

# Inner-shell multiphoton multiple ionization dynamics of Xe atoms by x-ray free-electron laser pulses

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**Center for Free-Electron Laser Science**

CFEL is a scientific cooperation of the three organizations:  
DESY – Max Planck Society – University of Hamburg



# Collaboration

**LCLS experiment**

**SACLA experiment**

## Max-Planck ASG at CFEL



Daniel Rolles



Artem Rudenko



Benedikt Rudek

## Tohoku Univ.



Kiyoshi Ueda

- Hironobu Fukuzawa
- Koji Motomura

# Introduction

## > Why heavy atoms?

- multiphoton multiple ionization dynamics characterized by a sequence of one-photon ionization and relaxations
- heavy atom: 

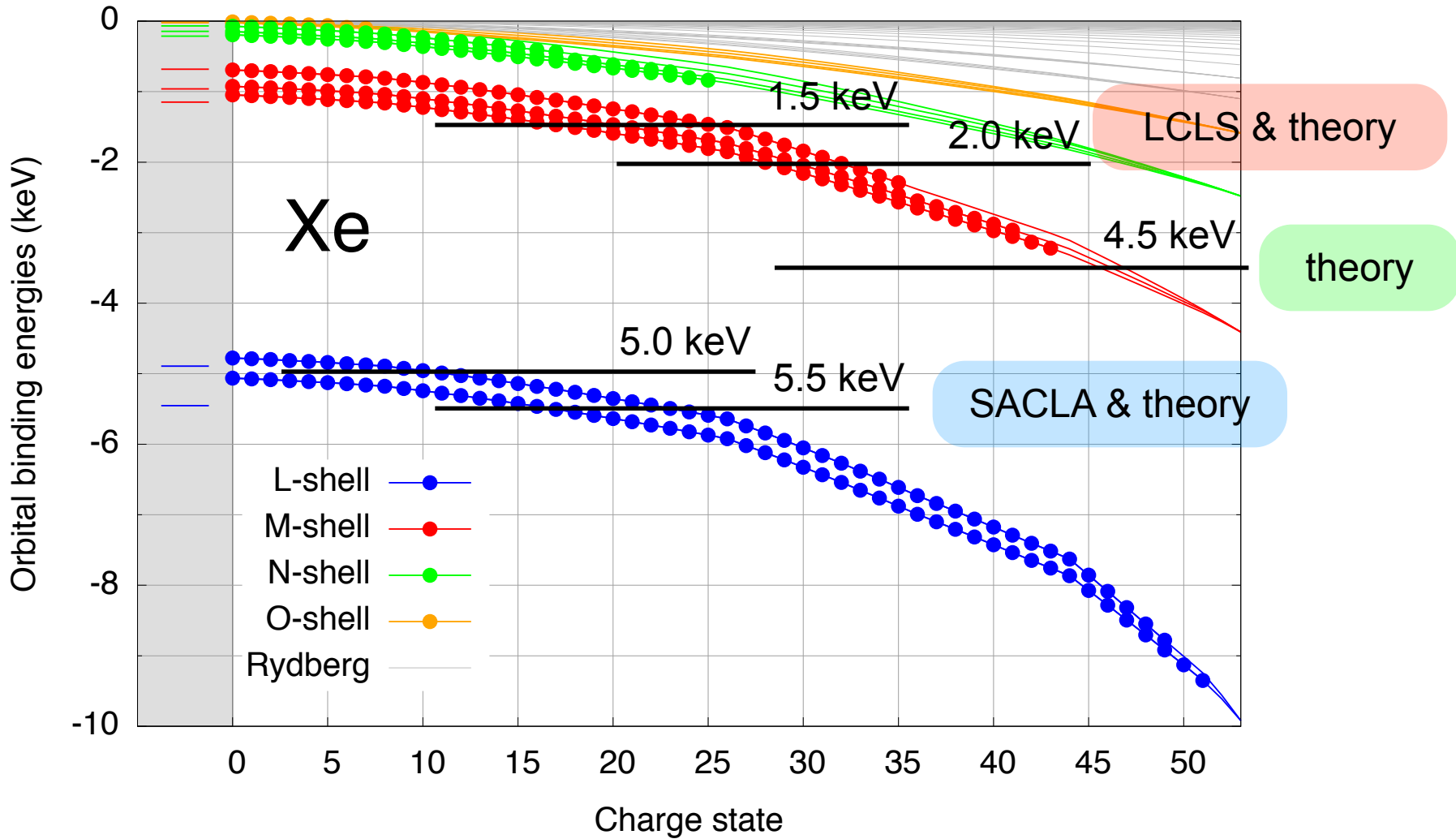
[	many electrons	]	newly unveiled physics
	many processes		
	many ionization pathways		
- electronic damage dynamics of heavy atoms: direct relevance for high-resolution x-ray imaging

## > Why theory needed?

- to reveal the ionization mechanism
- to guide future experiments, ex) MAD at high x-ray intensity

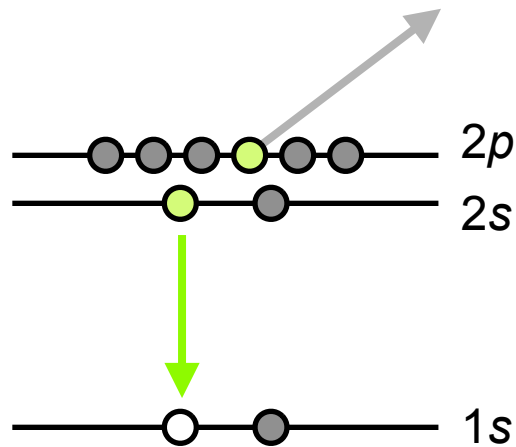
Son, Chapman & Santra,  
*Phys. Rev. Lett.* **107**, 218102 (2011).

# Ionization thresholds of Xe ions

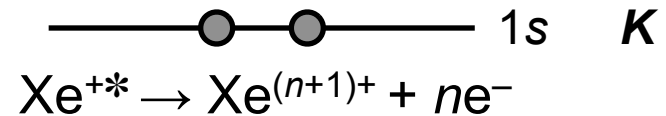
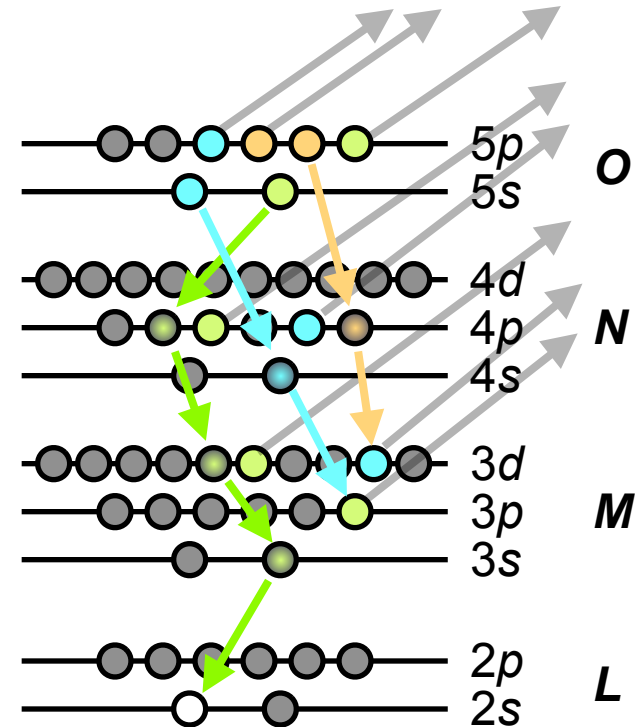


# Complex inner-shell decay cascade

## Ne



## Xe

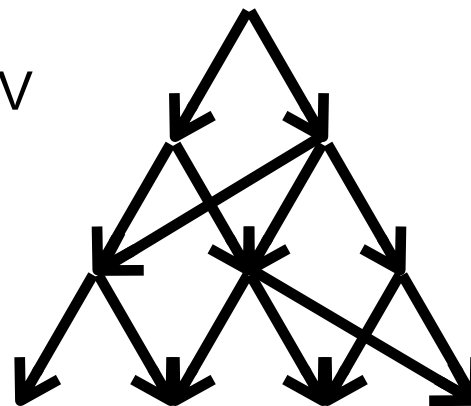


Auger (Coster-Kronig) decay cascade

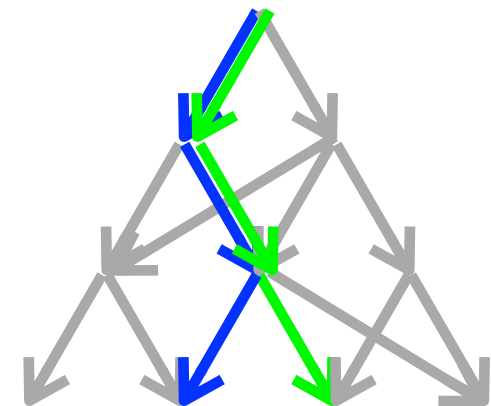
# Ionization dynamics: Monte Carlo method

- > How many coupled rate equations needed?
  - **Ne:** 63
  - **Xe:** 1 million for *M*-shell ionization  
>20 millions for *L*-shell ionization
- > How many physical processes to be considered?
  - **Ne:** 815 at 2 keV
  - **Xe:** 42 millions at 2 keV  
>2 billions at 5.5 keV
- > **XATOM** toolkit extended by the Monte Carlo method

Son & Santra, *Phys. Rev. A*  
**85**, 063415 (2012).



direct solution

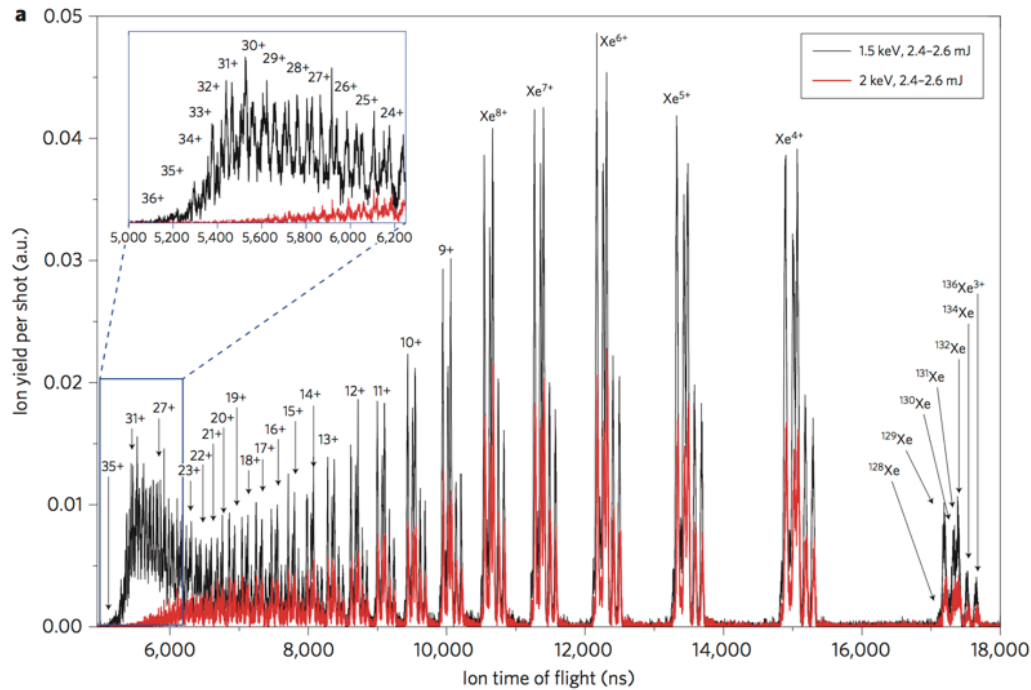


Monte Carlo approach

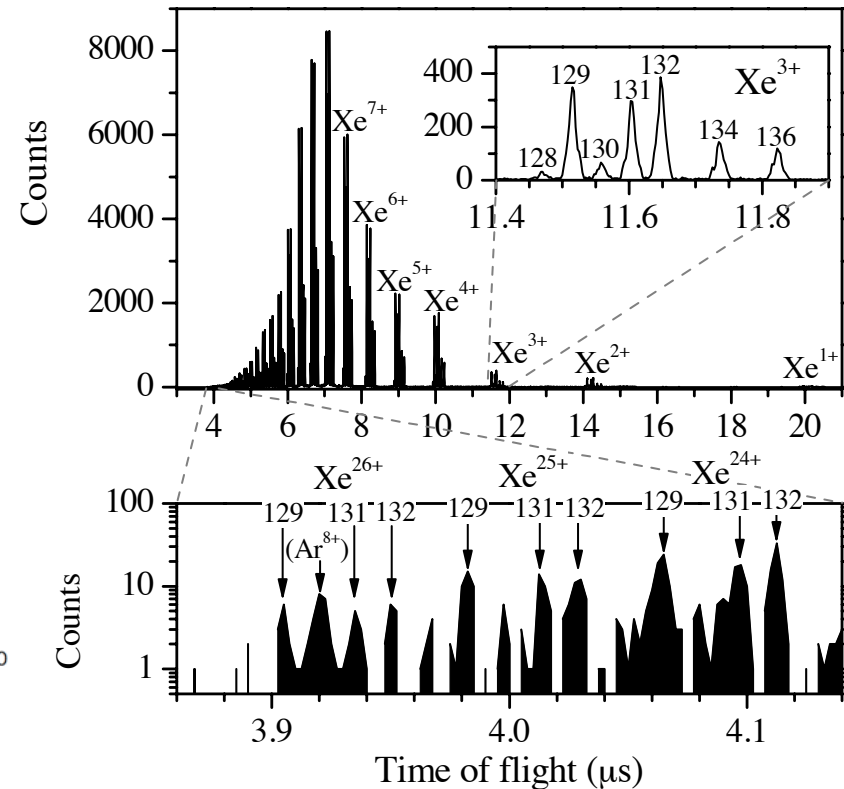
# Experiment: ion time-of-flight spectra

LCLS at  
1.5 keV & 2 keV

SACLA at  
5.5 keV

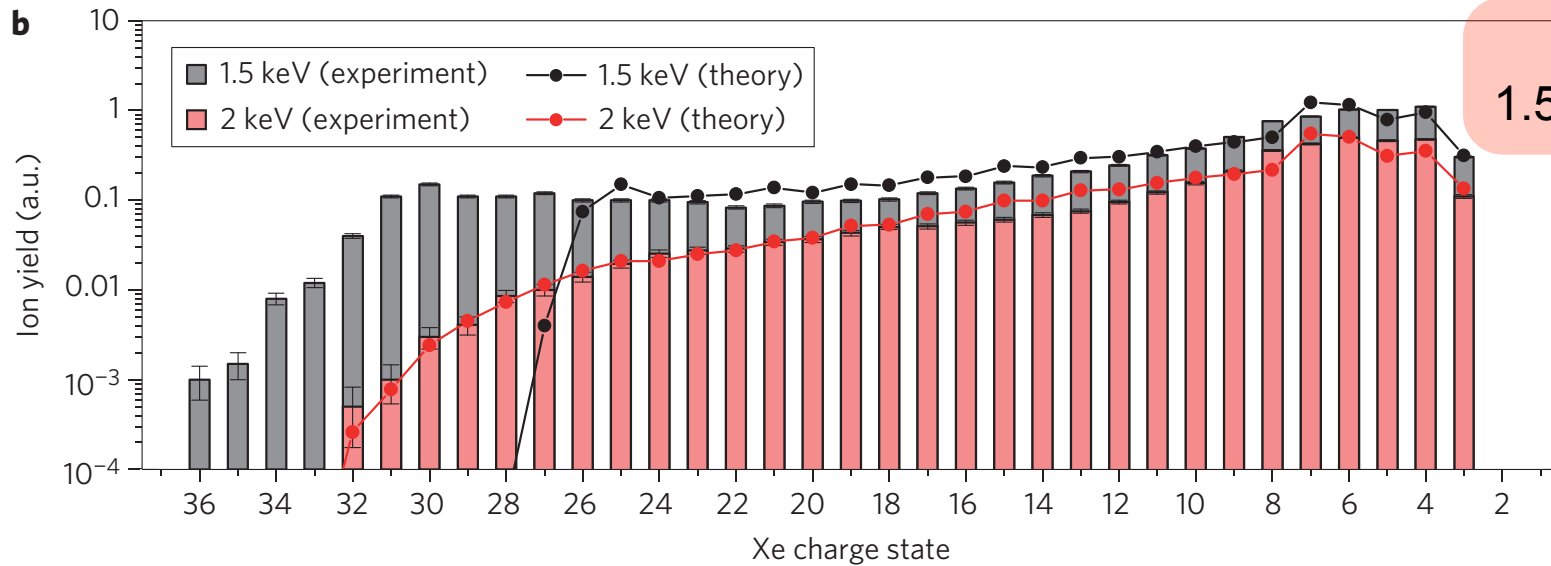


Rudek *et al.*, *Nature Photon.* **6**, 858 (2012).



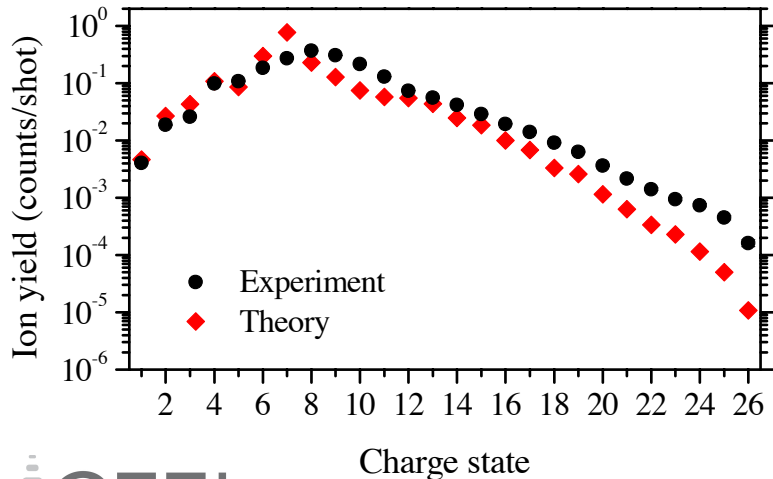
Fukuzawa *et al.*, (submitted),  
arXiv:1210.0673.

# Comparison b/w experiment and theory



LCLS at  
1.5 keV & 2 keV

Rudek *et al.*,  
*Nature Photon.*  
6, 858 (2012).

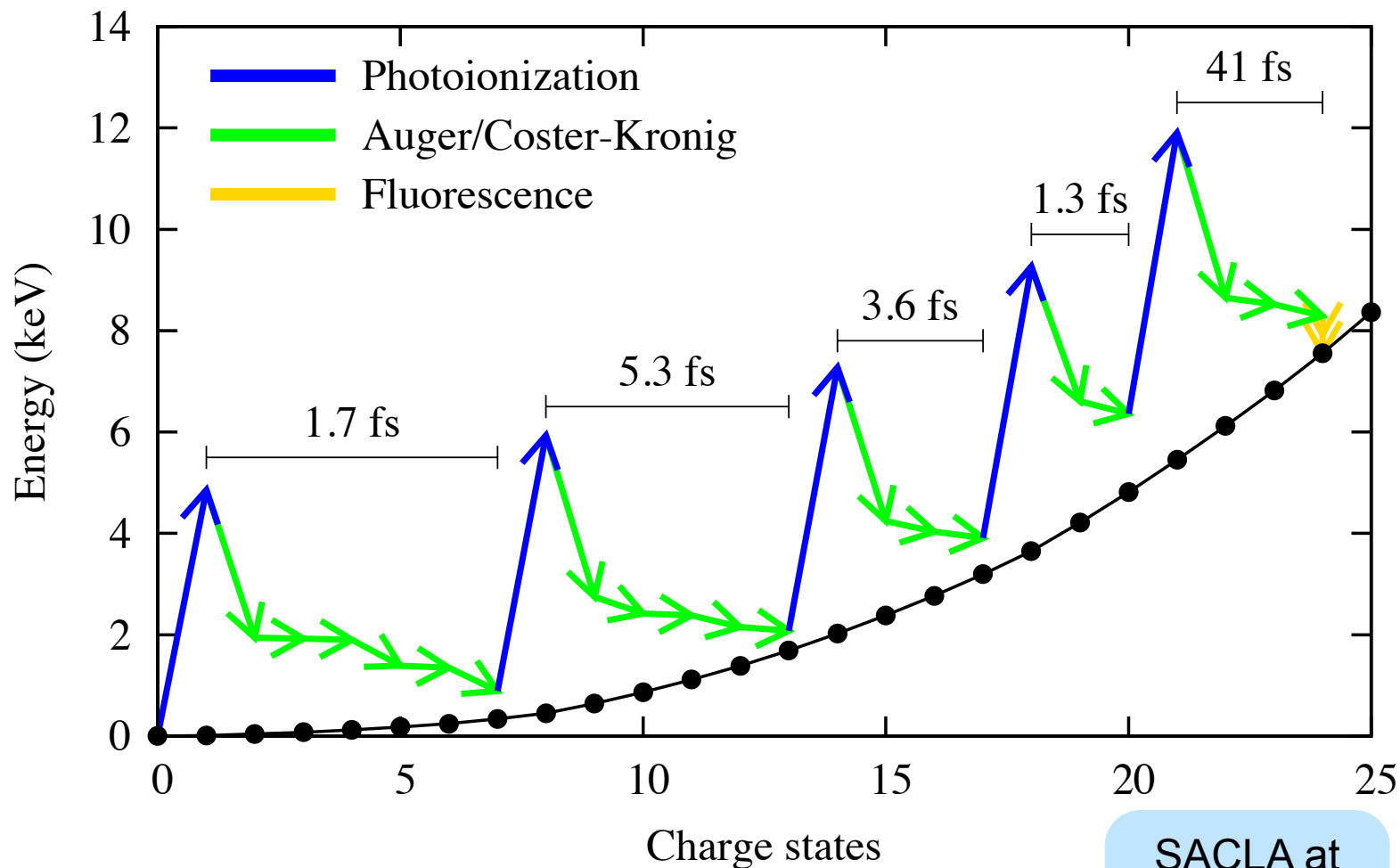


SACLA at  
5.5 keV

Fukuzawa *et al.*, (submitted),  
arXiv:1210.0673.



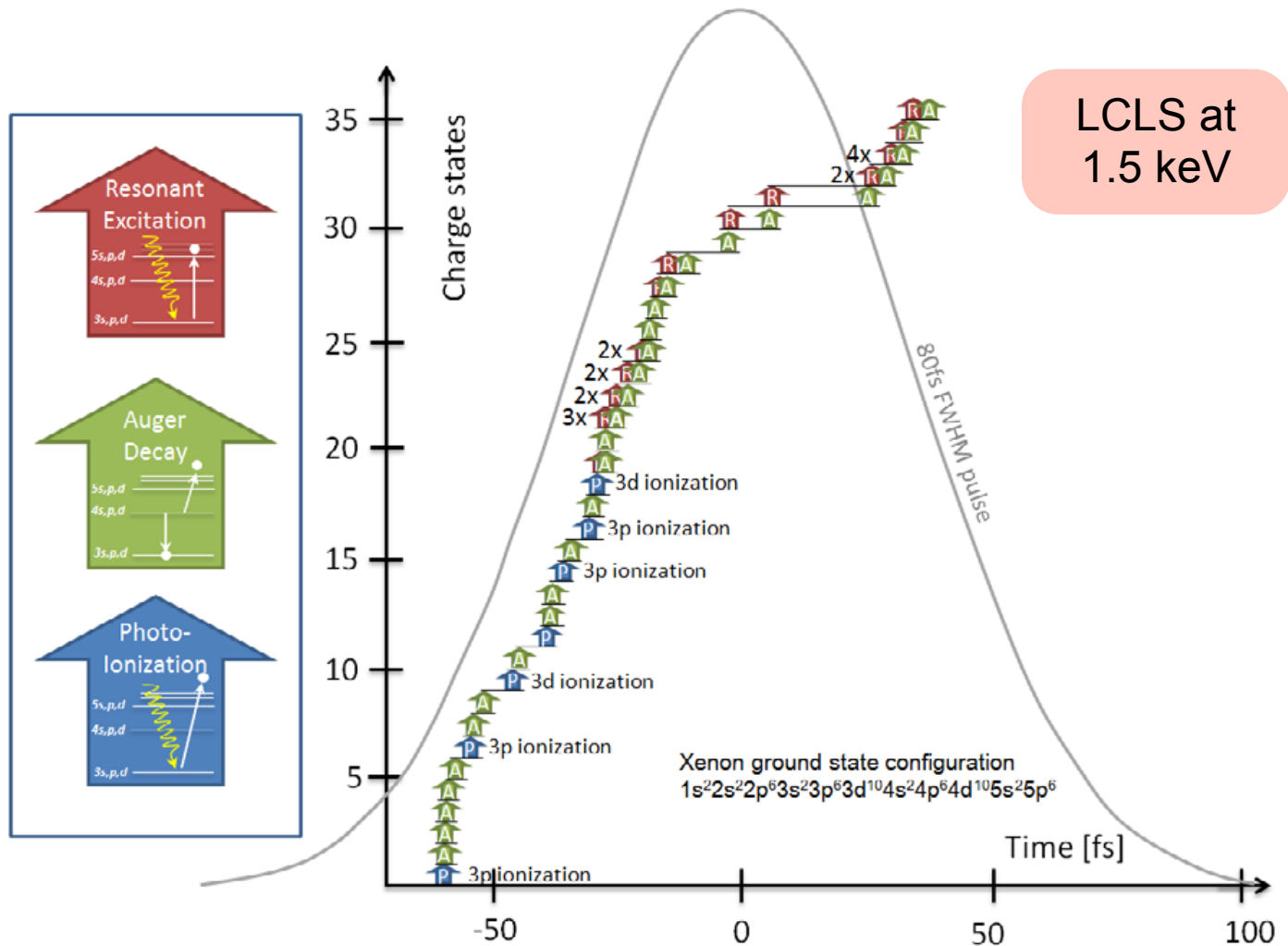
# Ionization energetics



Fukuzawa *et al.*, (submitted), arXiv:1210.0673.

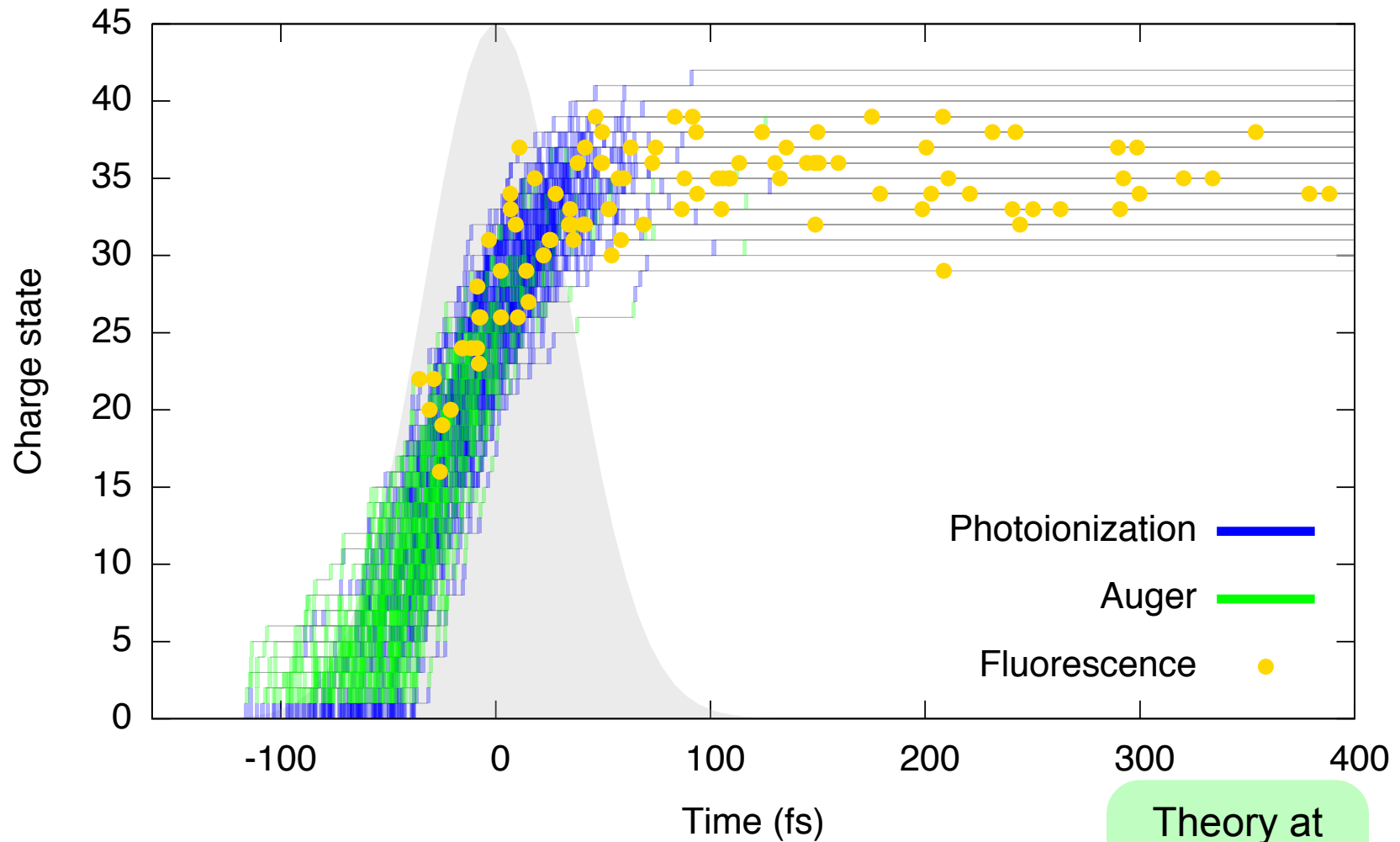
SACLA at  
5.5 keV

# Ionization pathway: one trajectory



Rudek et al., *Nature Photon.* **6**, 858 (2012).

# Ionization pathway: many trajectories



Son & Santra, *Phys. Rev. A* **85**, 063415 (2012).

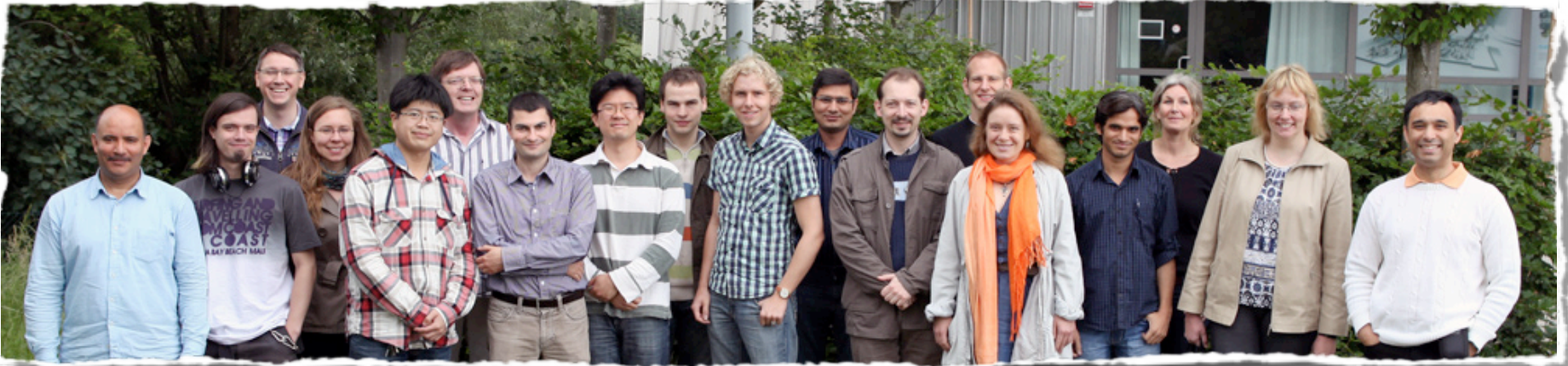
Theory at  
4.5 keV

# Conclusion

- > Atoms and molecules are highly ionized when exposed to XFEL pulses.
- > XFEL experiments of heavy atoms:
  - *M*-shell ionization of Xe at LCLS (1.5 keV and 2 keV)
  - *L*-shell ionization of Xe at SACLA (5 keV and 5.5 keV)
- > Heavy atoms have a rich manifold of ionization channels involving complex inner-shell decay cascade.
- > **XATOM** toolkit has been extended to treat multiphoton multiple ionization dynamics of heavy atoms by the Monte Carlo method.
- > The ionization mechanism of heavy atoms is visualized with ionization energetics and ionization dynamics.

# Acknowledgment

## CFEL Theory Division



*Thank you for your attention!*