Relativistic and resonant effects on x-ray multiphoton multiple ionization of heavy atoms

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HELMHOLTZ
RESEARCH FOR GRAND CHALLENGES

CFEL SCIENCE

Center for Free-Electron Laser Science
CFEL is a scientific cooperation of the three organizations:
DESY – Max Planck Society – University of Hamburg

DESY.

Collaboration

Theory

Koudai Toyota
at CFEL, DESY

Robin Santra
at CFEL, DESY

Experiment

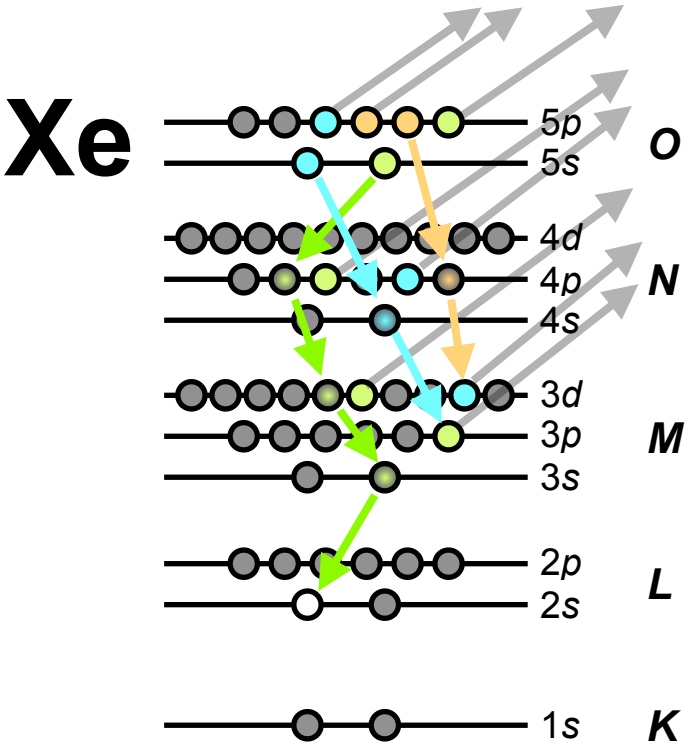
Benedikt Rudek
at PTB

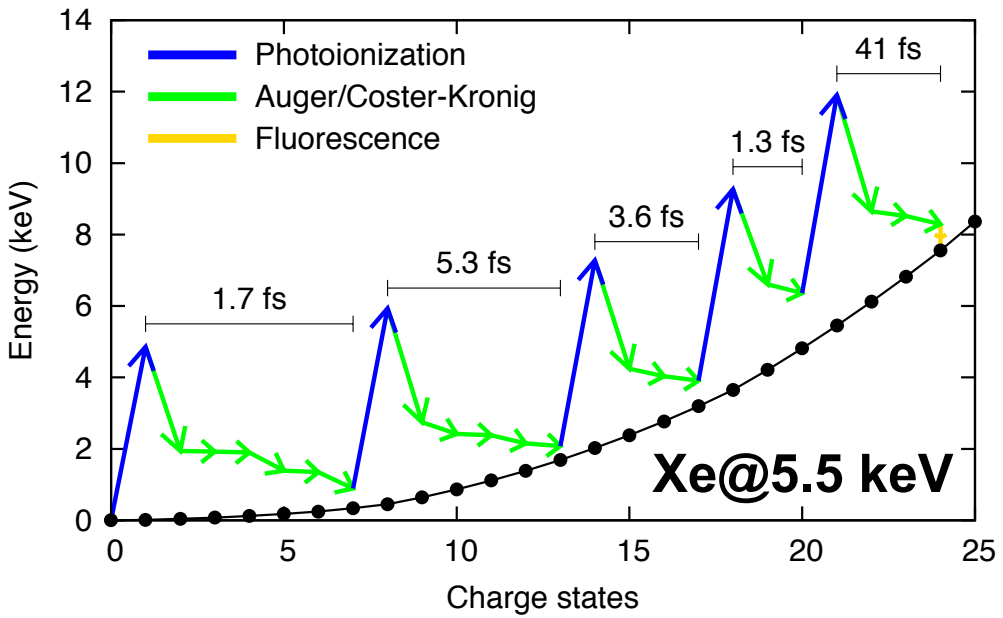
Artem Rudenko
at KSU

Daniel Rolles
at KSU

L. Foucar (MPI-MF), B. Erk, C. Bomme, J. Correa (DESY), R. Boll (EuXFEL), S. Carron, S. Boutet, G. J. Williams, K. R. Ferguson, R. Alonso-Mori, J. E. Koglin, T. Gorkhover, M. Bucher (LCLS), C. S. Lehmann, B. Krässig, S. Southworth, L. Young, Ch. Bostedt (ANL), K. Ueda (Tohoku), T. Marchenko, M. Simon (UPMC), Z. Jurek (CFEL)

X-ray multiphoton multiple ionization





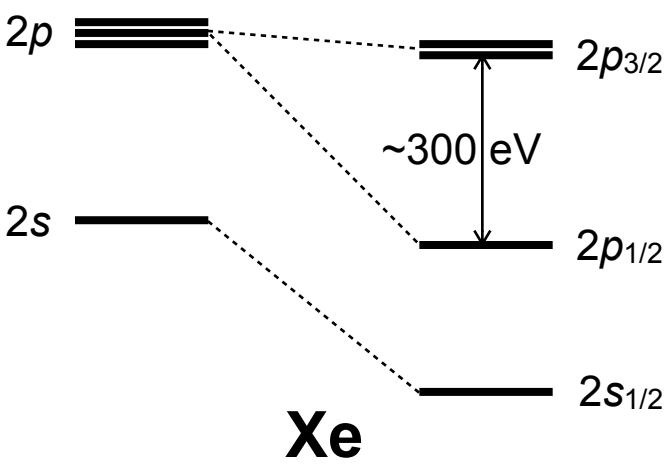
Fukuzawa *et al.*, *Phys. Rev. Lett.* **110**, 173005 (2013).

- Extremely complicated multiphoton multiple ionization dynamics
- No standard quantum chemistry code available

XATOM: computer program suite to describe dynamical behavior of atoms interacting with XFEL pulses

Jurek, Son, Ziaja & Santra, *J. Appl. Cryst.* **49**, 1048 (2016).
Download executables: http://www.desy.de/~xraypac

Relativistic effects in heavy atoms

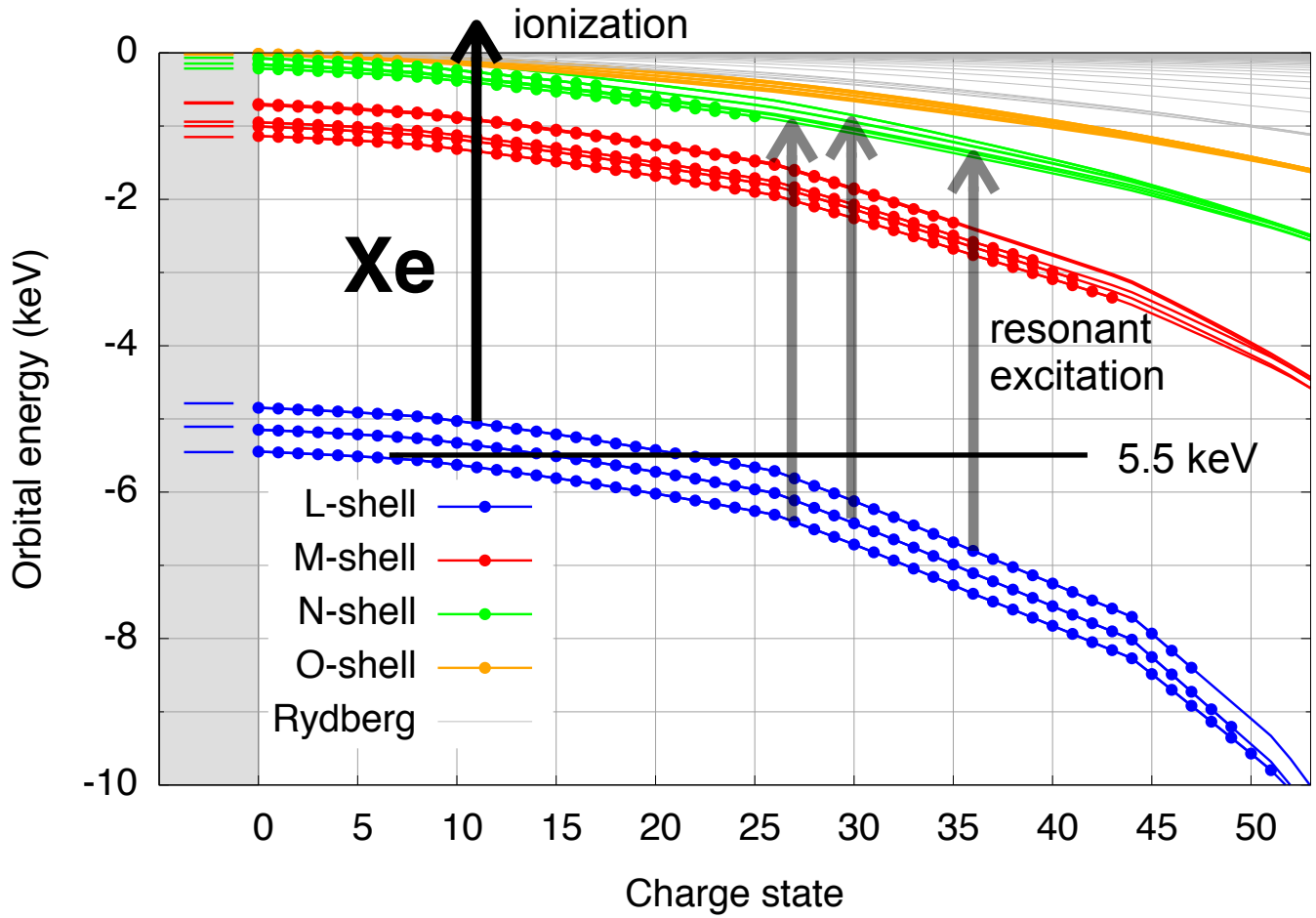


Group	Nonrel	Rel
$L_1 - X$	6.33×10^{-3}	8.03×10^{-3}
$L_1 - XY$	6.07×10^{-2}	5.63×10^{-2}
$L_1 - L_{23}X$	8.19×10^{-2}	6.76×10^{-2}
$L_2 - X$	1.04×10^{-2}	1.32×10^{-2}
$L_2 - XY$	9.38×10^{-2}	8.70×10^{-2}
$L_2 - L_3X$	Forbidden	2.01×10^{-2}
$L_3 - X$	$(=L_2 - X)$	1.08×10^{-2}
$L_3 - XY$	$(=L_2 - XY)$	9.28×10^{-2}

- Open new Coster-Kronig decay channels due to spin-orbit splitting
- Close photoionization earlier due to relativistic energy corrections
- XATOM: relativistic energy correction within first-order perturbation theory

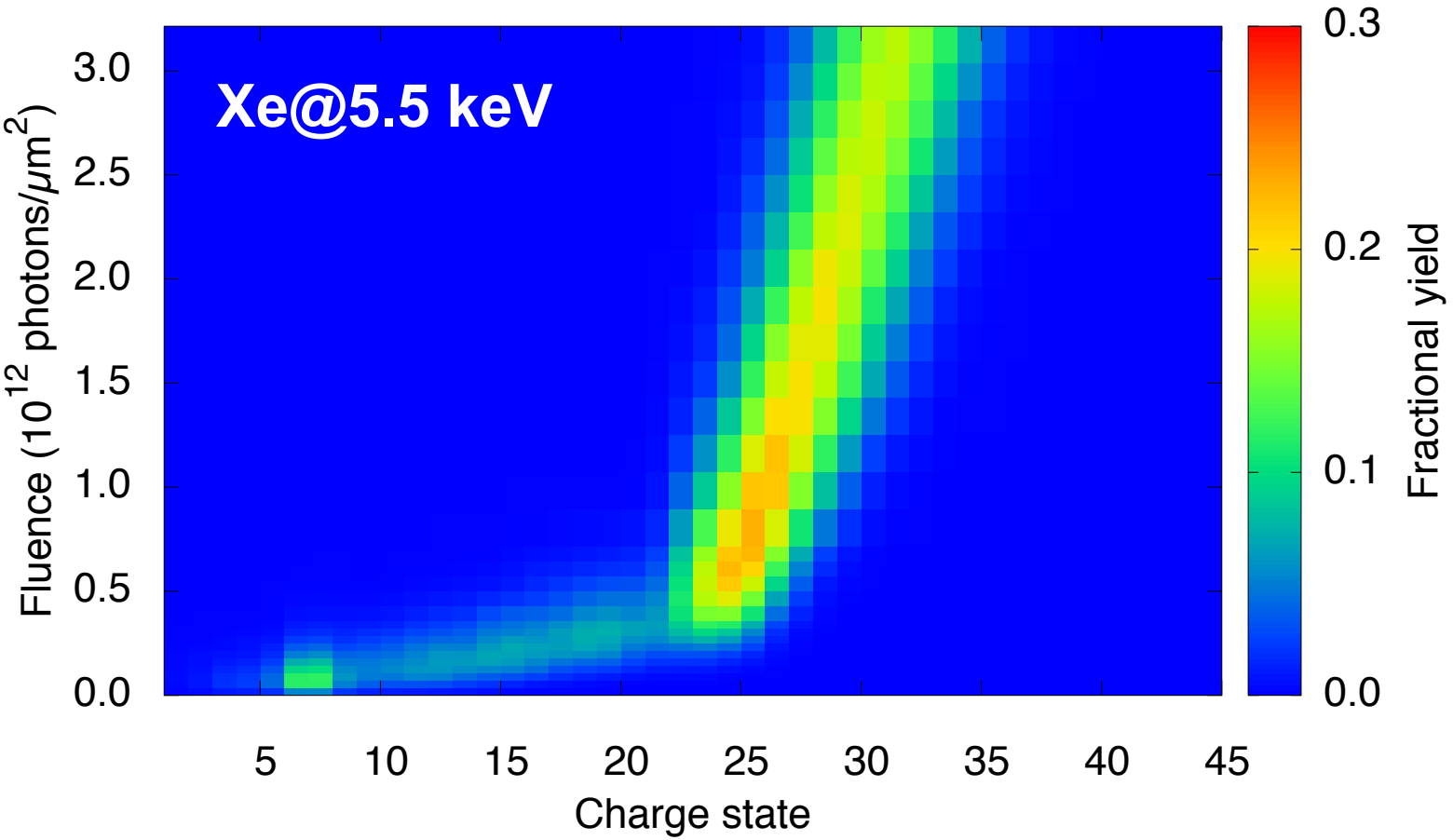
  Toyota, Son & Santra, *Phys. Rev. A* **95**, 043412 (2017).
- *N* of coupled rate eqs: ~20 million (non-rel: *n*,*l*) ➔ ~5 billion (rel: *n*,*l*,*j*)

Resonances in x-ray ionization dynamics



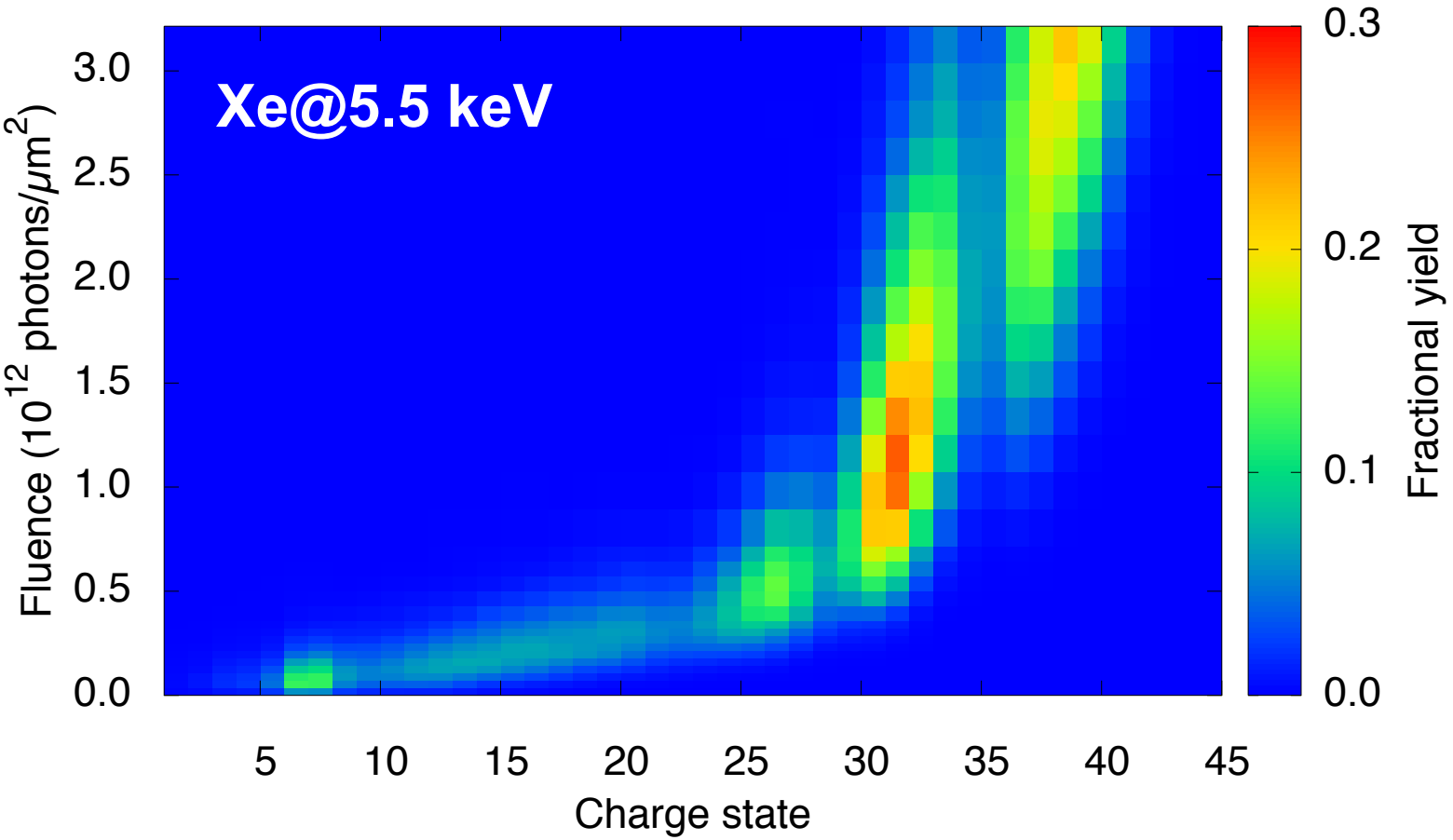
- REXMI: resonance-enhanced x-ray multiple ionization
- *N* of coupled rate eqs. ~2.6×10^{68} ➔ solved via Monte Carlo on-the-fly

Xe CSD without resonance & relativity



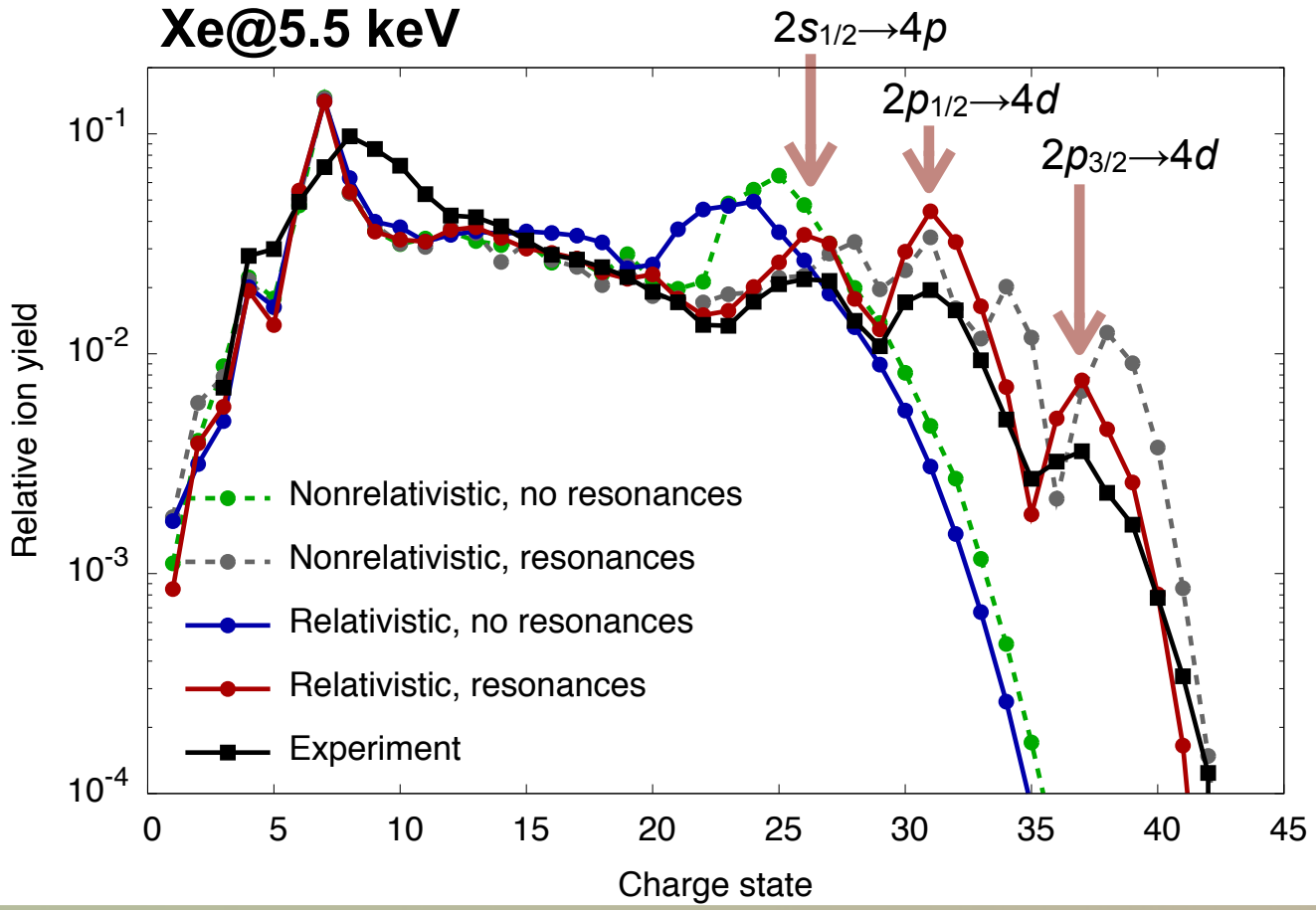
Rudek, Toyota, *et al.*, *Nature Commun.* **9**, 4200 (2018).

Xe CSD with resonance & relativity



Rudek, Toyota, *et al.*, *Nature Commun.* **9**, 4200 (2018).

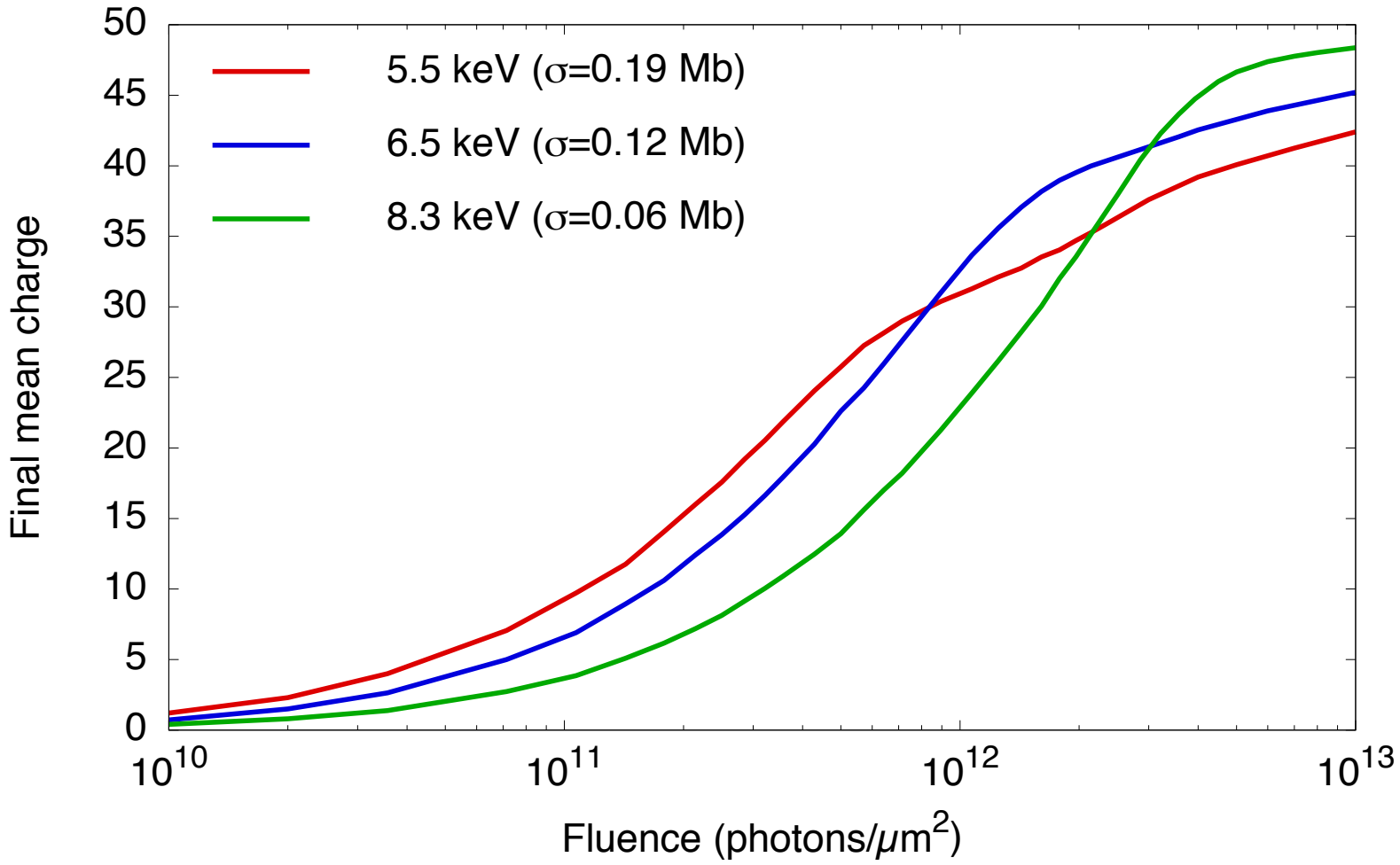
Comparison between theory & experiment



First quantitative comparison for resonance-enhanced ionization with relativity

Rudek, Toyota, *et al.*, *Nature Commun.* **9**, 4200 (2018).

Benchmark of atomic x-ray ionization



Rudek, Toyota, *et al.*, *Nature Commun.* **9**, 4200 (2018).

Conclusion

- XATOM: enabling tool for investigating x-ray multiphoton physics of atoms exposed to XFEL pulses
- X-ray multiphoton inner-shell ionization of Xe: experiment and theory
- Interplay between resonance and relativistic effects
- Benchmark of atomic x-ray ionization
  - molecular x-ray ionization
  - warm-dense-matter formation
  - electronic radiation damage for molecular imaging

MO20.7: Ludger Inhester's talk (now)
SYXR1.4: Daniel Rolles's talk
U Audimax at 14:00–16:00

CFEL-DESY
Theory Division

https://desy-theory.cfel.de