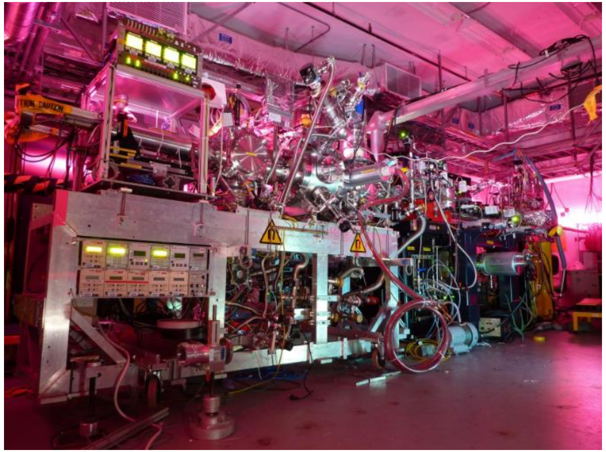
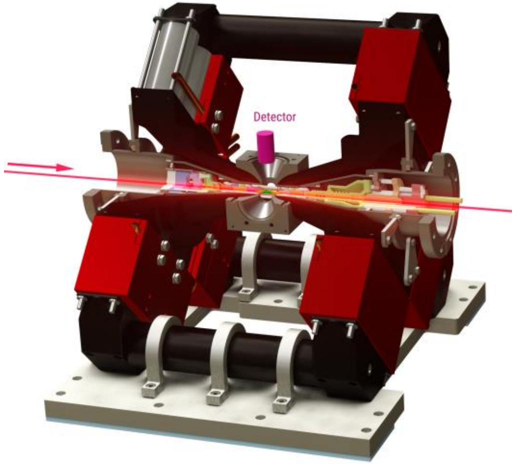
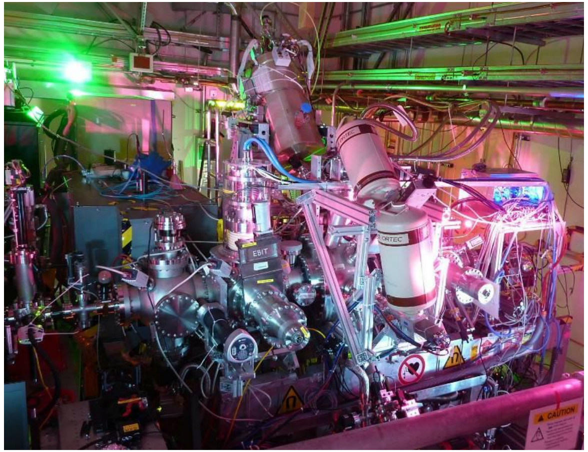
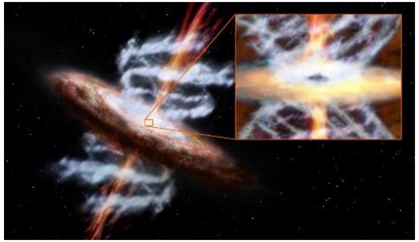
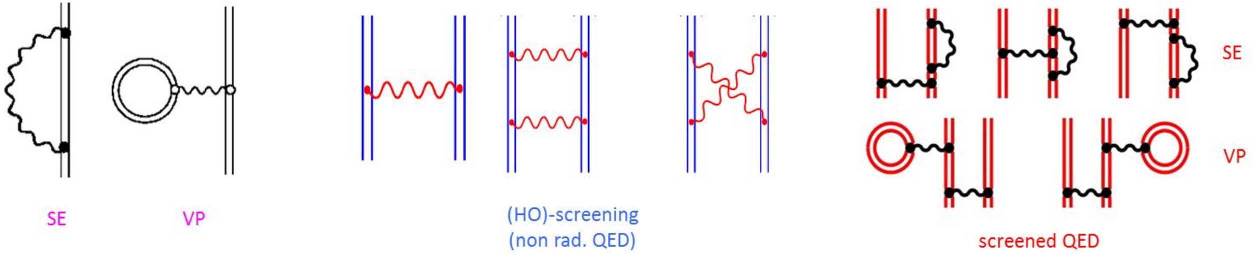
Highly charged ions research at SXP











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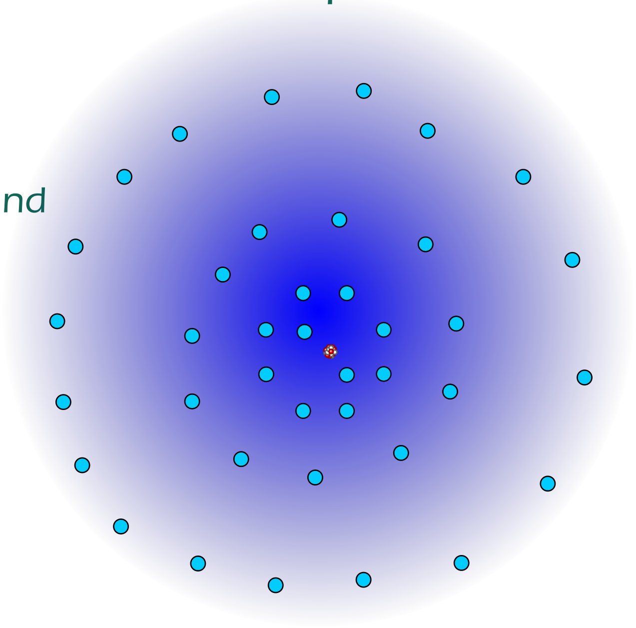
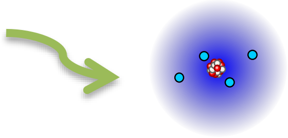
Highly charged ions (HCI)

- Study of hydrogen lead to quantum mechanics, relativistic fine structure and spin, hyperfine structure, QED..., proton size, antimatter asymmetry...
- HCI: Expanding to ~90 H-like ions, plus all other isoelectronic sequences

Atoms:
- size: 100 pm
- outer electrons weakly bound
- strong correlation effects



HCI:
- size: few pm
- few strongly bound electrons
- large electron-nucleus overlap



- Binding energy ~ Z^2
- Fine structure ~ Z^4
- QED effects ~ Z^4
- nuclear size effects ~ Z^6
- PNC contributions ~ Z^5
- Stark shifts, light shifts ~ $1/Z^6$

Bound-state quantum electrodynamics

- QED describes atomic, molecular and photonic interactions, and is the most accurate physical theory
- QED is the best understood quantum field theory, and serves as paradigm for all others
- In stable, bound systems, QED can be tested with ultimate precision
- For many-electron bound systems, QED calculations are essentially perturbative, and require approximations which still have to be benchmarked by experiments

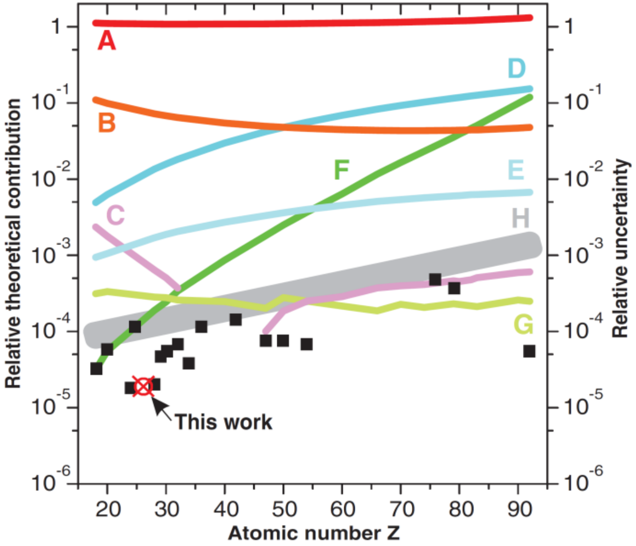
Bound-state quantum electrodynamics

- Understanding relativistic and QED effects is important to correctly model atoms (gold is yellow…) and molecules, and their interactions with X rays from first principles
- Every atom contains a core which can be investigated in detail using HCI
- Trapped HCI allow one to study QED and other interactions in a precise and controlled, steady-state fashion
- This stands in contrast to experiments using transient HCI sources with a very fast temporal evolution, strong spatial inhomogeneity, and density gradients
- In the XFEL world of ultra-high intensities, HCI become the natural survivors and can handle extremely powerful photon fluxes

Bound-state quantum electrodynamics

- Isoelectronic sequences of few-electron ions are the ideal testing ground for QED, providing a controlled scaling of QED strength and electron-correlation effects
- Analogously, nuclear-size effects also scale with high powers of Z and become important for an accurate description of the system

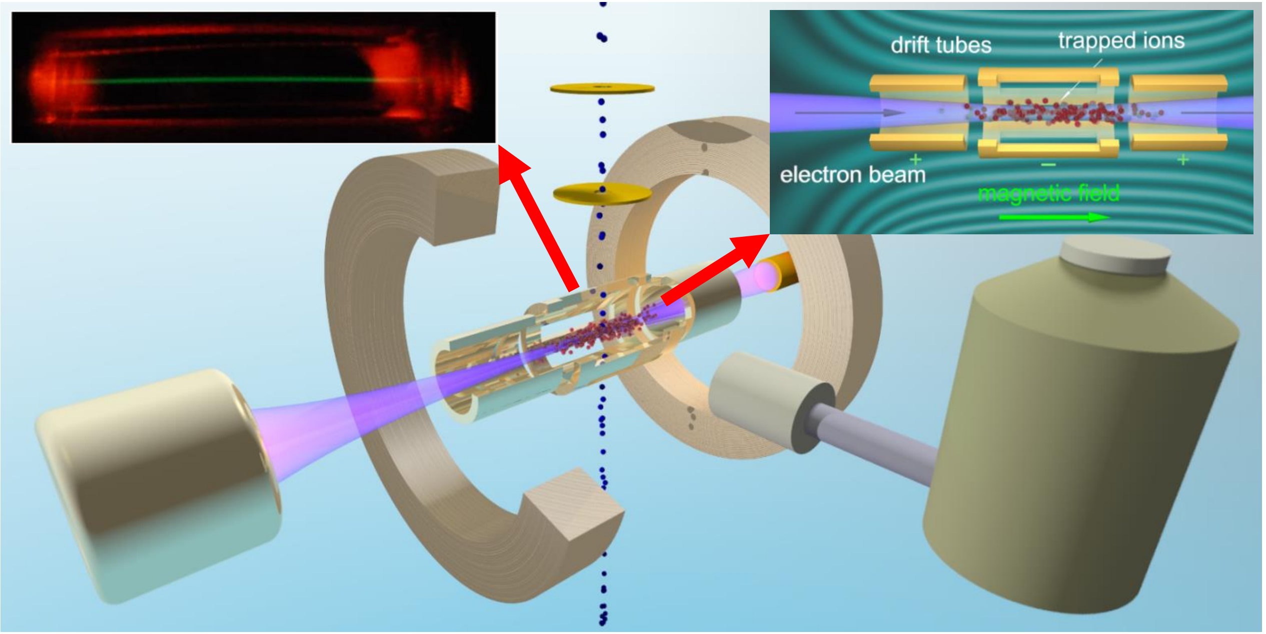
FIG. 4 (color). Different relative contributions (left scale) to the total $1s^2 2s - 1s^2 2p_{1/2}$ transition energy in Li-like HCI as a function of Z [18–20]. Interelectronic: (A) one, (B) two, and (C) three virtual photon exchange between the valence and core electrons. Radiative corrections: (D) one-loop self energy + vacuum polarization (H-like), (E) screening of (D) by core electrons. Nuclear corrections: (F) finite nuclear size, (G) relativistic recoil. Total relative uncertainties (right scale): (H) theoretical; (black squares) experimental ([15], [17,18], [23–26] and references therein), and (red cross) this work.



Production and experiments

- Electron beam ion traps (EBIT) are capable of producing and storing HCI in any charged state (from He^{+} to U^{92+})
- All x-ray spectroscopic measurements of HCI are limited by statistics and resolution, due to instrumental issues in both storage rings and EBITs
- At x-ray energies, photoexcitation cross sections (~10^{-16} cm^2) are many orders of magnitude higher than electron impact excitation cross sections (~10^{-22} cm^2)
- The combination of an XFEL and an EBIT provides enormous statistical and resolution advantages for bound-state QED studies

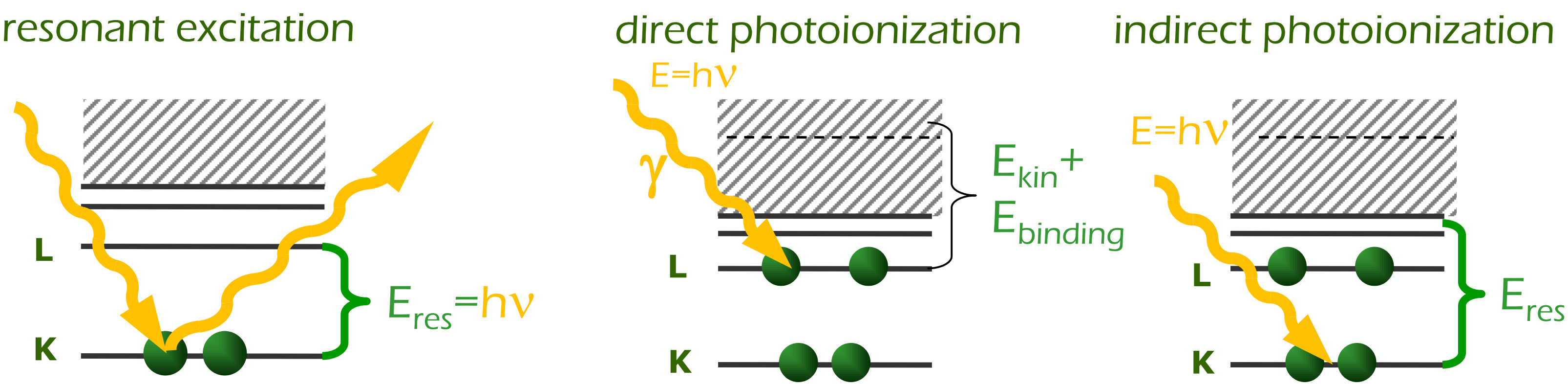
Electron beam ion trap (EBIT)



- *An electron beam produces, traps and excites HCI under well-defined, controlled conditions.*
- *Photon detectors, crystal and grating spectrometers, microcalorimeters, etc., are used for diagnostics from the optical to the hard x-ray range.*

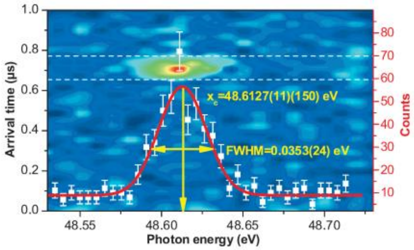
What is needed for X-ray laser spectroscopy?

1. Two bound states separated by x-ray energies
   - *Atoms are unsuitable at energies beyond their ionization potential*
   - Nuclei require much higher photon energies
2. Many photons of the right energy
   - Intensity, collimation and frequency control are much better with lasers than in other sources.



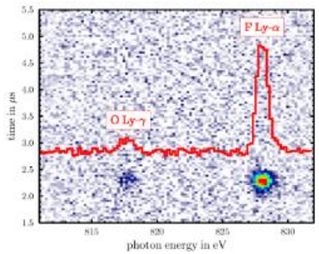
Resonantly photon-induced processes

50 eV: *2s-2p* in Fe^{23+}

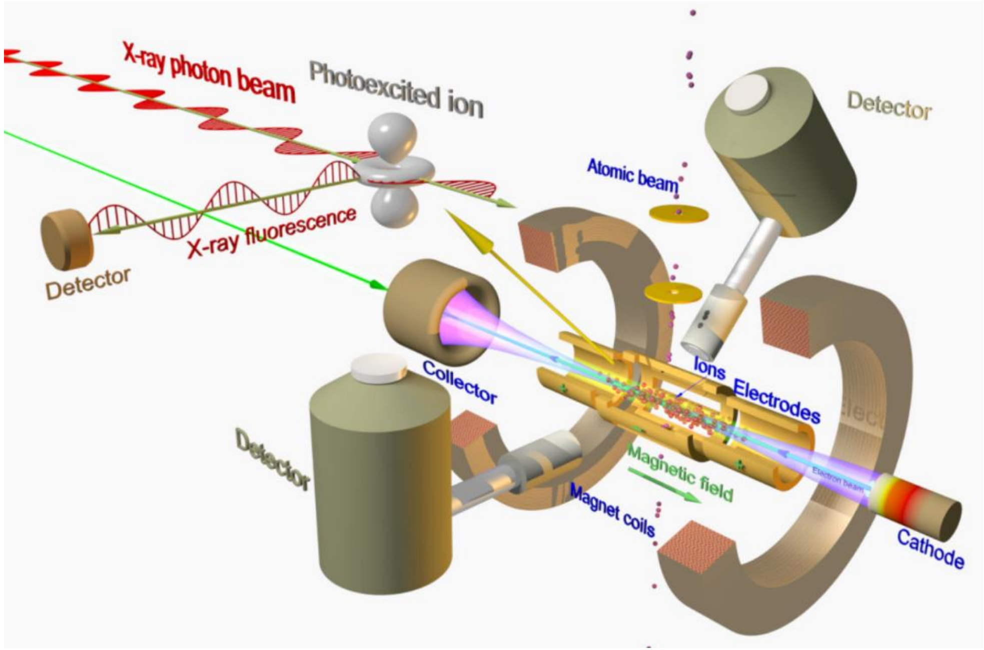


S. Epp et al.,
PRL **98**, 183001 (2007)

800 eV: *2p-3d* in Fe^{16+}

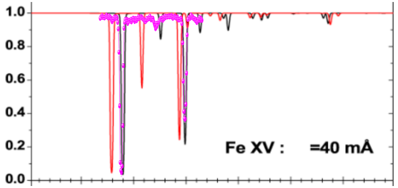


S. Bernitt et al.,
Nature **492**, 225 (2012)



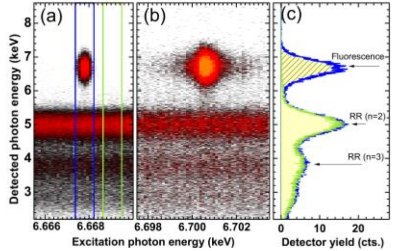
Free-electron lasers and synchrotrons provide X-rays with high power and energy resolution

800 eV: photoionization of Fe^{14+}



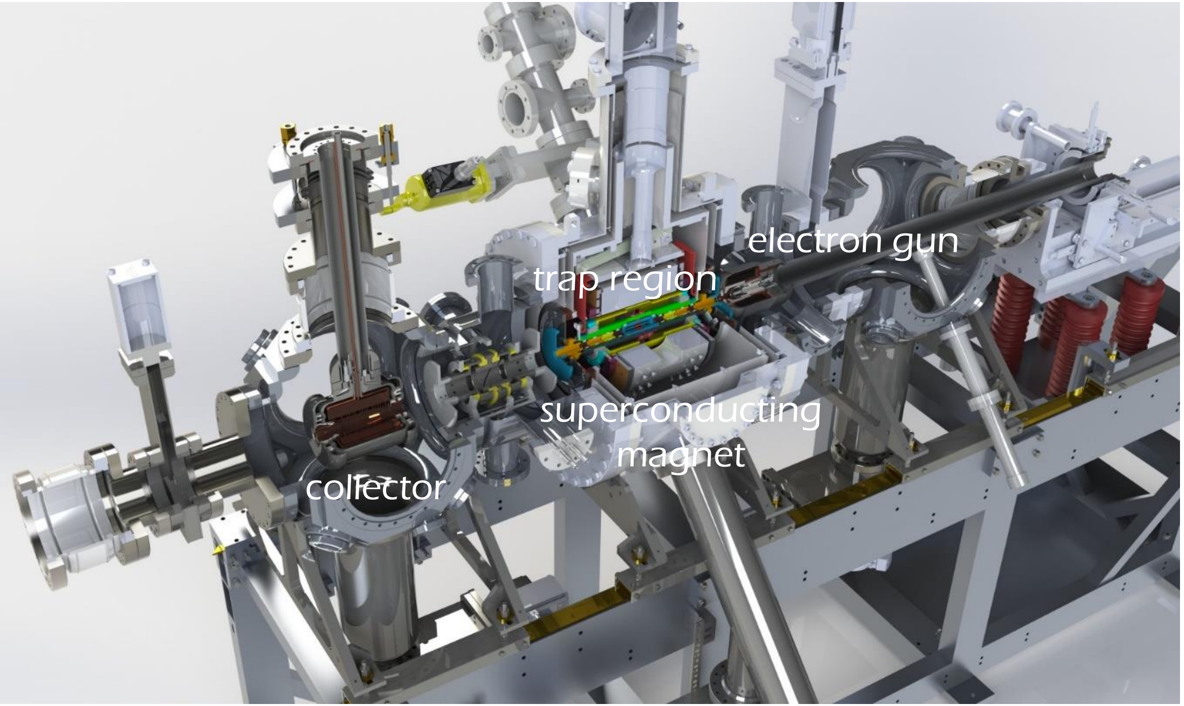
M. C. Simon et al.,
PRL **105** 183001 (2010)

6 keV: *1s-2p* in Fe^{24+}



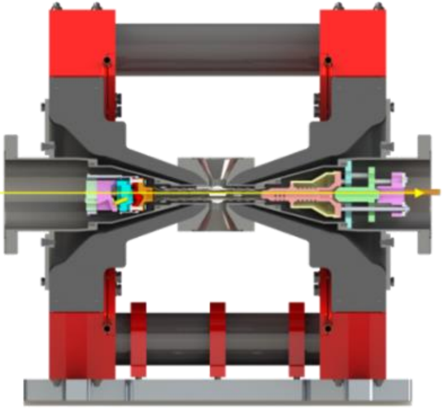
J. Rudolph et al.,
PRL **111**, 103002 (2013)

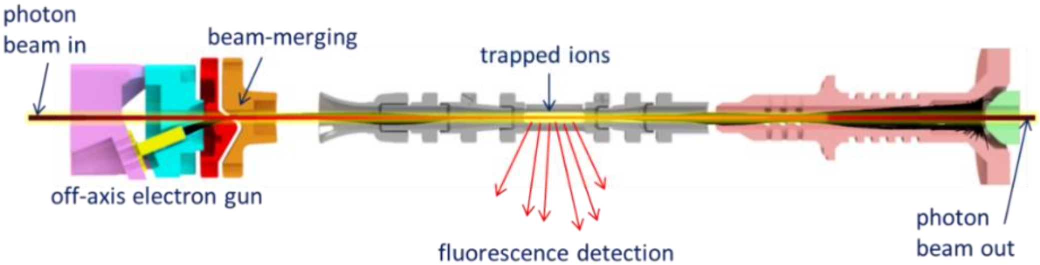
Electron beam ion trap (EBIT)



- EBITs used to be cryogenic and big in order to achieve efficient operation
- Recently, compact EBITs qualified for XFEL experiments have been developed

Compact EBITs for photon studies

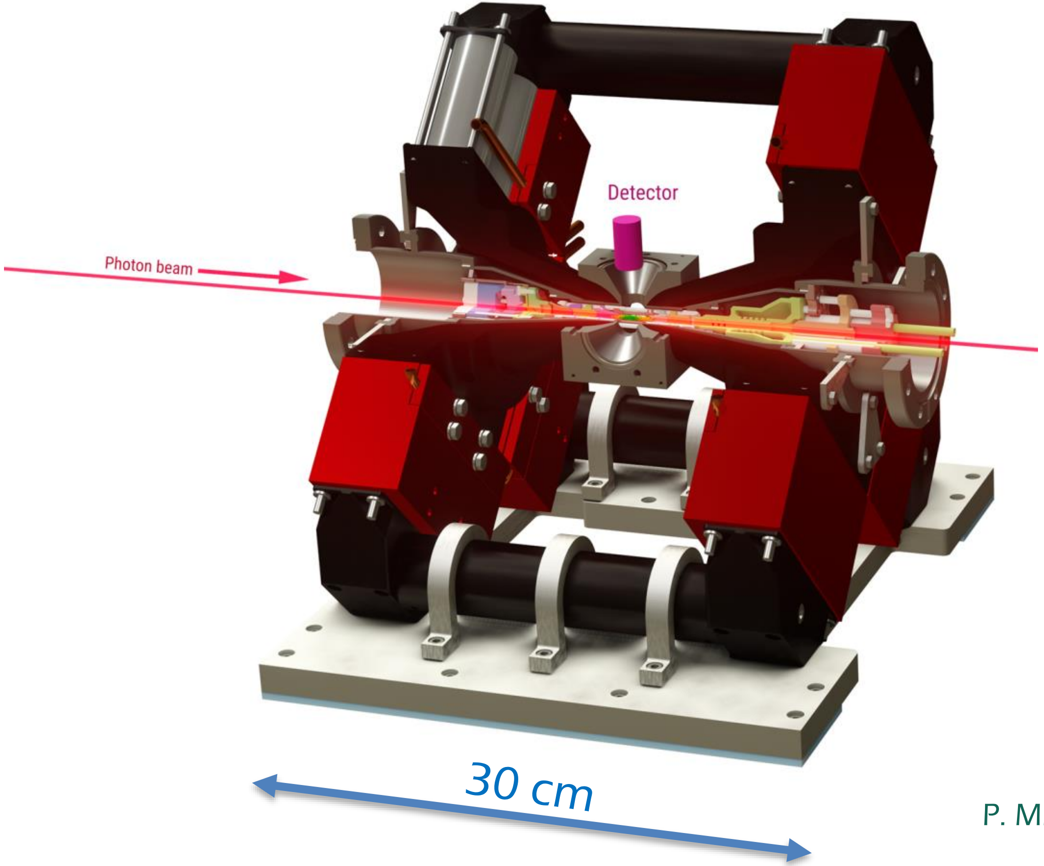




P. Micke et al.,
JRCLU, RSI (2018)

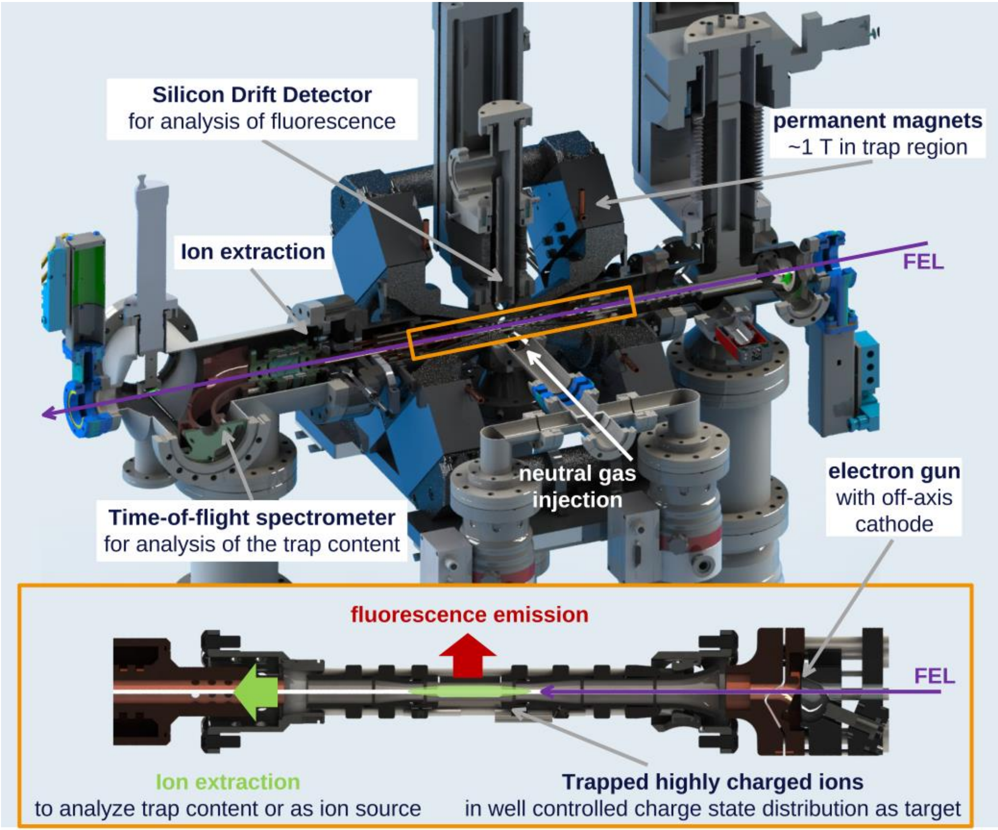
Polar-X EBIT and section through it. Bottom: Off-axis electron gun letting the photon beam to pass interaction region towards downstream experiments for pulse diagnostics.

Compact EBITs for photon studies



P. Micke et al., JRCLU, RSI (2018)

A miniature EBIT for EuXFEL



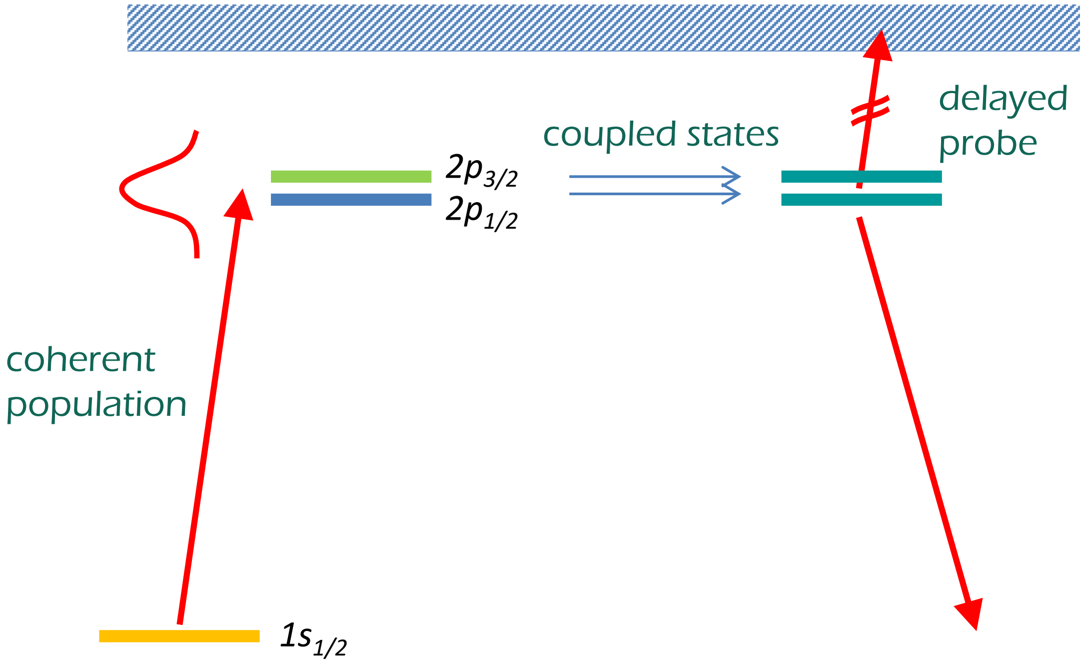
T. M. Baumann, M. Togawa, J.R. Crespo López-Urrutia, T. Pfeifer, M. Izquierdo, and M. Meyer, Poster UM EuXFEL (2022)

Electron excitation dynamics in the attosecond scale

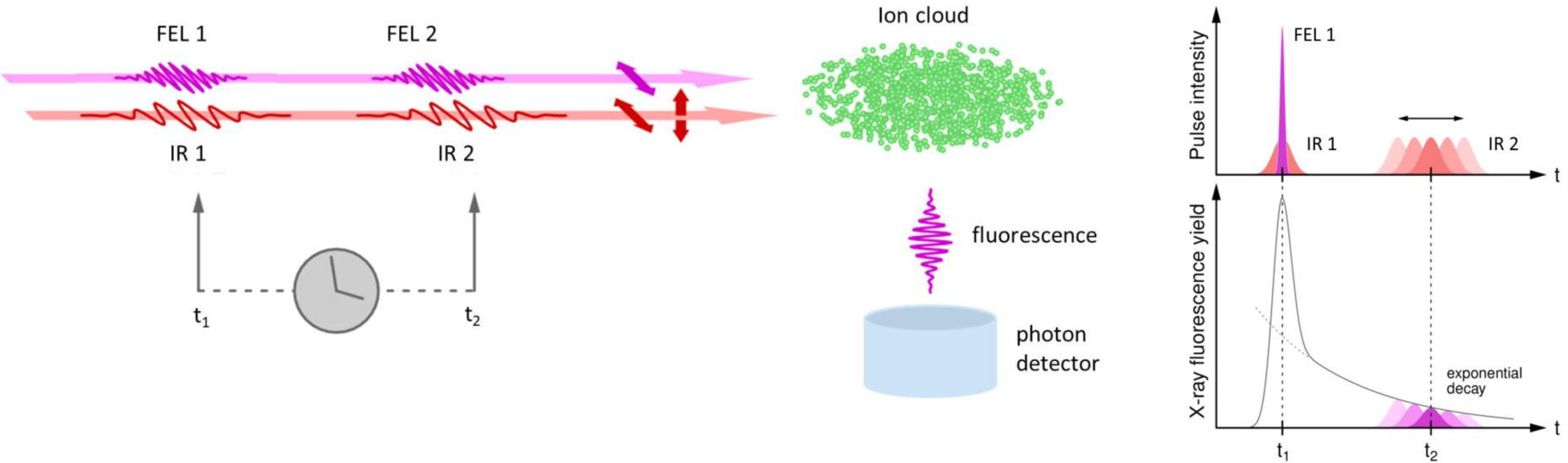
- Electronic wave packages (e. g., coupled spin states) can be prepared in systems which are impervious to Auger decay within the experimental time
- Multi-photon (sequential) absorption is possible in the 80 keV range
- Pump-probe experiments can track the dynamic evolution of the spin system recording both fluorescence and/or photoions (quantum beats, Ramsey-type methods)
- Such experiments could, e. g., allow to better understand the role of the Breit interaction (spin-spin) in strongly bound, relativistic electrons by exaggerating those effects in a well-defined way

Generic pump-probe experiments

- Fine structure and hyperfine/isotopic energy differences in the meV…eV range result in fs-scale beatings that can be used to analyze energy differences and spontaneous transition rates



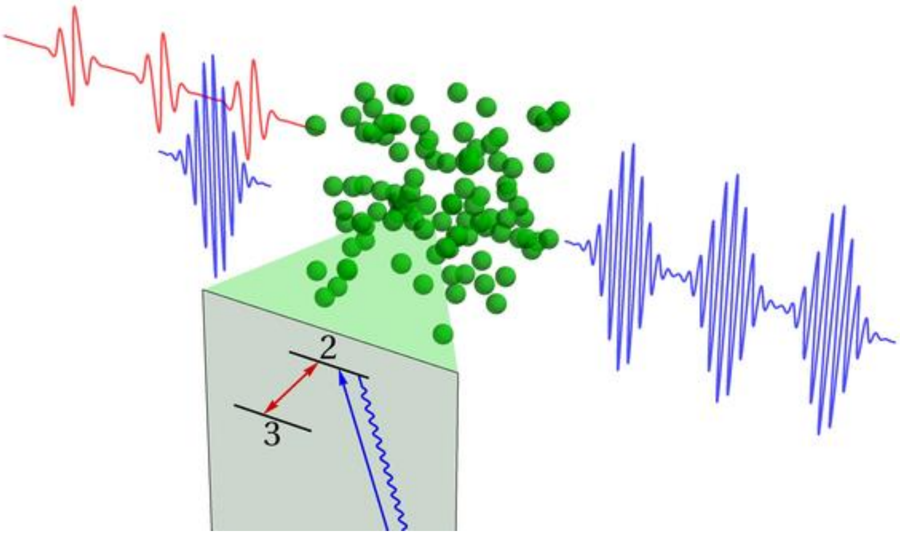
Pump-probe experiments



- Combined XFEL-IR pump-probe experiments with HCI, time evolution of state population
- Initial peak due to the *E1*-excited transition decays much faster than population shifted into metastable level by an IR pulse.
- Delayed IR pulses coupling the metastable state to fast-decaying ones cause fluorescence.

S. M. Cavaletto *et al.*, Phys. Rev. A **88**, 063402 (2013)
S. M. Cavaletto *et al.*, Nature Photonics **8**, 520 (2014)
O. Postavaru, Z. Harman, and C. H. Keitel, Phys. Rev. Lett. **106**, 033001 (2011)

X-ray frequency comb generation



Coherent superpositions of states in hard X-ray driven systems can be modulated by optical or VUV frequency combs for the generation of X-ray frequency combs

S. M. Cavaletto *et al.*, Phys. Rev. A **88**, 063402 (2013)

S. M. Cavaletto *et al.*, Nature Photonics **8**, 520 (2014)

O. Postavaru, Z. Harman, and C. H. Keitel, Phys. Rev. Lett. **106**, 033001 (2011)

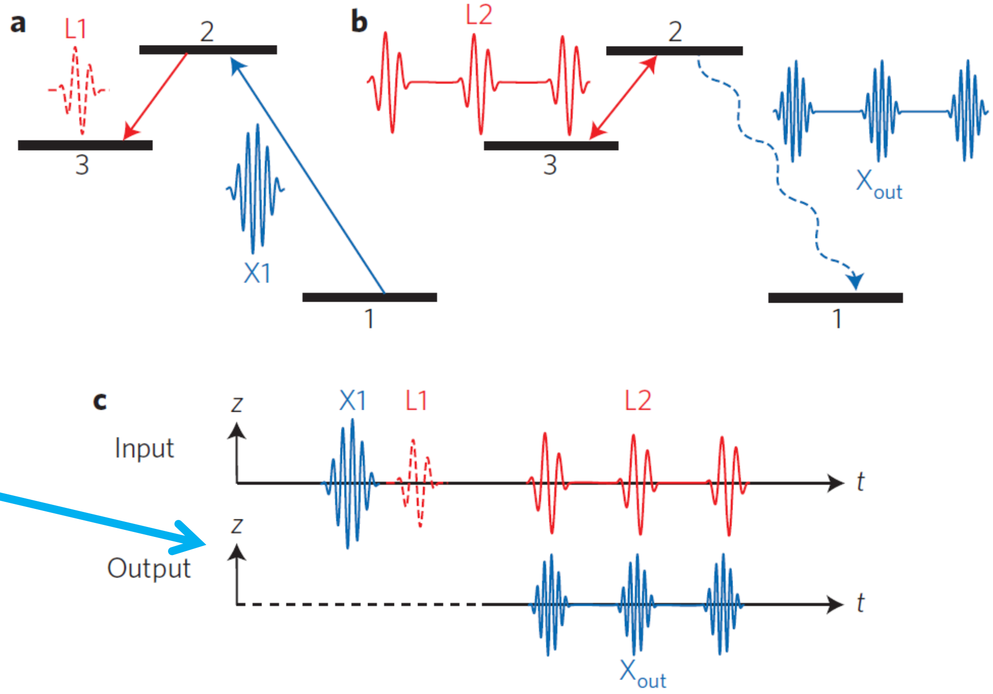
Frequency comb generation

Coherent superpositions of states in hard X-ray driven systems can be modulated by optical or VUV frequency combs for the generation of X-ray frequency combs

a) An ion ensemble is driven by an ultrashort, broadband X-ray pulse (X1) exciting from **1** the fast-decaying level **2**, which an optical pulse (L1) couples to the metastable state **3**. This generates a superposition of **1** and **3**.

b) An optical frequency comb (L2) drives **2**↔**3**. The emitted X-rays (X_{out}) amplify or attenuate X1 as it propagates through the medium, and constitute an X-ray comb.

c) All pulses from a) and b) are polarized and co-propagating.

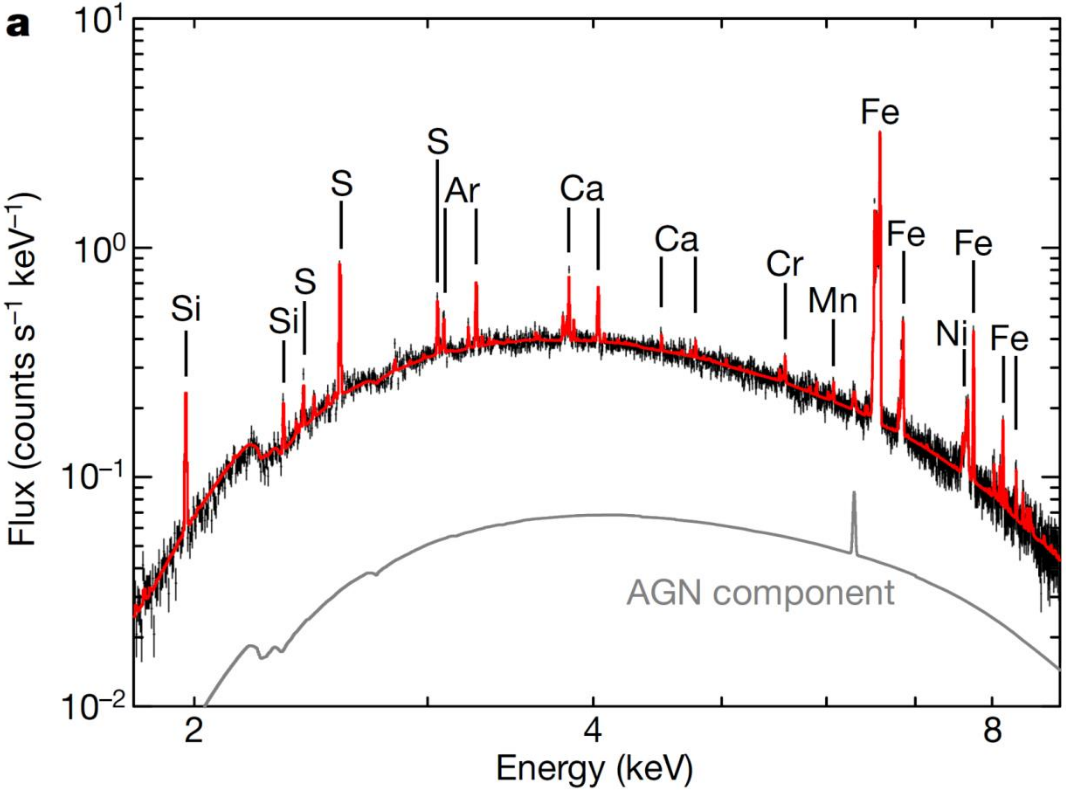


Broadband high-resolution X-ray frequency combs, S. M. Cavaletto et al., Nature Photonics **8**, 520 (2014)

X-ray astrophysics observatories

- Most of the baryonic matter is highly ionized; the strongest X-ray emitters at stellar, galactic, and intergalactic scales are HCI
- The first high-resolution X-ray microcalorimeter mission, *Hitomi*, has shaken many theories in only a few days of test operation before its untimely demise
- Several space missions equipped with microcalorimeters (Athena, XRISM Resolve, Arcus…) will be launched in the next decade for studying the 'violent universe'
- Observational high-resolution X-ray data require laboratory astrophysics for testing atomic structure and dynamics in order to understand astrophysical plasmas

Hitomi SXS spectra of the Perseus cluster of galaxies

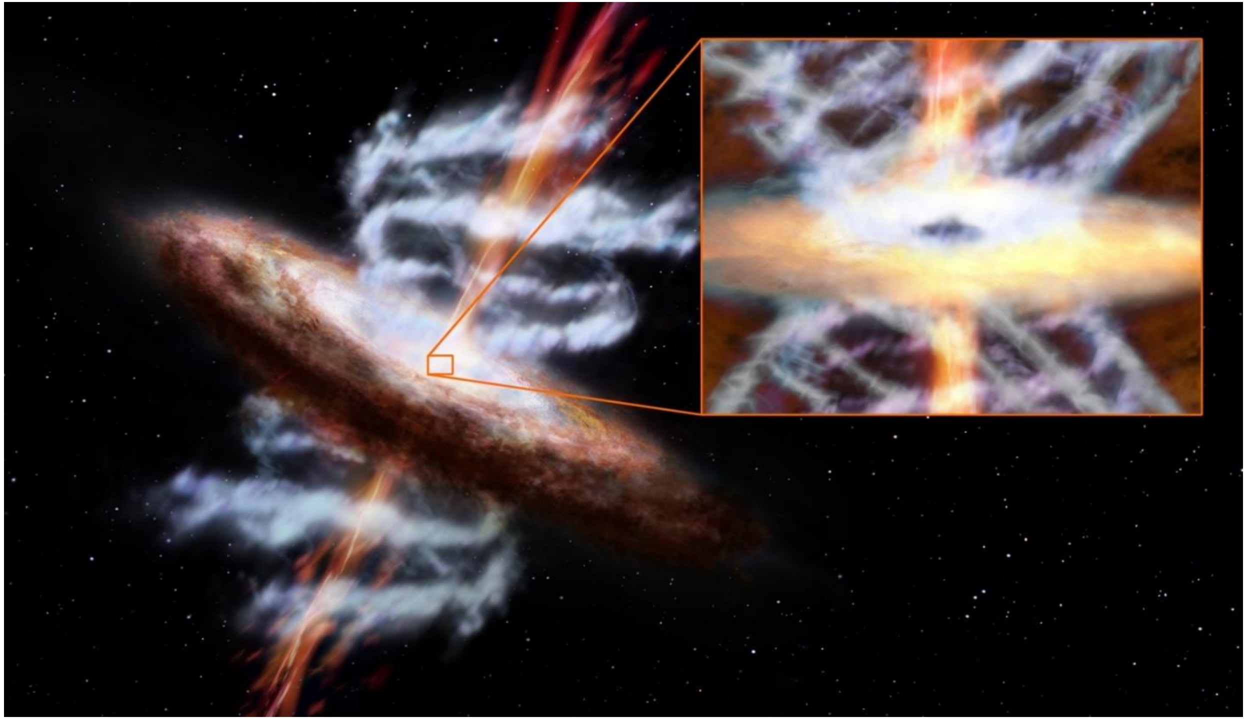


X-ray lines from H-like, He-like and Li-like ions

kTe = 3.97 ± 0.02 keV
Fe/H= 0.63 ± 0.01
(relative to solar abundance)

Solar abundance ratios of the iron-peak elements in the Perseus cluster, Hitomi Collaboration, Nature (2017)

Ultra-fast outflows



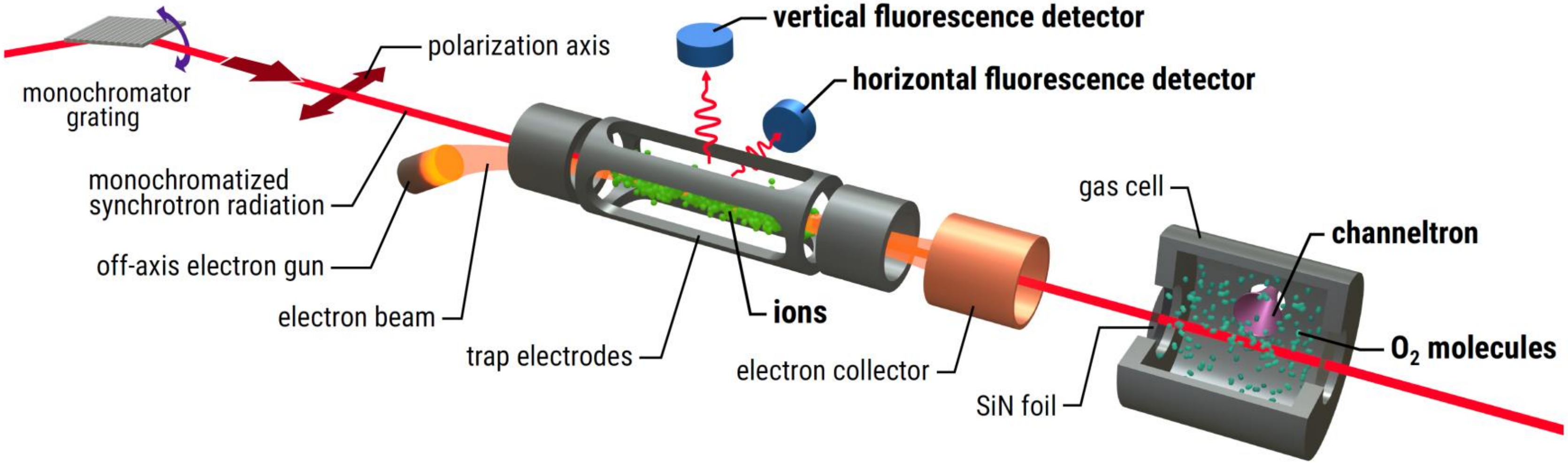
Supermassive black holes produce narrow particle jets (orange) and wider streams of gas (blue-gray) which can regulate both galactic star formation and the growth of the black hole

F. Tombesi et al., ApJ, MNRAS 2010,2011,2012

Photoionized plasmas in astrophysics and HCI traps

- In particular, photoionized plasmas produced by active galactic nuclei (AGN) are very interesting, since they can yield information about the most energetic processes driving galaxy formation
- XFELs are currently the only tools capable of generating photon-dominated plasmas
- Inside a trap (magnetic trapping mode EBIT, Penning or RF traps) the 'educt' HCI can be prepared, and the interaction products can be analyzed in great detail both in terms of structure and dynamics
- Photon-beam ion source (PhoBIS) is an old concept that XFELs could enable

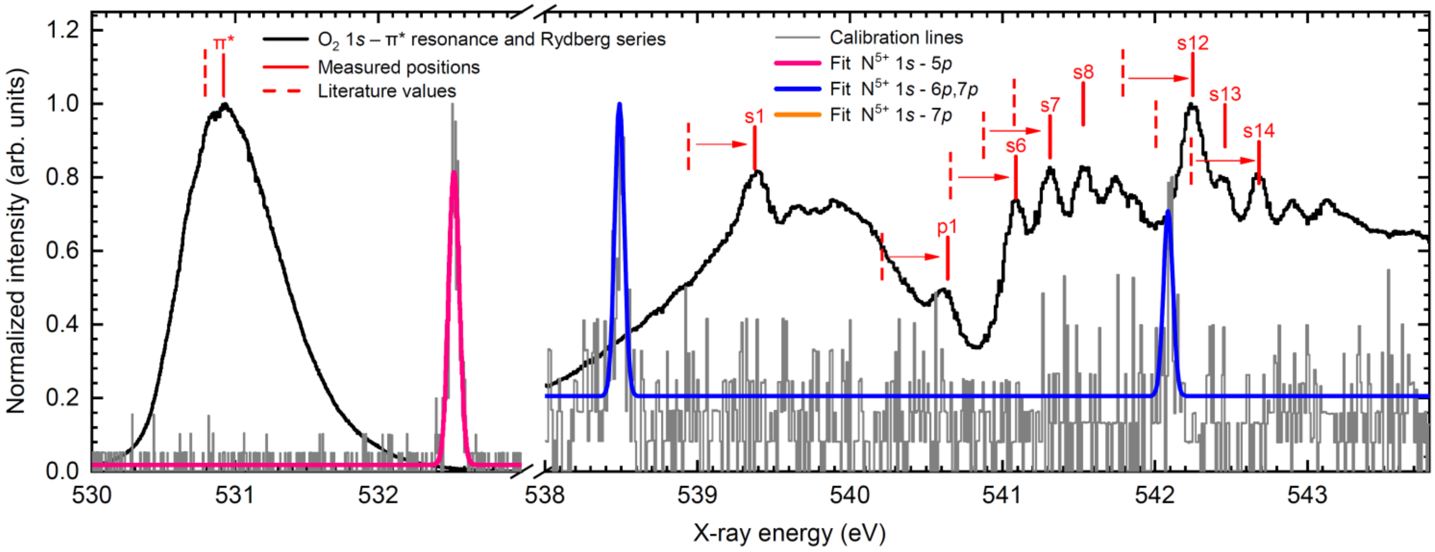
HCI and neutrals: PolarX-EBIT and gas-cell setup



Simultaneous measurements of molecular oxygen photabsorption and X-ray fluorescence of O VII and other HCI

M. Leutenegger et al., JRCLU, PRL 2020

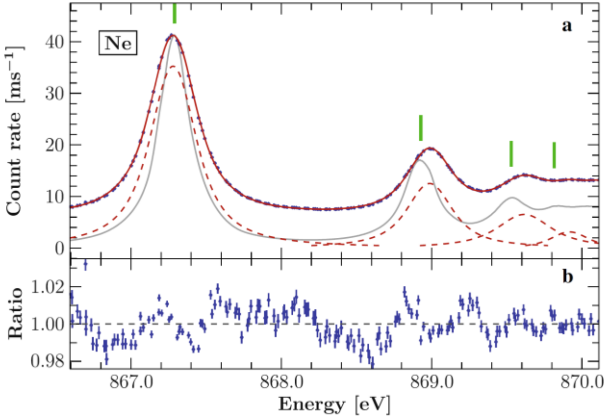
Interstellar oxygen brought to rest

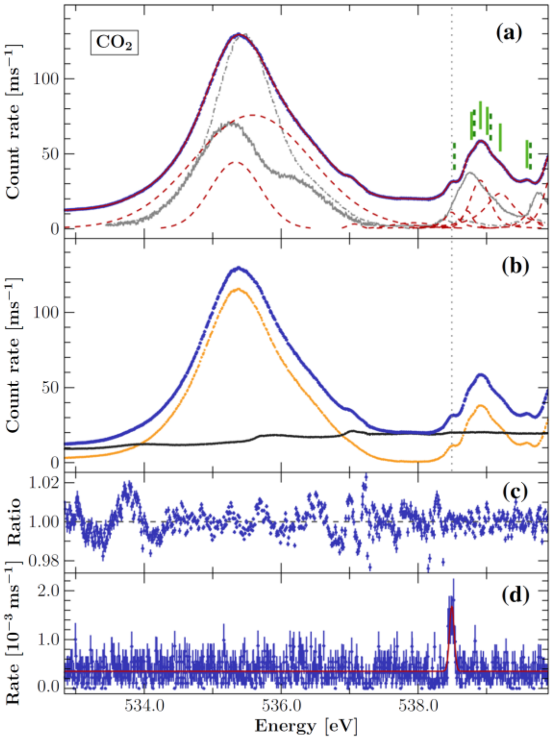


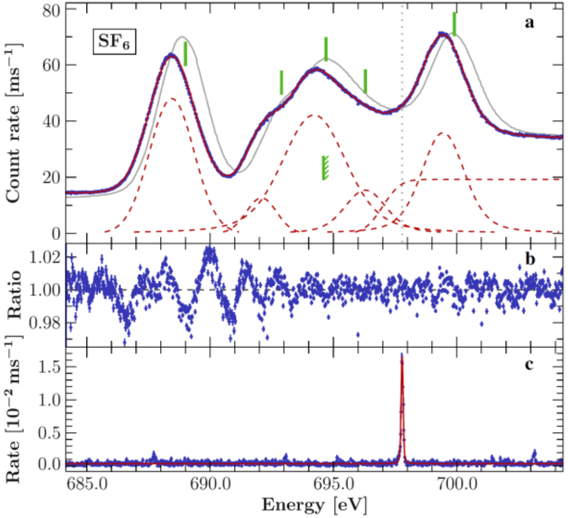
Recalibration of O_2 absorption spectrum by simultaneously measuring Kδ (1s-5p), Kϵ (1s-6p), and Kζ (1s-7p) transitions in He-like N^{5+} as energy references. Positions of spectral features in O_2 from literature (dashed red vertical markers) and our measurements (full red vertical markers) clearly showing an 0.42 eV offset.

M. Leutenegger et al., JRCLU, PRL 2020

Recalibration of calibration standards







- Statistical uncertainty 1–10 meV with HCI calibration
- Systematic ~ 40–100 meV, mainly due to monochromator angular scale stability (solvable!)

- Green vertical bars indicate earlier reported values
- HCI calibration references: panels (d), c

A new benchmark of soft X-ray transition energies of Ne, CO2, and SF6: paving a pathway towards ppm accuracy

J. Stierhof et al., JRCLU, M. A. Leutenegger, Eur. J. Phys. D 76, 38 (2022)

Summary of results

- X-ray energy standards from HCI:
  - $Fe^{15+...17+}$ resonance transitions at ~800 eV
  - Ly-series lines of F^{8+} and O^{7+} at ~800 eV
  - Fe Kα in $Fe^{21+...24+}$ ions excited at 6.7 keV
  - Kr^{34+}, Br^{33+} high-resolution studies up to 14 keV
  - Calibrations with $\Delta E \approx 10$ meV still limited by monochromator reproducibility
- HCI energy standards surpass in reproducibility, stability and calculability the present ones, and serve users of XFEL and synchrotron radiation facilities
- Oscillator strengths, line widths determined
- Photoionization studies from N^{3+} to Fe^{23+}
- Applications to the analysis and diagnostics of astrophysical plasmas
- Fundamental science (QED, BSQED, many-electron-systems) with HCI
- Miniature EBITs perform well at these tasks

Further science possibilities

- Highly polarized ion (beams) by X-ray optical pumping in combination with polarized XFEL photon beams:
  - Studies of parity non-conservation & Lorentz invariance with deeply bound electrons
  - Probing 'long range' (fm to pm) hypothetical Yukawa interactions
  - Providing accurate electronic binding energies for neutrino mass determinations physics
  - Pump-probe (soft and hard) X-ray studies of lifetimes, mixings between different multipole matrix elements in few-electron systems
- Ultra-cold ions in RF traps: Momentum transfer as a tool for atom interferometry with non-negligible relativistic component
- Absolute energy determinations in X-ray in direct comparison with Mössbauer transitions, transfer of frequency stability from Mössbauer to XFELO…
- Combination with VUV frequency combs for X-ray comb modulation

MPIK

S. Bernitt, S. W. Epp, S. Kühn, P. Micke, C. Shah, M. Togawa, K. Fujii, S. Dobrodey, M. Blessenohl, R. Steinbrügge, J. Rudolph, C. Beilmann, M. C. Simon, K. M. Rosner, T. Pfeifer, JRCLU

MPIK Theory Division C. H. Keitel: Z. Harman, C. Lyu

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EuXFEL

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S. M. Cavaletto *et al.*, Nature Photonics **8**, 520 (2014)

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