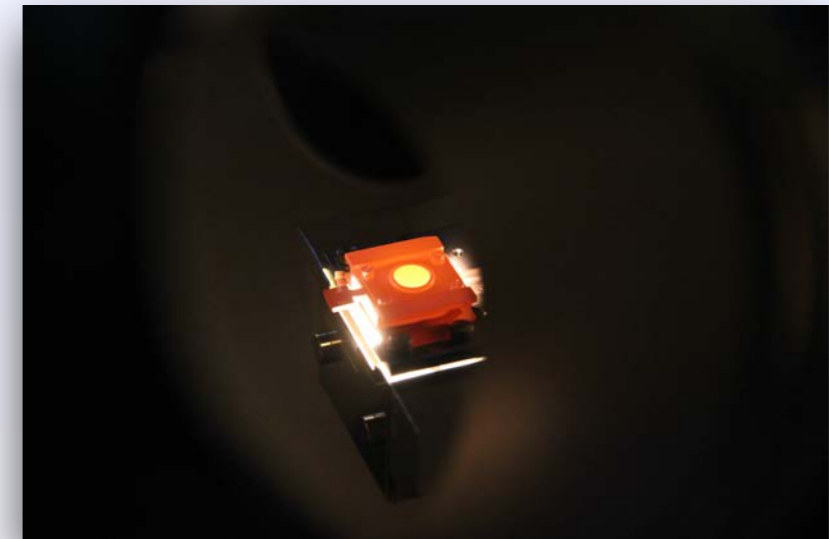


FR et al. submitted to *Nat. Commun.*

Research possibilities - TUBAF

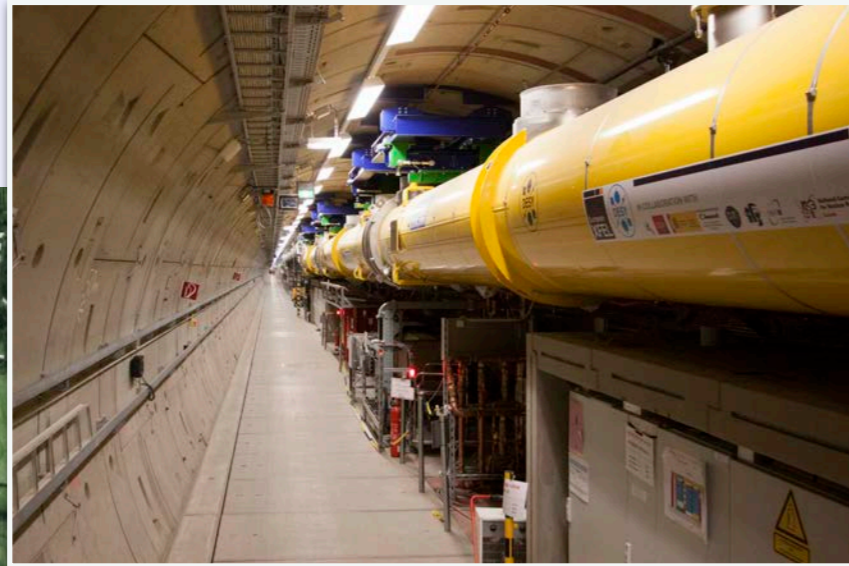
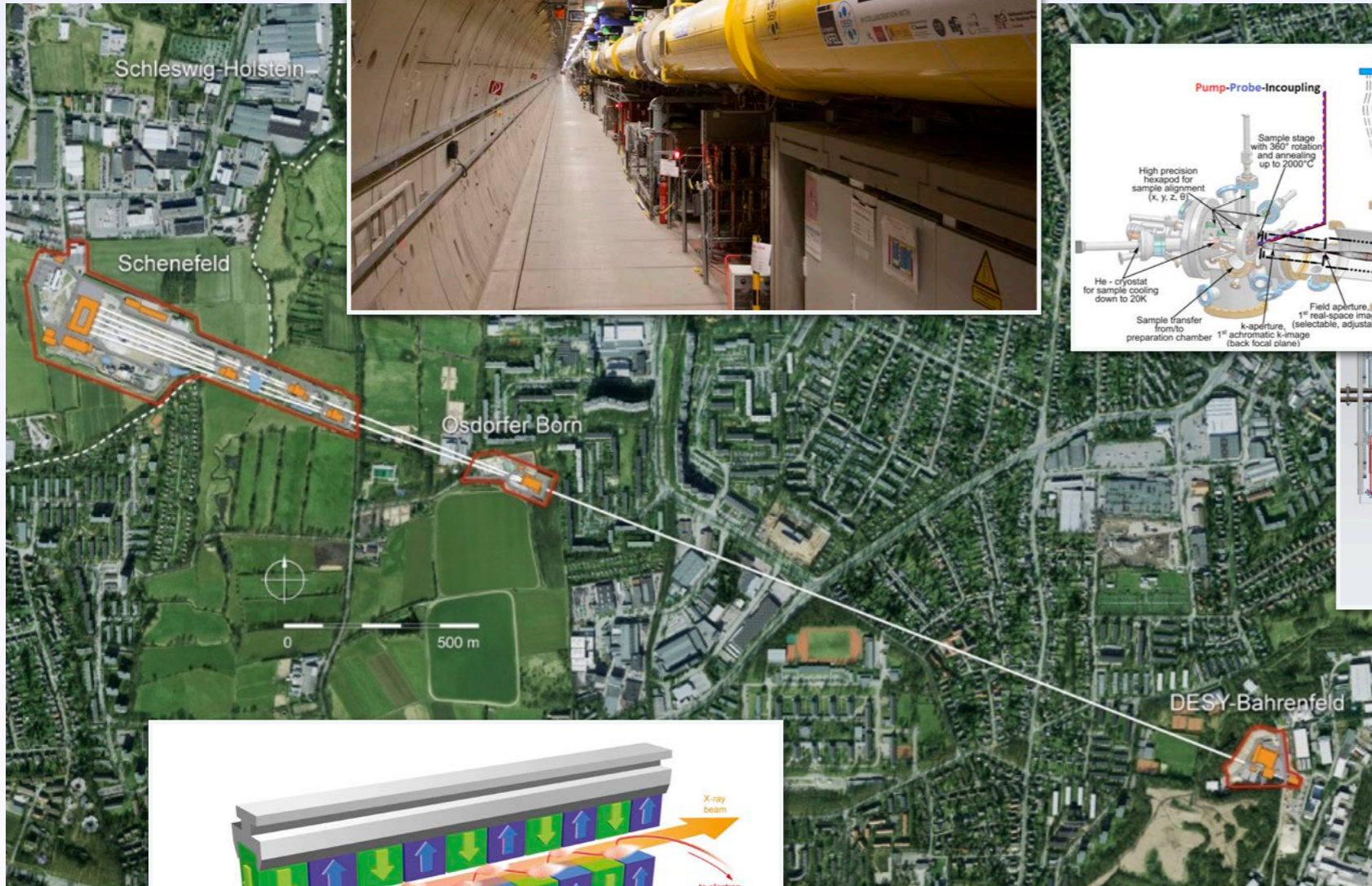


HT-PES System

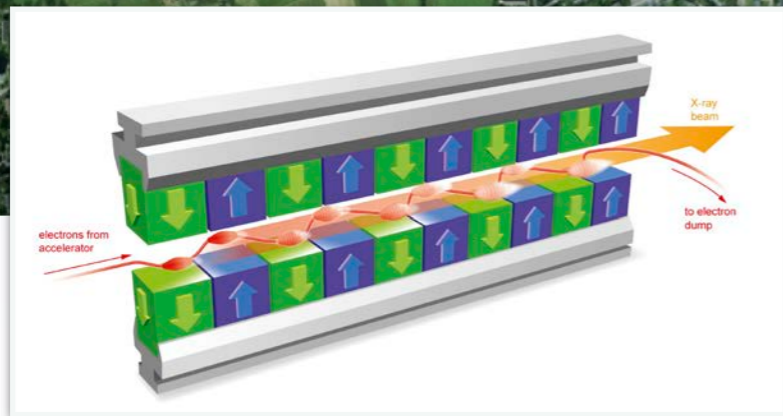
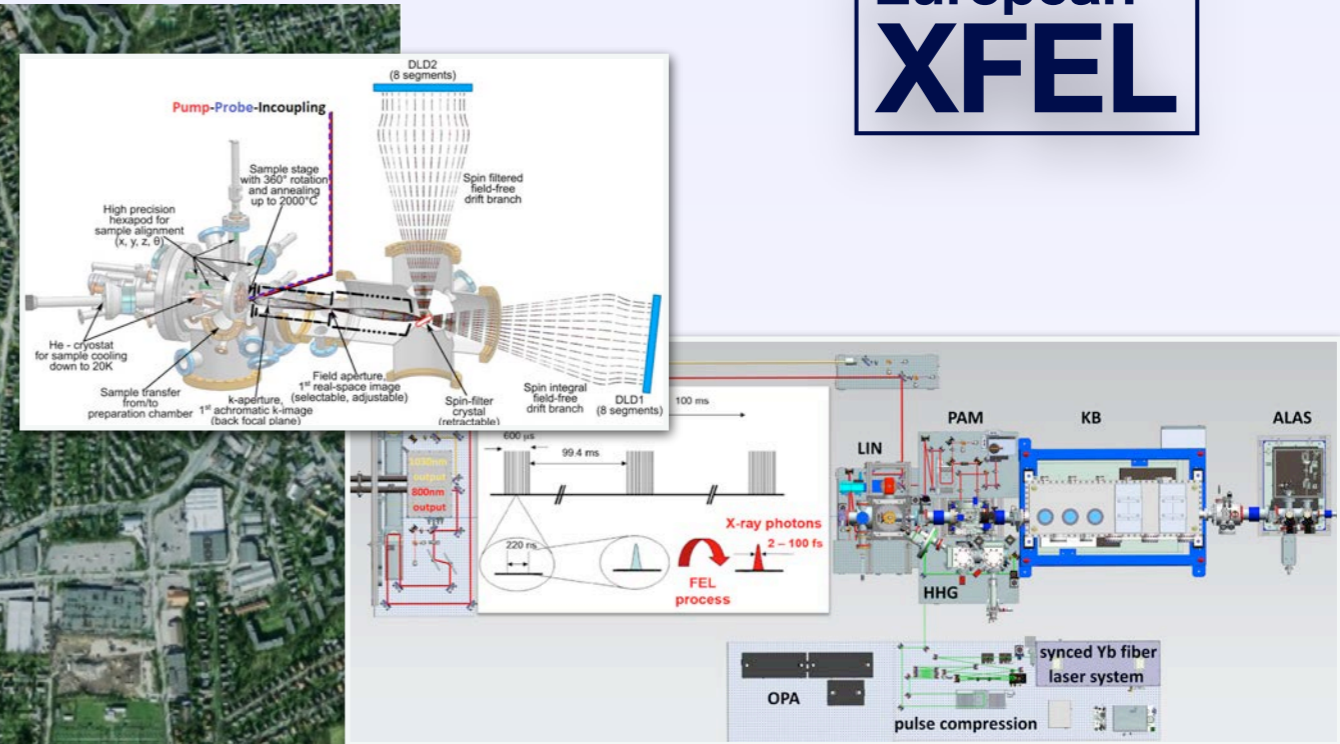


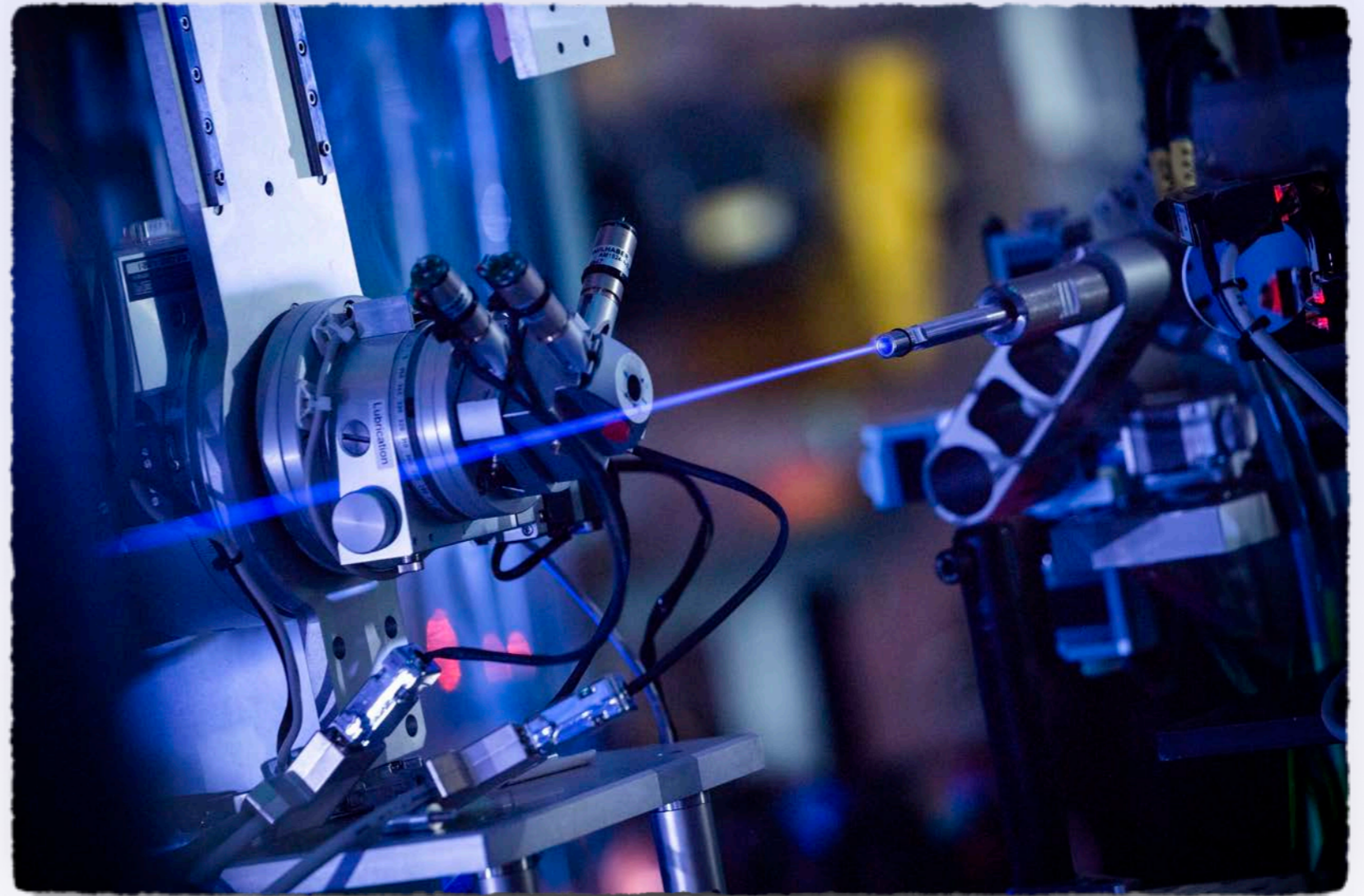


Tr-XPS @ FELs



Soft X-ray Port (SXP)





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Contact us

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friedrich.roth@physik.tu-freiberg.de