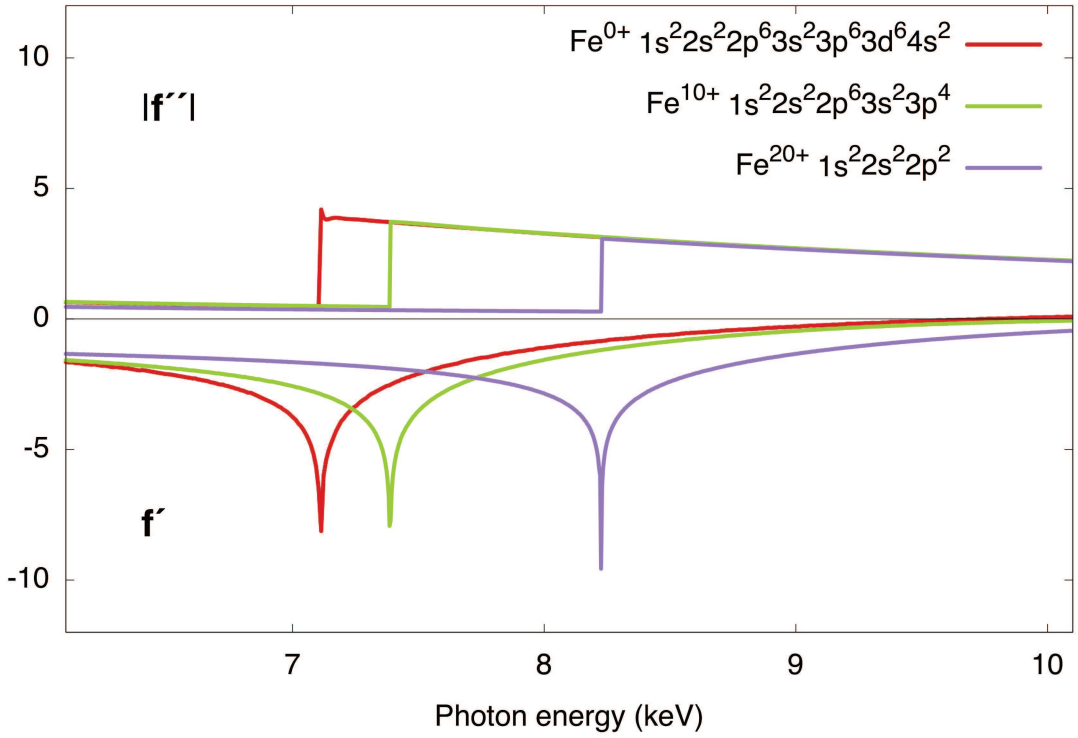
Dispersion corrections to atomic form factors

$$f(\mathbf{Q},\omega) = f^0(\mathbf{Q}) + f'(\omega) + if''(\omega)$$



Calculation using XATOM

S.-K. Son, H. N. Chapman, and R. Santra, Phys. Rev. Lett. **107**, 218102 (2011).

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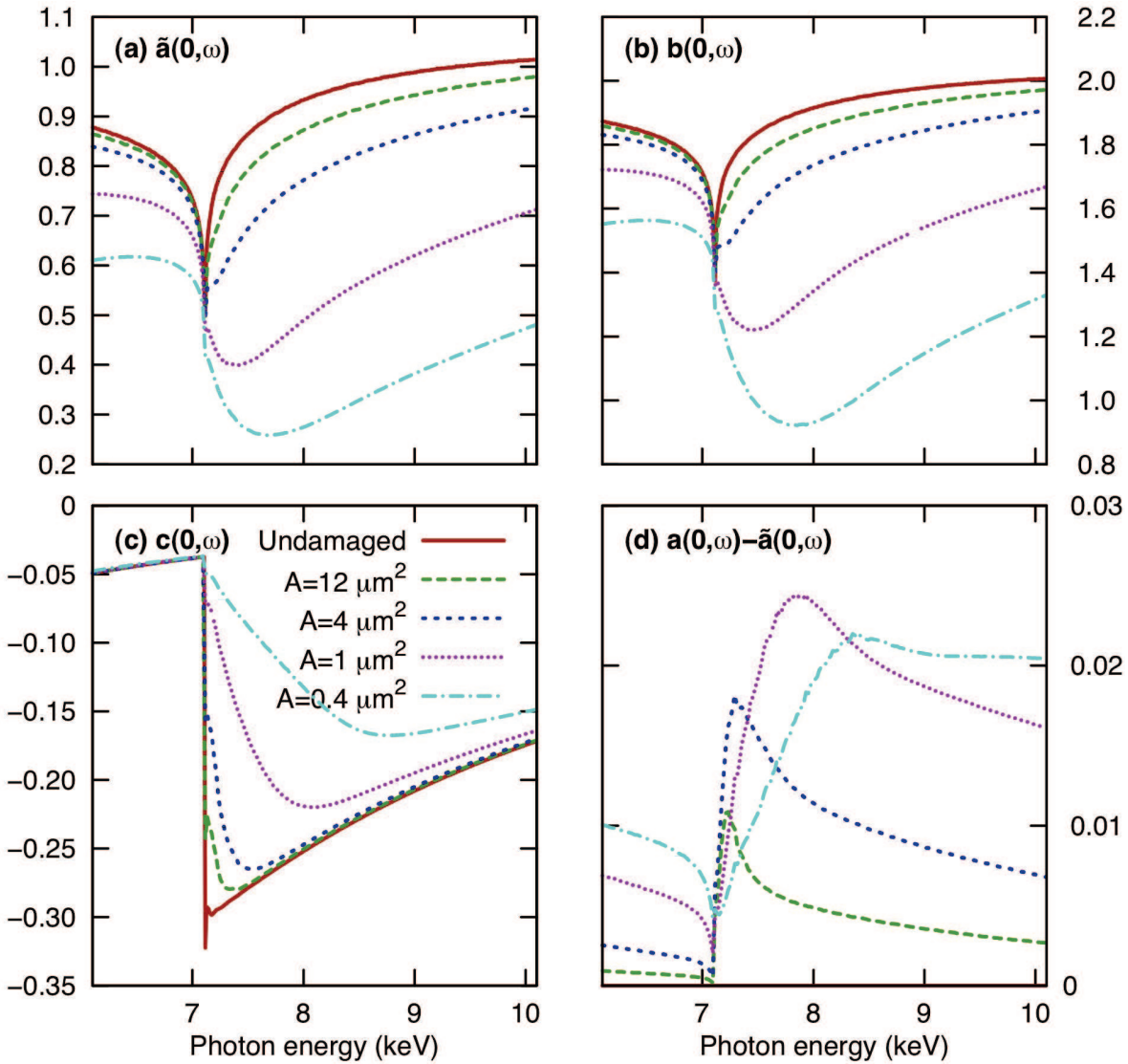
MAD coefficients calculated using XATOM



Fe in an x-ray pulse with 2×10^{12} photons and 10 fs FWHM

S.-K. Son, H. N. Chapman, and R. Santra, Phys. Rev. Lett. **107**, 218102 (2011).

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Experimental tests of XATOM

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X-ray multiphoton ionization of xenon at photon energies of 1.5 keV and 2 keV

Experiment carried out at the
Linac Coherent Light Source (LCLS) at SLAC

Xe: $[1s^2\ 2s^2\ 2p^6]\ 3s^2\ 3p^6\ 3d^{10}\ 4s^2\ 4p^6\ 4d^{10}\ 5s^2\ 5p^6$

→ ***1,120,581*** coupled rate equations
(excluding ionization from the K and L shells)

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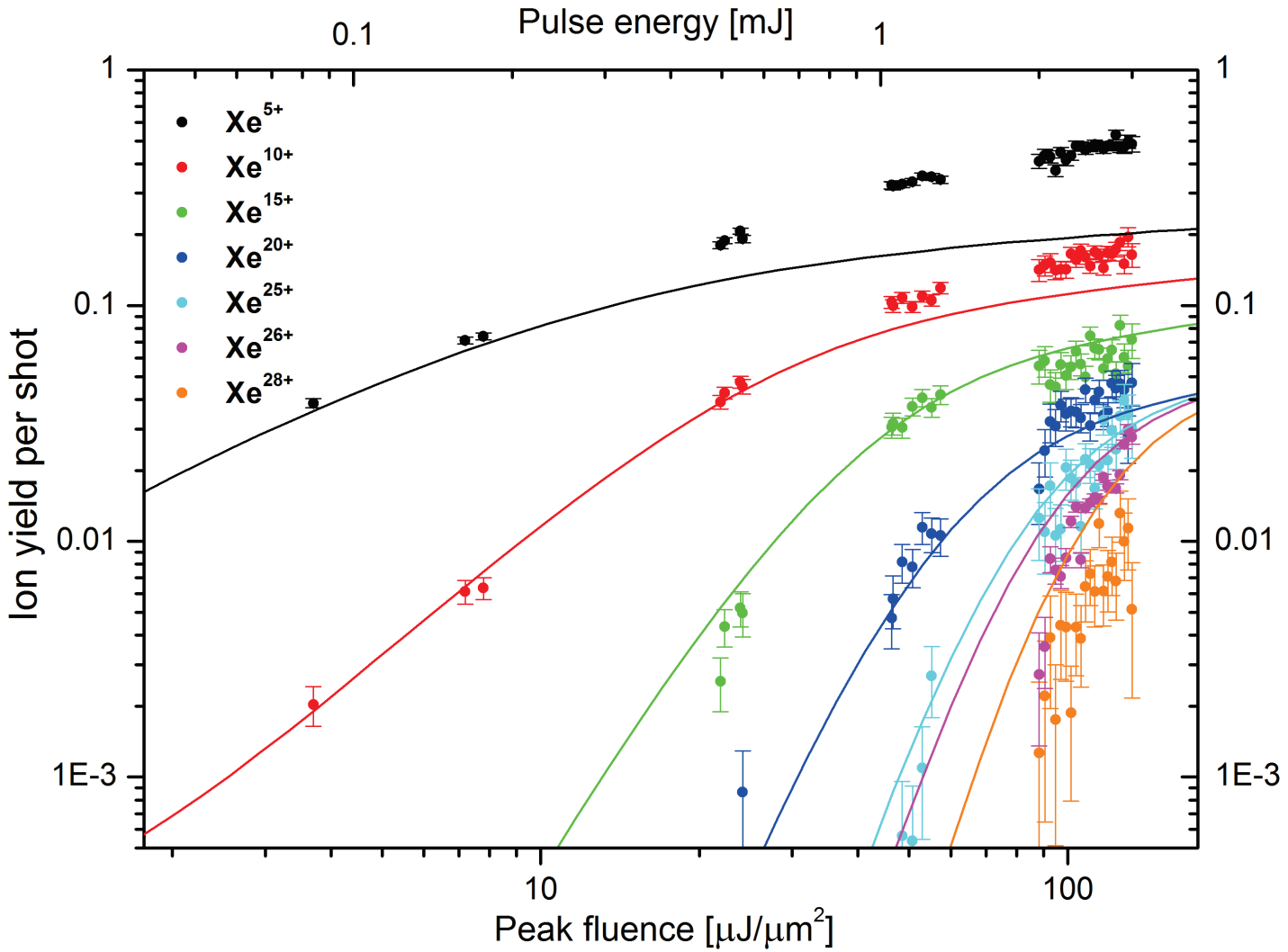
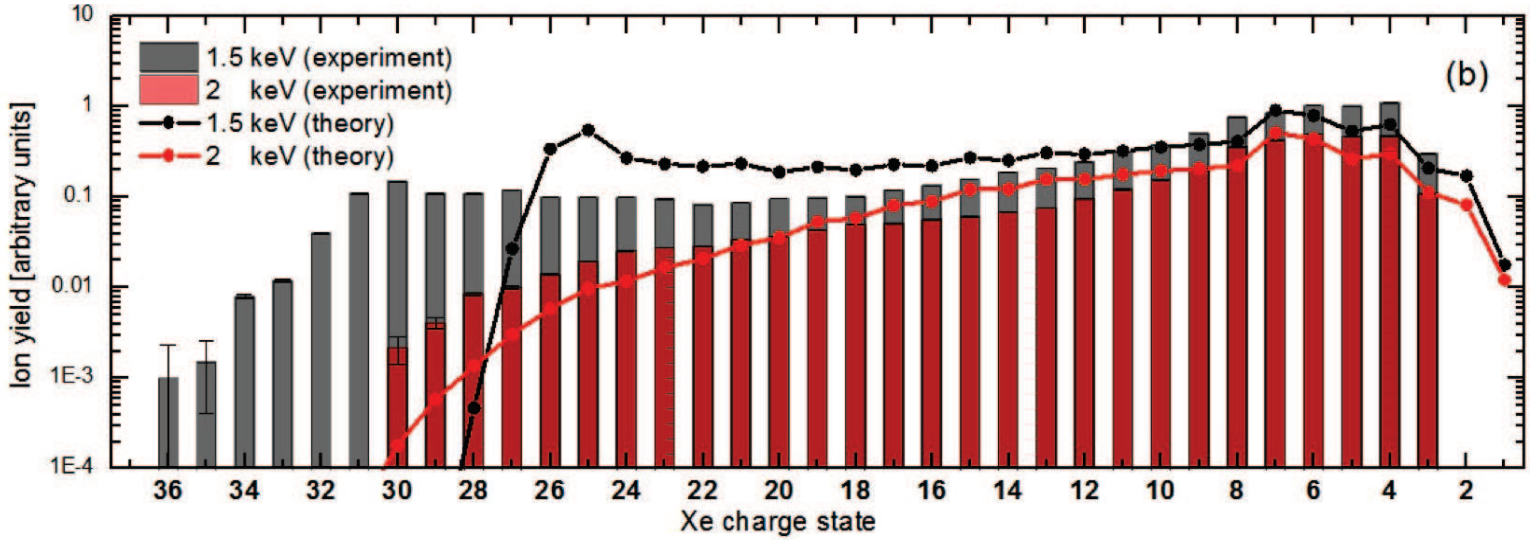
Comparison between experiment and theory at 2 keV



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

Enhancement of ionization via resonances



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

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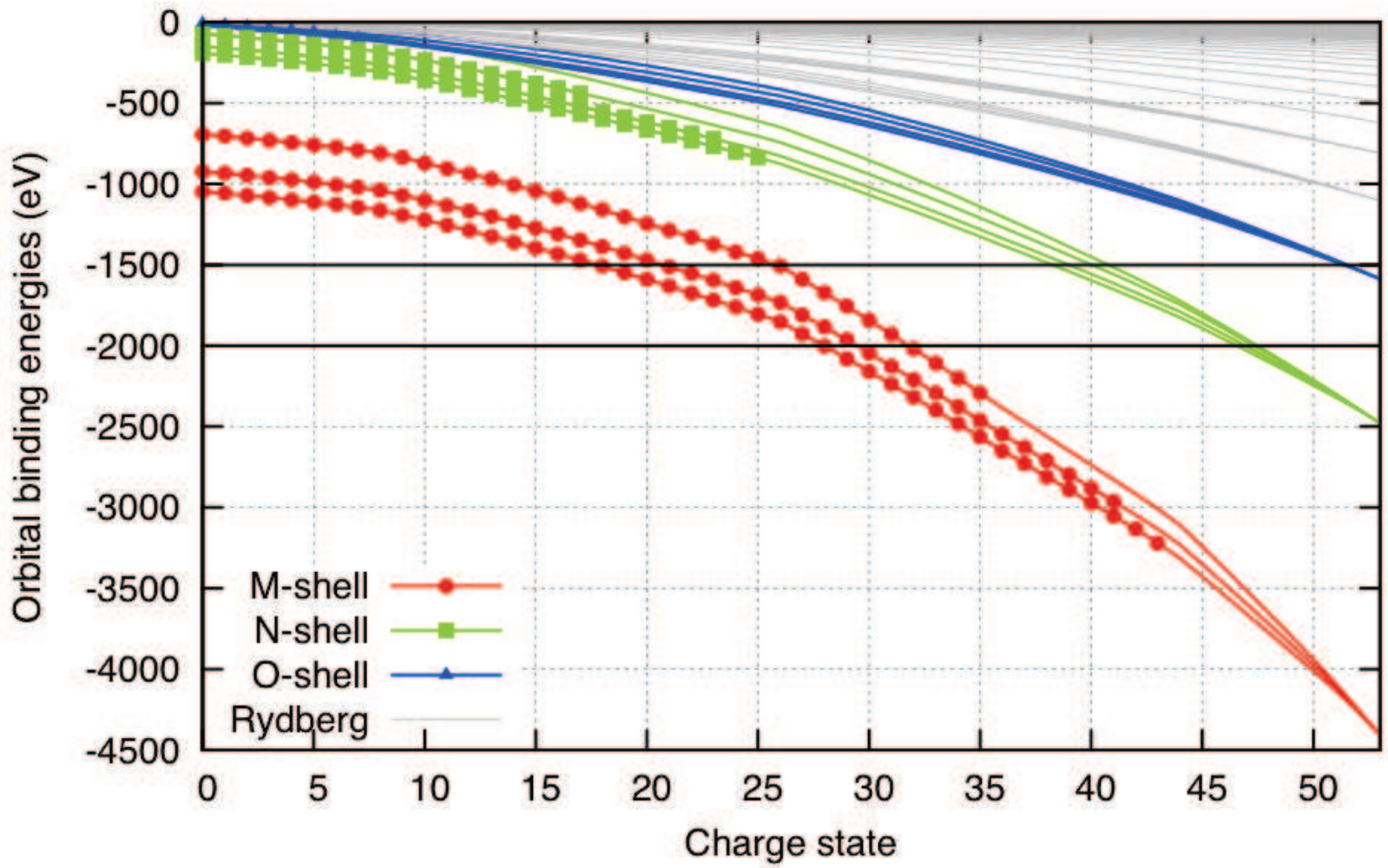
Orbital energies of the ground configuration of Xe^{q+}



S.-K. Son and R. Santra, Phys. Rev. A **85**, 063415 (2012).

Acknowledgments

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X-ray multiphoton ionization of xenon at a photon energy of 5.5 keV

Experiment carried out at SACLA in Japan

Xe: $[1s^2]\ 2s^2\ 2p^6\ \mathit{3s^2}\ \mathit{3p^6}\ \mathit{3d^{10}}\ \mathit{4s^2}\ \mathit{4p^6}\ \mathit{4d^{10}}\ \mathit{5s^2}\ \mathit{5p^6}$

→ ***~24 million*** coupled rate equations
(excluding ionization from the K shell)

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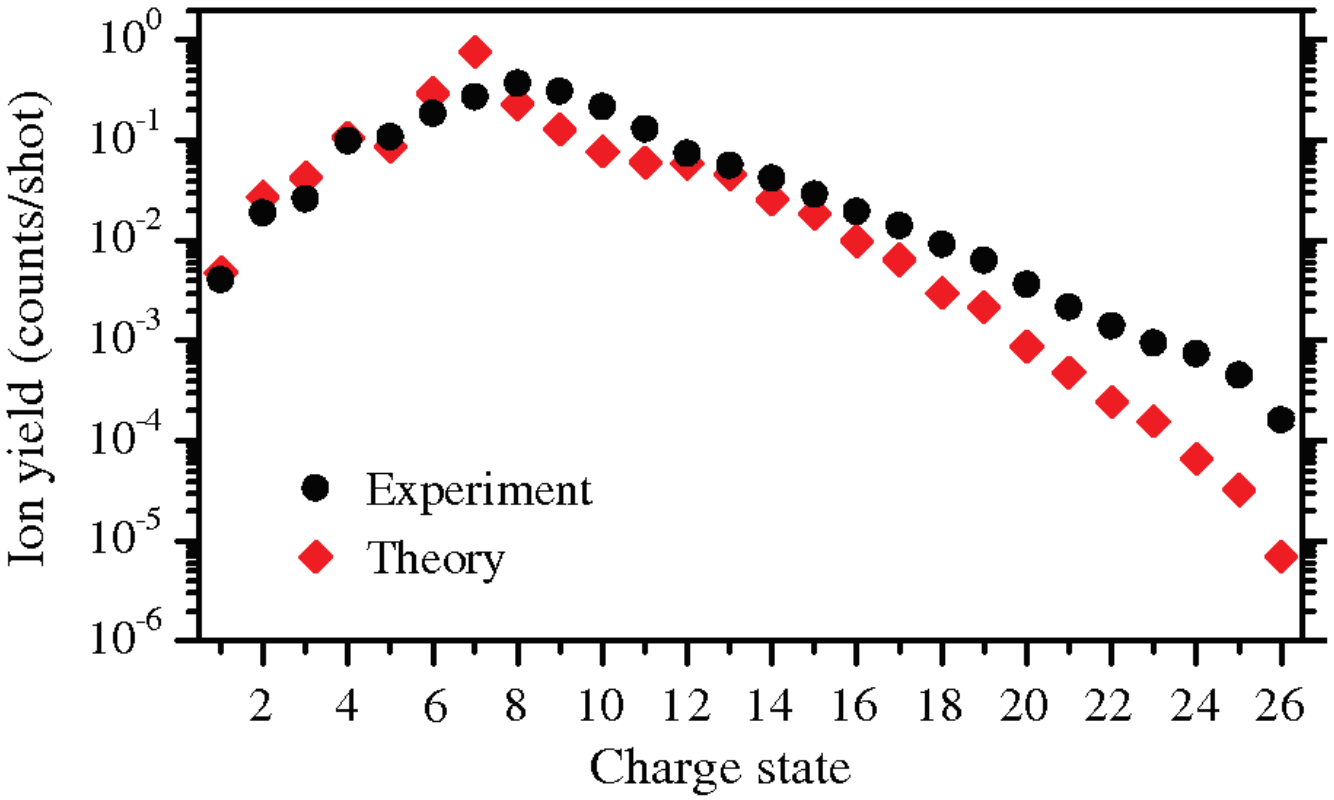
Xe charge-state distribution (5.5 keV, 70 μJ/μm^2)



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

The model neglects shake-off and relativistic effects, which tend to increase the yield of higher charge states.

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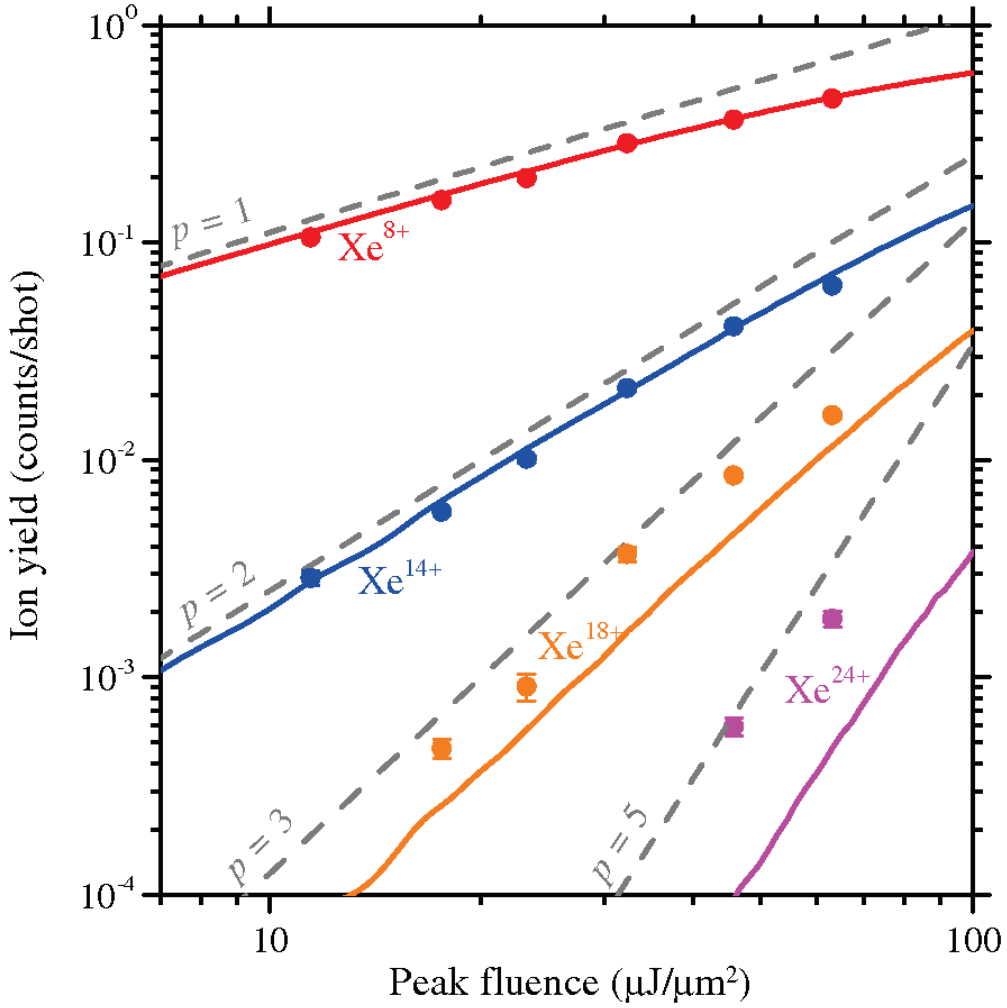
Fluence dependence of the xenon ion yield (5.5 keV)



Xe^{24+} produced via five-photon absorption.

On average, each photon causes the ejection of ~five electrons.

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

Acknowledgments

H. Fukuzawa,[1, 2] **S.-K. Son**,[3] K. Motomura,[1] S. Mondal,[1] K. Nagaya,[2, 4] S. Wada,[2, 5] X.-J. Liu,[6] R. Feifel,[7] T. Tachibana,[1] Y. Ito,[1] M. Kimura,[1] T. Sakai,[4] K. Matsunami,[4] H. Hayashita,[5] J. Kajikawa,[5] P. Johnsson,[8] M. Siano,[9] E. Kukk,[10] B. Rudek,[11, 12] B. Erk,[11, 12] L. Foucar,[11, 13] E. Robert,[6] C. Miron,[6] K. Tono,[14] Y. Inubushi,[2] T. Hatsui,[2] M. Yabashi,[2] M. Yao,[4] **K. Ueda**[1, 2]

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Conclusions

- Our analysis suggests that it should be possible, even under conditions of high x-ray intensity, to solve the phase problem of coherent x-ray scattering by using MAD.
- This is important for molecular structure determination using serial femtosecond crystallography at x-ray free-electron lasers.
- For MAD at high x-ray intensity to work, one must be able to determine the dynamical behavior of the electronic structure of heavy atoms exposed to high-intensity x-ray pulses.

- Multiphoton processes in xenon have been observed at photon energies as high as 5.5 keV.
- XATOM successfully describes these processes, but not in the near-threshold region, which is of particular relevance for MAD.
- Necessary developments:
  - Bound-to-bound transitions
  - Relativistic effects
  - Environment effects

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