Theoretical investigation of direct two-photon ionization

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CFEL Theory
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HELMHOLTZ

CFEL SCIENCE

DESY.

Acknowledgement

Thank you very much!

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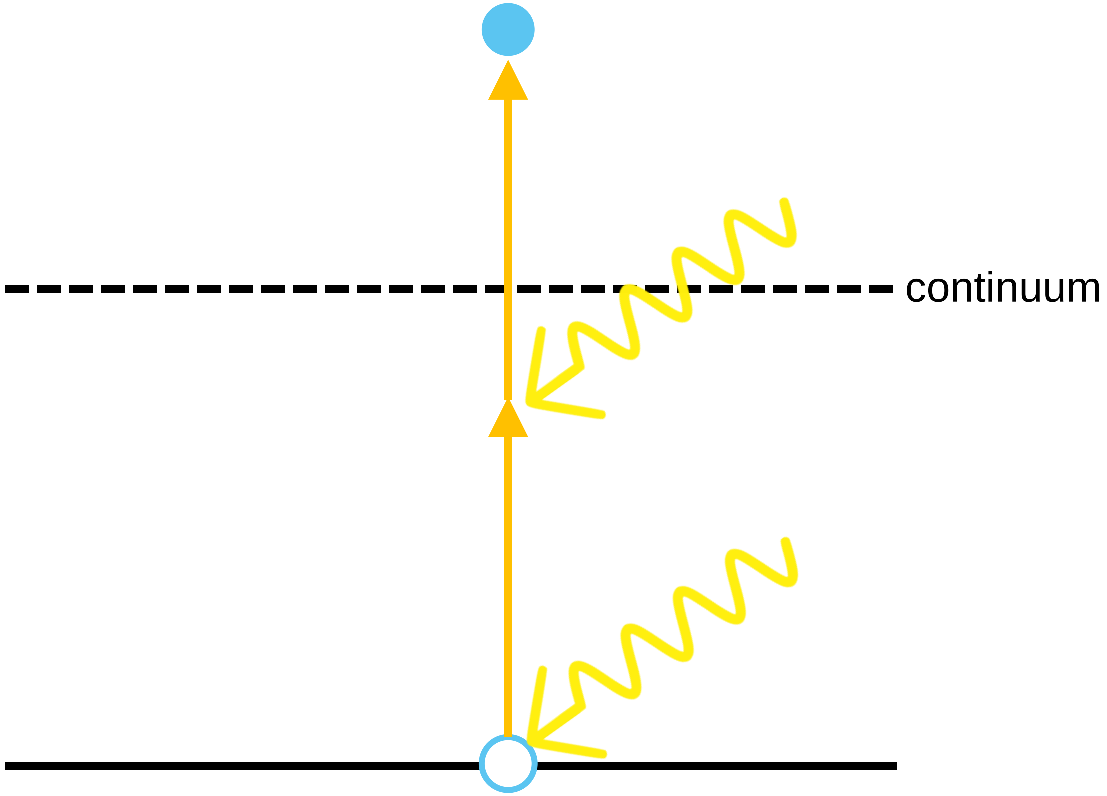
Physics:	Anthony Ferté, Ludger Inhester
Organizers:	Olaf Behnke et al.

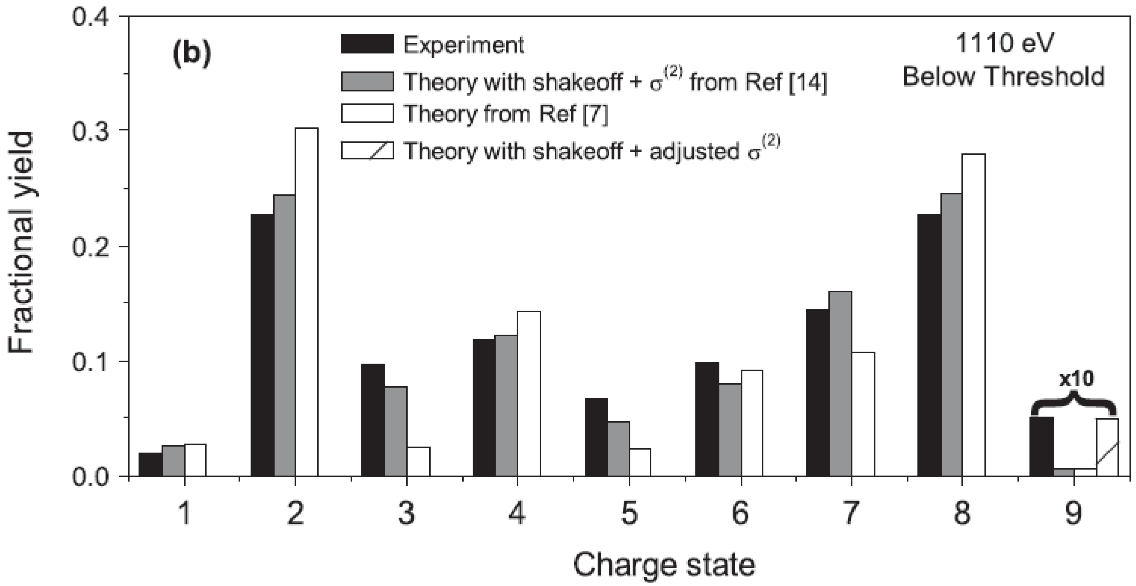
Motivation

What is direct two-photon ionization and why is it relevant?

What?



Why?



not enough higher charged states

→ new channel for ionization

Math and Theory

What is the TPCS in equations?

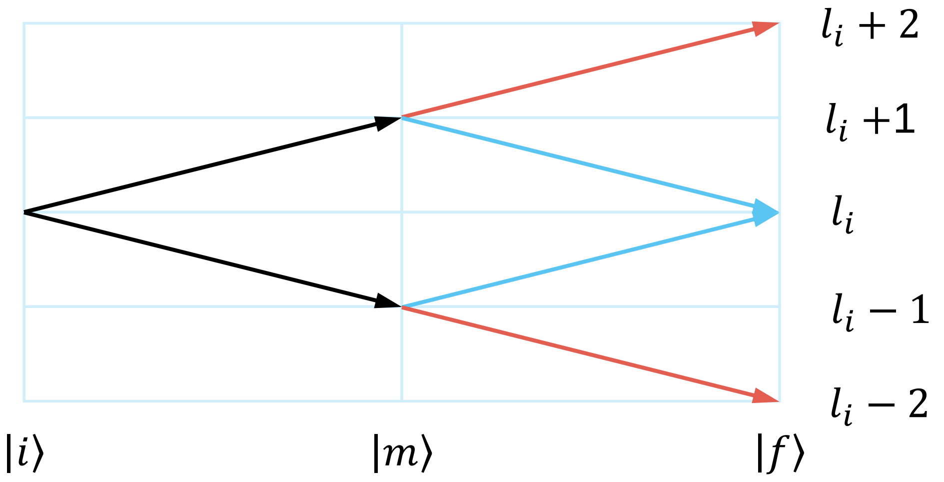
$$\sigma^{(2)}_{\mathrm{LOPT}}(\omega) = \pi(4\pi\alpha\omega)^2 \sum_f \delta(\varepsilon - \omega_i - 2\omega) \left| \sum_m \frac{\langle f|\hat{z}|m\rangle \langle m|\hat{z}|i\rangle}{\omega_i + \omega - \omega_m + i\Gamma_m/2} \right|^2 \quad \text{with} \quad |i\rangle = \frac{u_{n_i,l_i}}{r} Y_{l_i,m_i}$$

$$= \frac{\pi(4\pi\alpha\omega)^2}{15(2l_i+1)} \times \left[\sum_{\Delta l} C_1^{(\Delta l)} \left| S_{fmi}^{(2\Delta l,\Delta l)} \right|^2 + \sum_{\Delta l} C_2^{(\Delta l)} \left| S_{fmi}^{(+0,\Delta l)} \right|^2 + C_3 2\mathrm{Re}\left(S_{fmi}^{*(+0,+1)} S_{fmi}^{(+0,-1)} \right) \right]$$

with

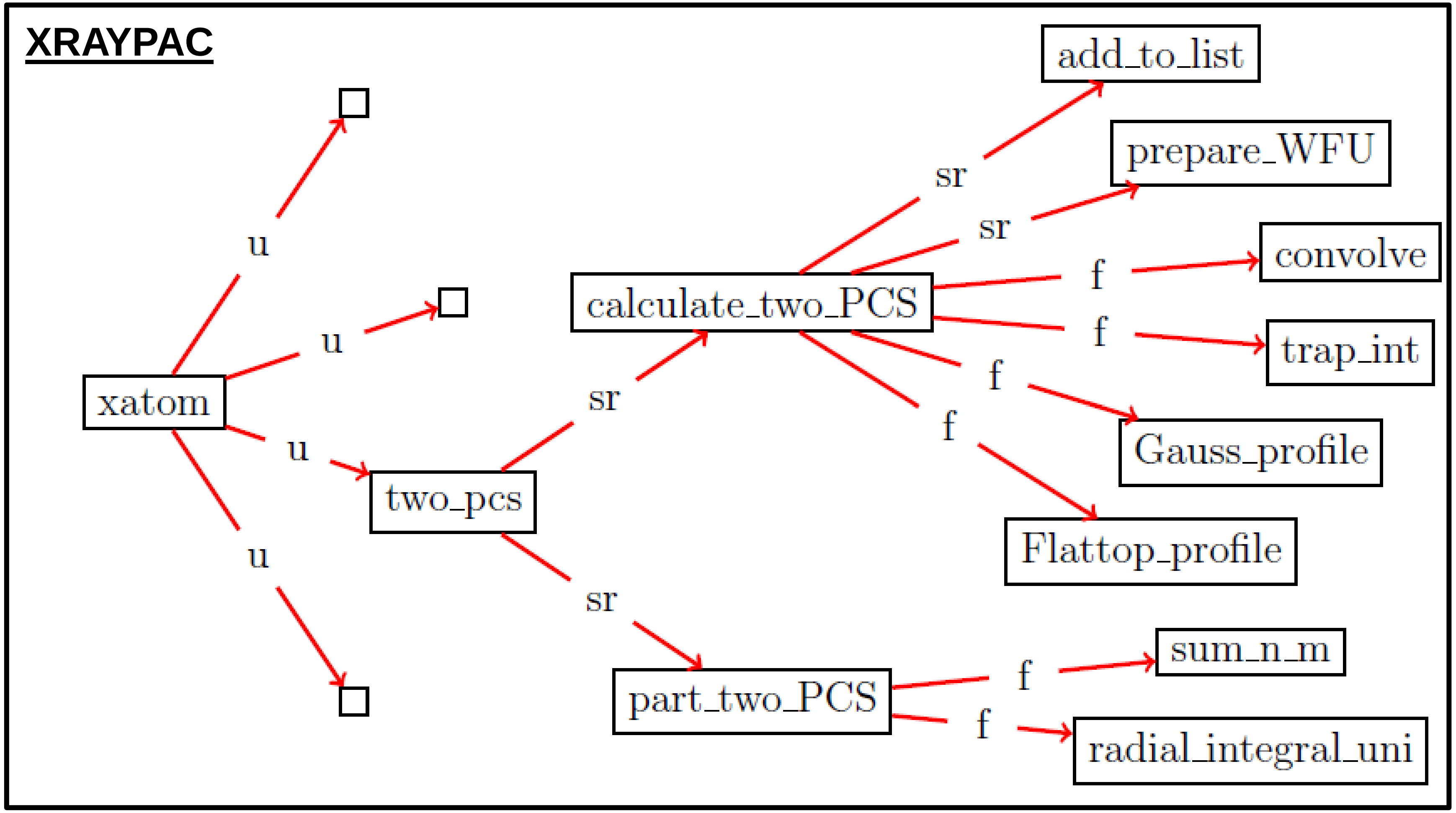
$$S_{fmi}^{(\Delta l_f,\Delta l_m)} = \sum_{n_m=1}^{\infty} \frac{R_{\varepsilon,l_i+\Delta l_f,n_m,l_i+\Delta l_m} R_{n_m,l_i+\Delta l_m,n_i,l_i}}{\omega_i + \omega - \omega_m + i\Gamma_m/2}$$

$$R_{n_1,l_1,n_2,l_2} = \int_0^\infty \mathrm{d}r\, u_{n_1,l_1}(r)\, r\, u_{n_2,l_2}(r)$$



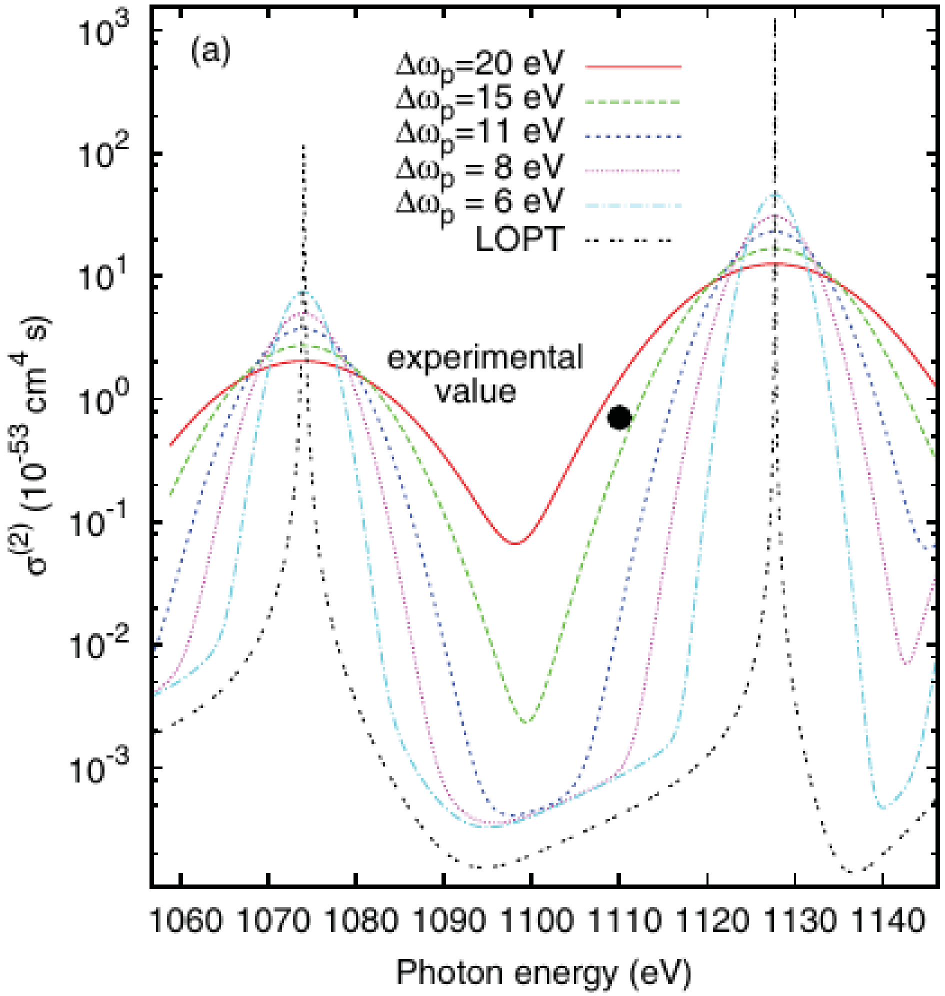
Code

What does the module do?

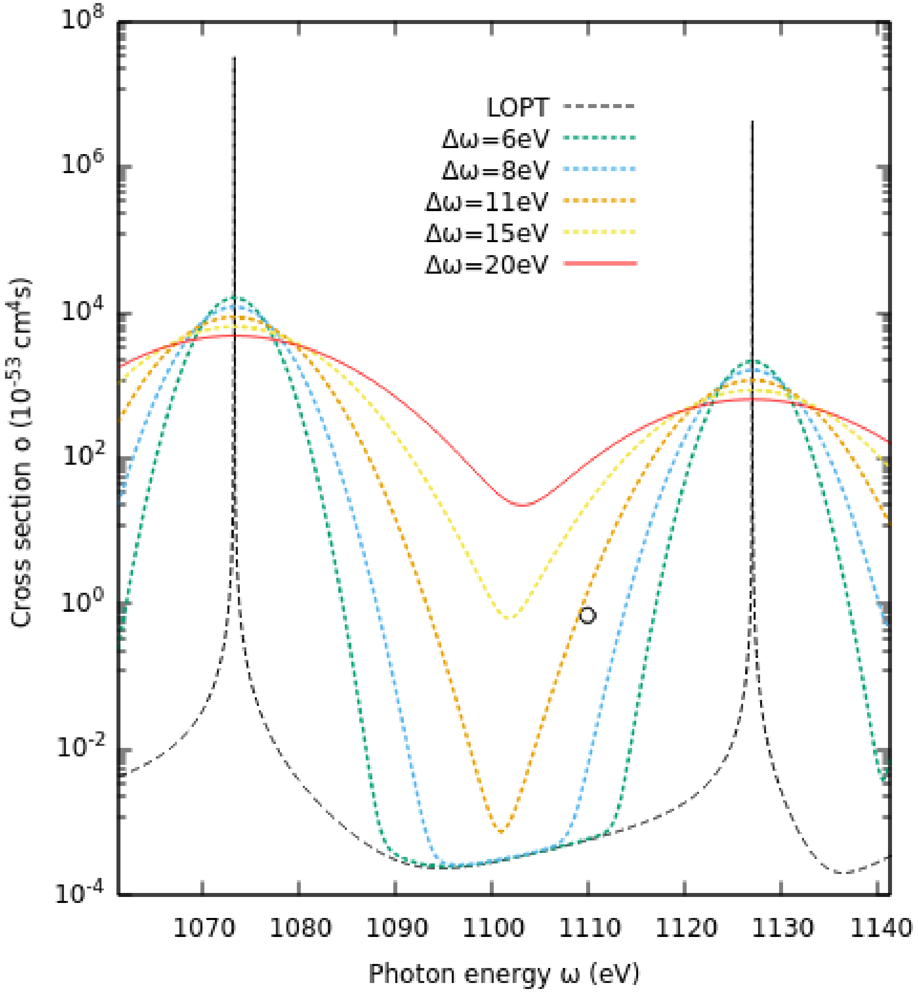


TPCS of Ne^{8+}

How do the results look like?



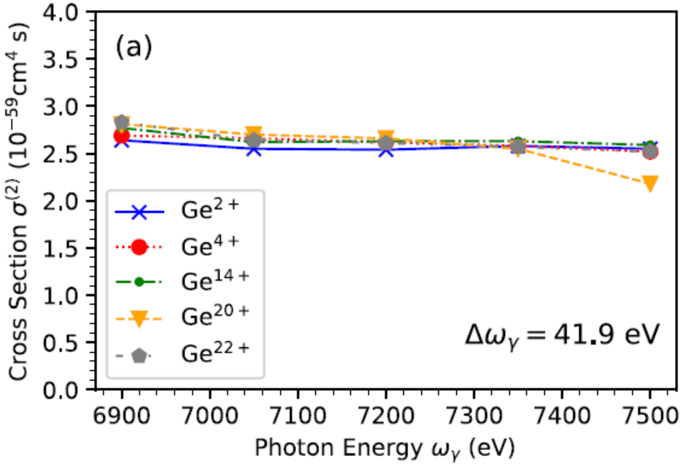
10.1103/PhysRevA.83.033402 [3]

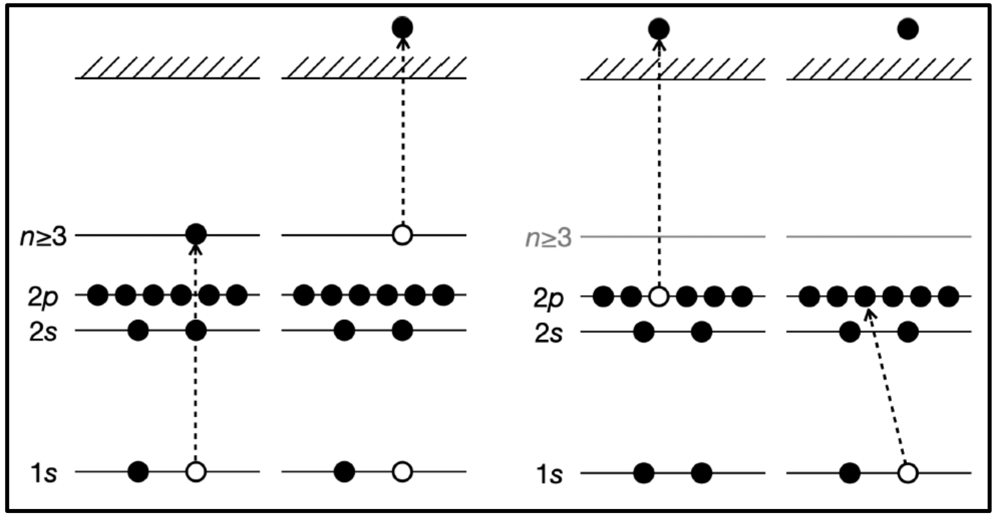


TPCS of Germanium ions

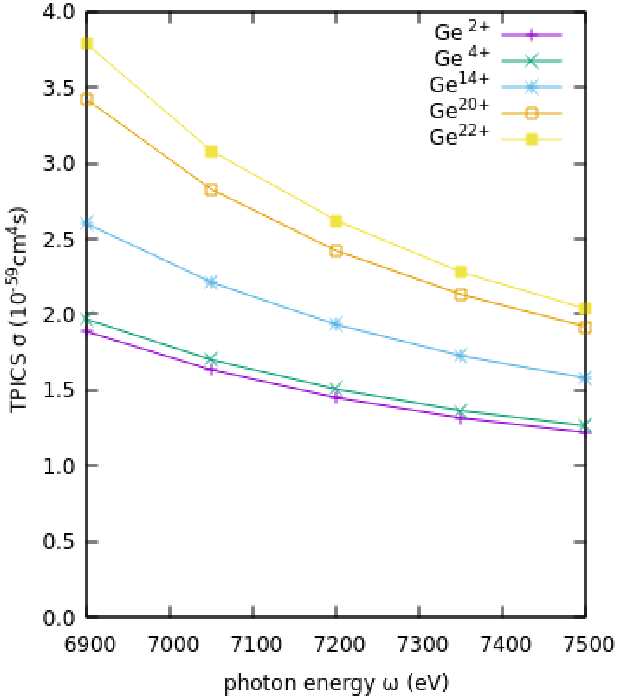
Is the code applicable to other atomic species?

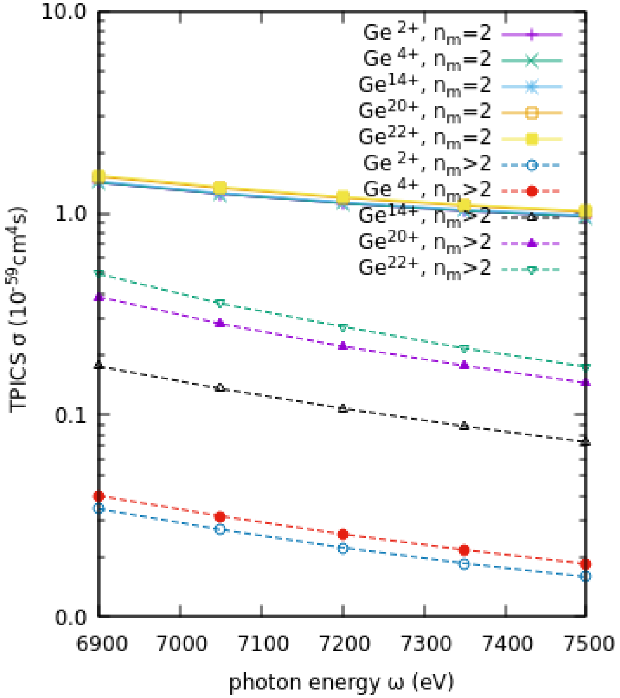
10.1103/PhysRevA.106.023118. [6]





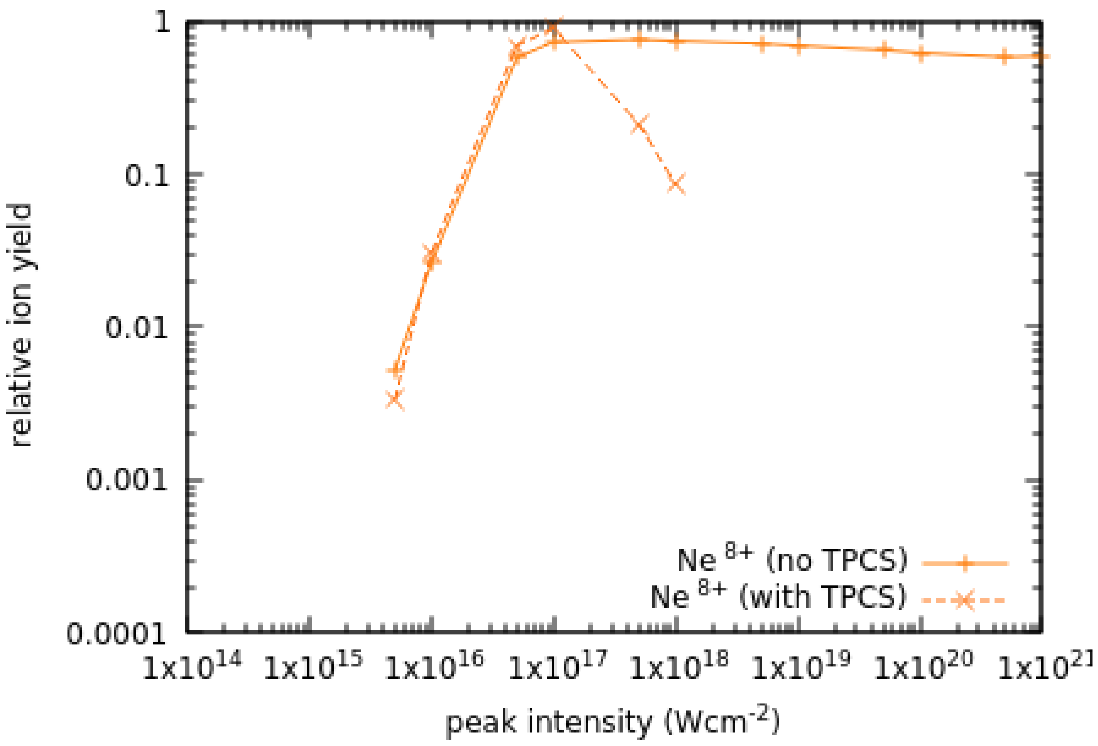
10.1103/PhysRevA.106.023118. [6]

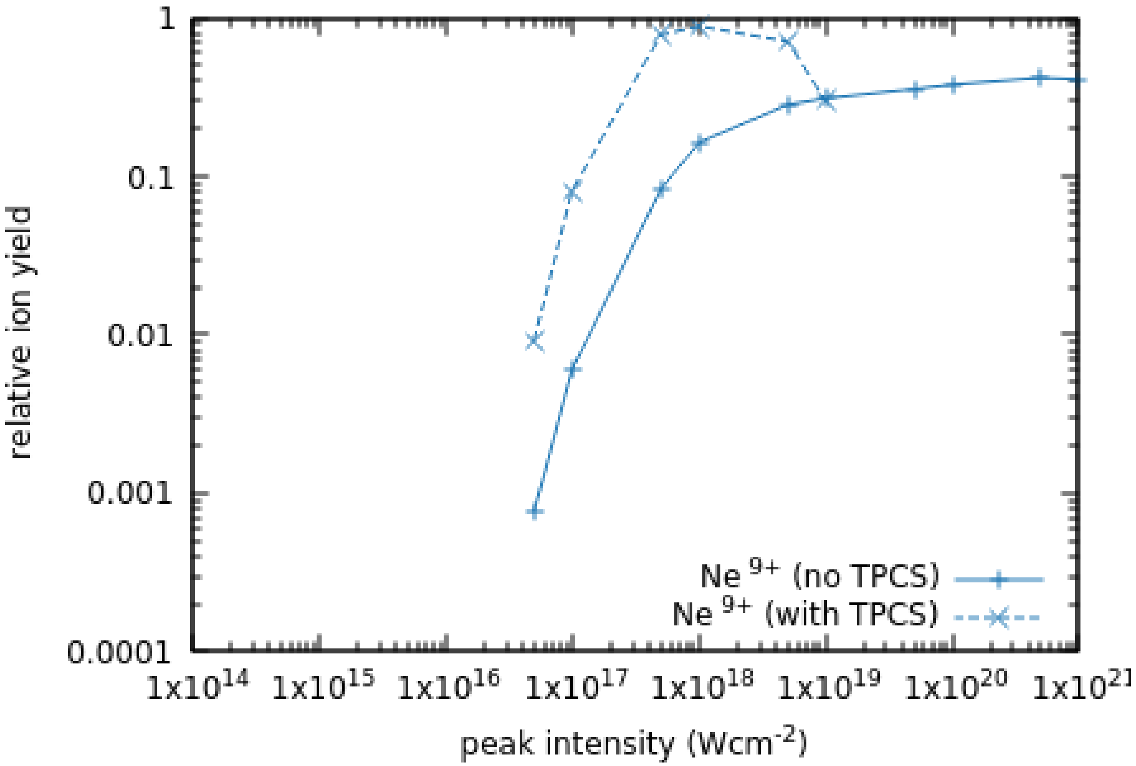




TPCS in ionization dynamics

How does TPCS impact ionization dynamics?





- minor effect at lower intensities / major effect at higher intensities

→ Need to consider direct two-photon ionization in simulations

Conclusion

What has been done?

- Derivation and implementation of LOPT TPCS in XATOM
- Reproduction of Ne^{8+} TPCS with good match to experiments
- Application to Germanium ions with new method
- Implementation in ionization dynamics and quantification of impact

References

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