X-ray Free Electron Laser Driven Resonance Pumping of Spectral Lines of Highly Charged Ions in Dense Plasmas

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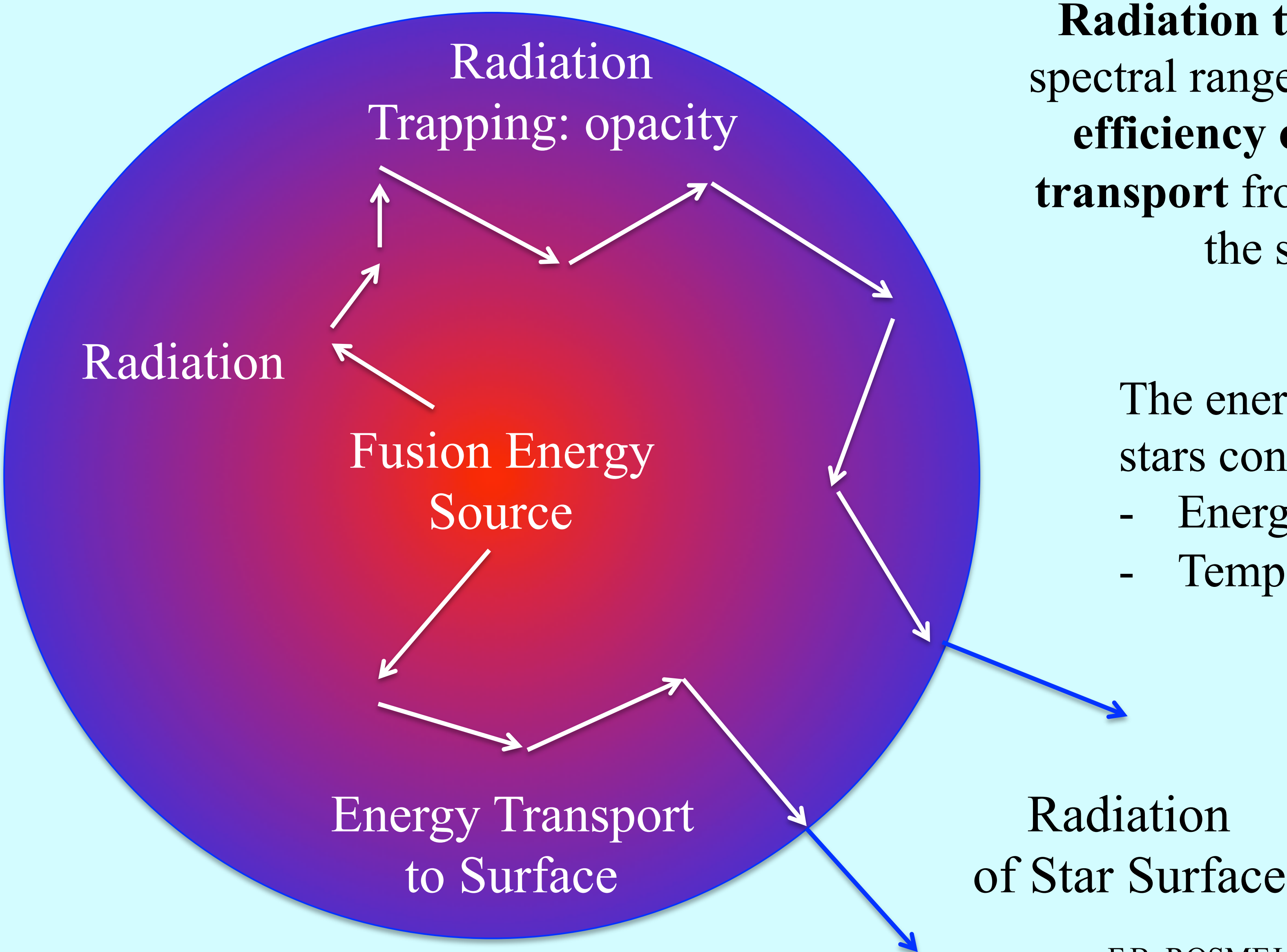
Contents

I. Motivation

Energy balance in astrophysical objects



Radiation trapping in all spectral range determines the **efficiency of the energy transport** from the center to the surface

The energy transport in stars controls:

- Energy balance
- Temperature profile

Opacity, Atomic Physics & Population Kinetics

$$d\tau_{\omega}^{(i,j)} = \kappa_{\omega}^{(i,j)} dl \propto \frac{f_{ij}}{\omega} \cdot n_i \cdot dl \cdot \varphi_{ij}\left(\omega, \omega_{ij}\right)$$

$\tau_{\omega}^{(i,j)}, \kappa_{\omega}^{(i,j)}$: *bound – bound opacity, absorption coefficient*

$\hbar\omega$: *photon energy of absorption*

$\hbar\omega_{ij}$: *atomic absorption energy*

f_{ij} : *oscillator strength*

n_i : *absorbing lower state density*

L : *source size*

φ_{ij} : *absorption profile*

Opacity is a complex measure composed from detailed atomic physics properties and population kinetics

Bound-bound opacity: strongly width-dependent

$$d\tau^{(i,j)}_{\omega=\omega_{ij}} = \kappa^{(i,j)}_{\omega=\omega_{ij}} \cdot dl \propto \frac{f_{ij}}{\omega_{ij}} \cdot n_i \cdot \frac{1}{FWHM} \cdot dl$$

$\tau^{(i,j)}_{\omega_{ij}}, \kappa^{(i,j)}_{\omega_{ij}}$: *b − b line center opacity, absorption coefficient*

$\hbar\omega_{ij}$: *atomic absorption energy*

f_{ij} : *oscillator strength*

n_i : *absorbing lower state density*

dl : *source size*

FWHM: Full width at half maximum

The greater the broadening the smaller the local absorption coefficient !

Emissivity

$$\varepsilon_{\omega}^{(j,i)} \propto \omega \cdot A_{ji} \cdot n_j \cdot \varphi_{ji}\left(\omega, \omega_{ji}\right)$$

$\varepsilon_{\omega}^{(i,j)}$: *emission coefficient*

$\hbar\omega$: *photon energy of emission*

$\hbar\omega_{ij}$: *central atomic transition energy*

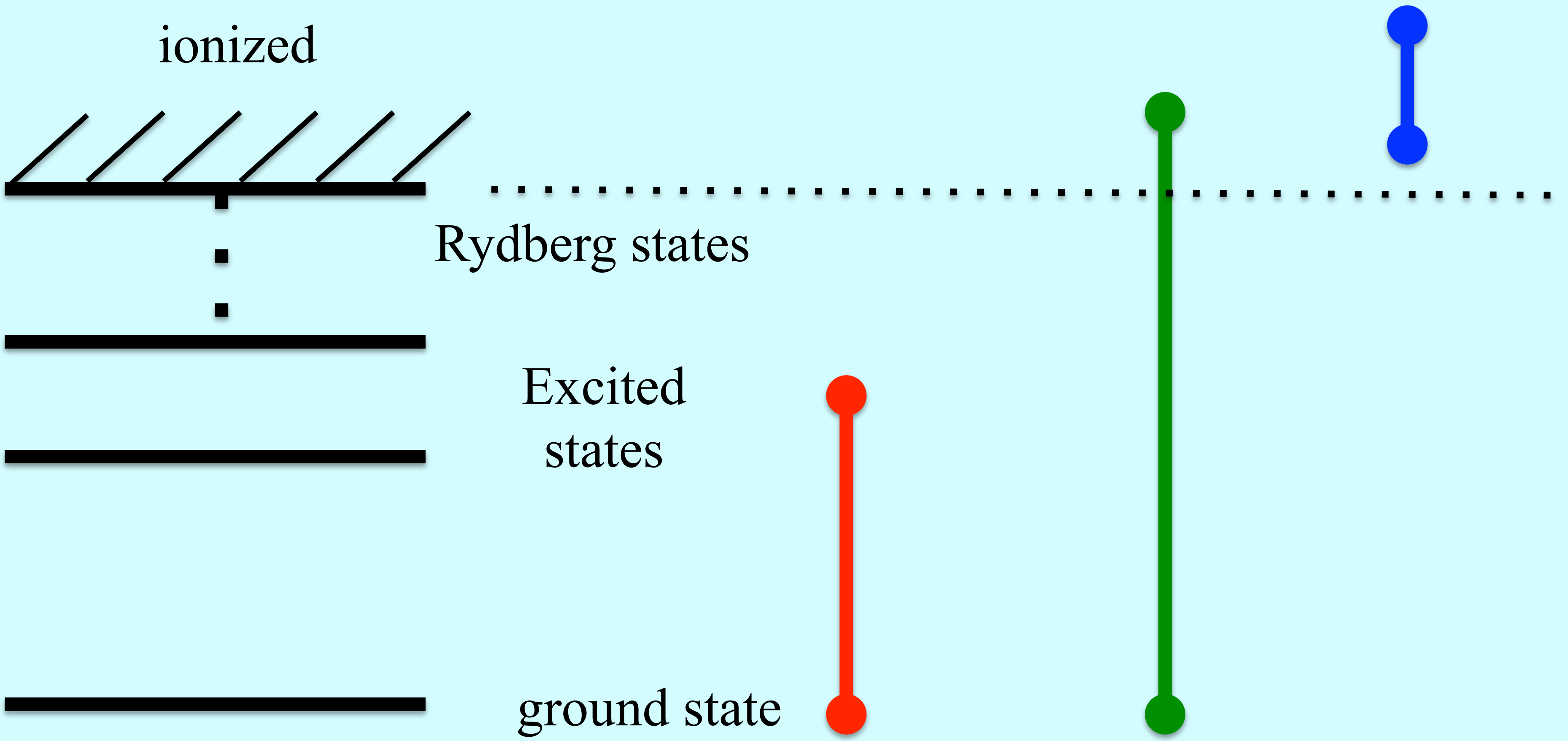
A_{ji} : *spontaneous transition rate*

n_j : *upper level density*

φ_{ji} : *emission profile*

Emissivity is a complex measure composed from detailed atomic physics properties and population kinetics

Total absorption: bound-bound + free part



$$\kappa_\omega^{(total)} = \kappa_\omega^{(bound-bound)} + \kappa_\omega^{(bound-free)} + \kappa_\omega^{(free-free)}$$

Ions, atoms   Ions, atoms   Free electrons

Radiation transport

Transport equation $$\frac{\partial I_\omega}{\partial \tau_\omega} = -I_\omega + S_\omega$$

Source function $$S_\omega = \varepsilon_\omega / \kappa_\omega$$

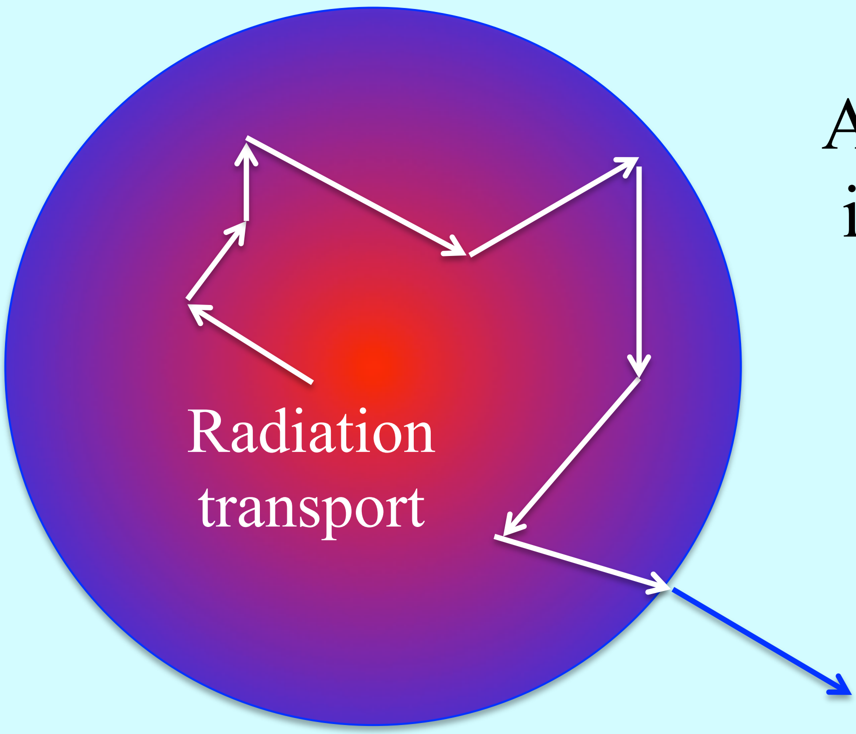
Absorption coefficient $$\kappa_\omega^{(total)} = \kappa_\omega^{(bb)} + \kappa_\omega^{(bf)} + \kappa_\omega^{(ff)}$$

Opacity $$d\tau_\omega = \kappa_\omega^{(total)} dx$$

=> Line transitions “bound-bound” are linked to the continuum via the absorption coefficient

II. Interest in complex configurations

What happens after absorption ?



After photo absorption….the photon is reemitted…absorbed…reemitted …. until it leaves the star…

Energy transport in stars couples opacity τ and emission I over the total frequency band !

Solar opacity is a problem of absorption & re-emission in large energy bands where line shapes are important

Energy transport: large frequency band

Radiation transport

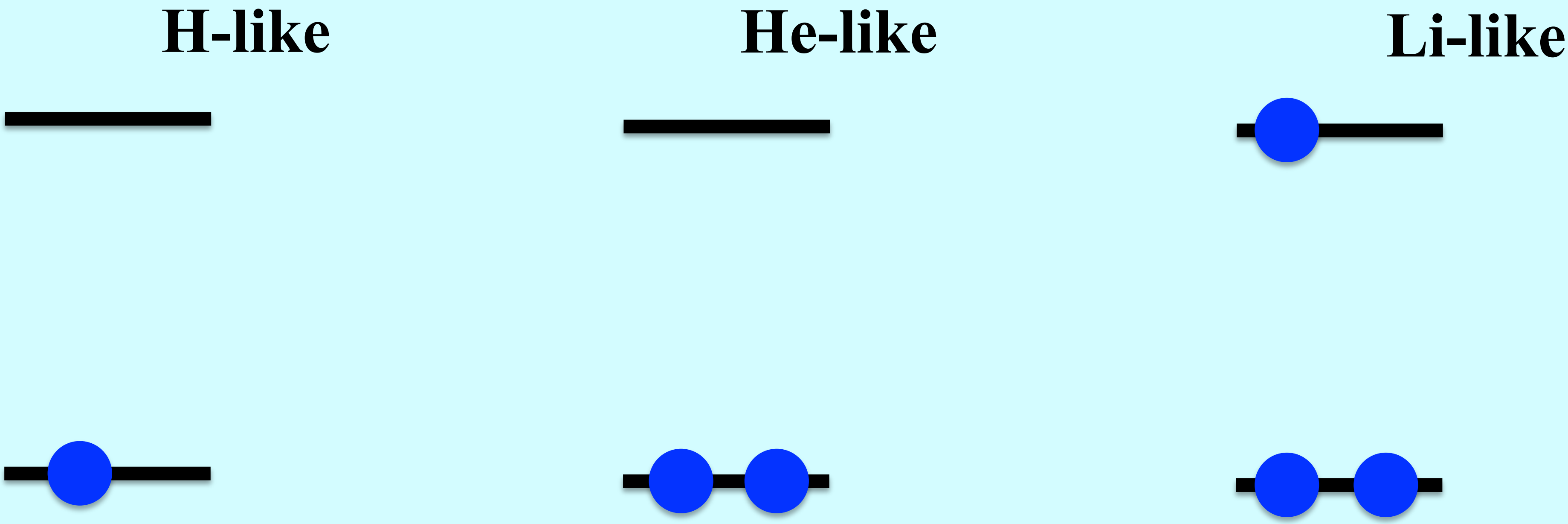
Absorption and emission in a large frequency band

Atomic physics language

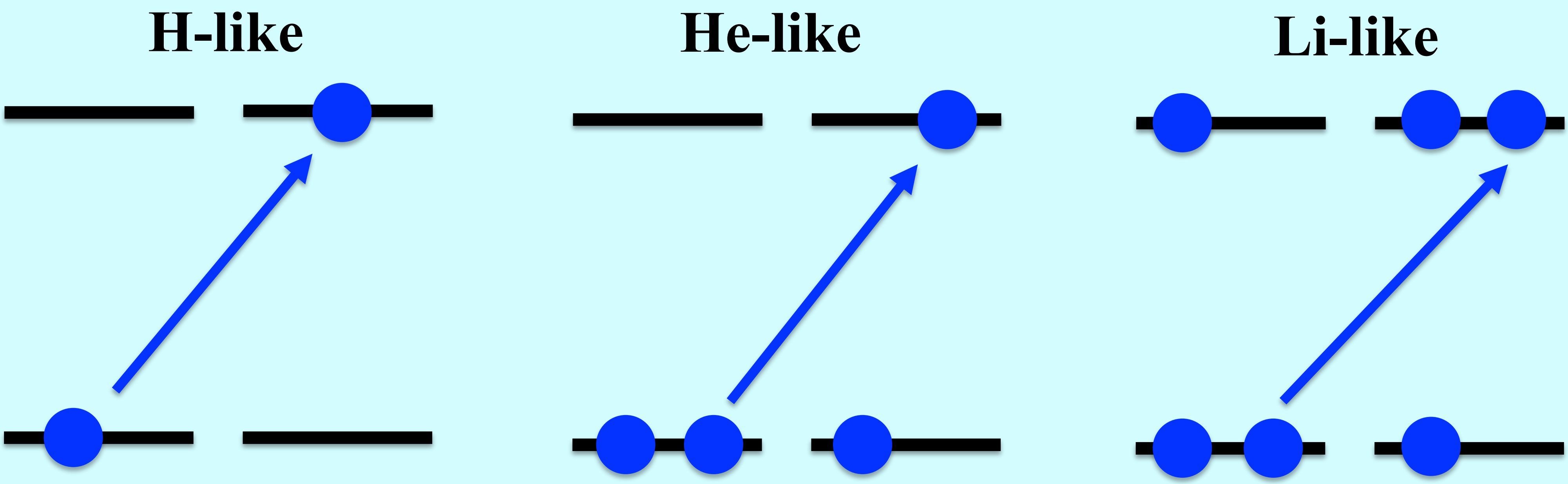
Transitions in atoms, partially and highly ionized ions

Transitions of simple and complex atomic configurations

Simple and complex configurations

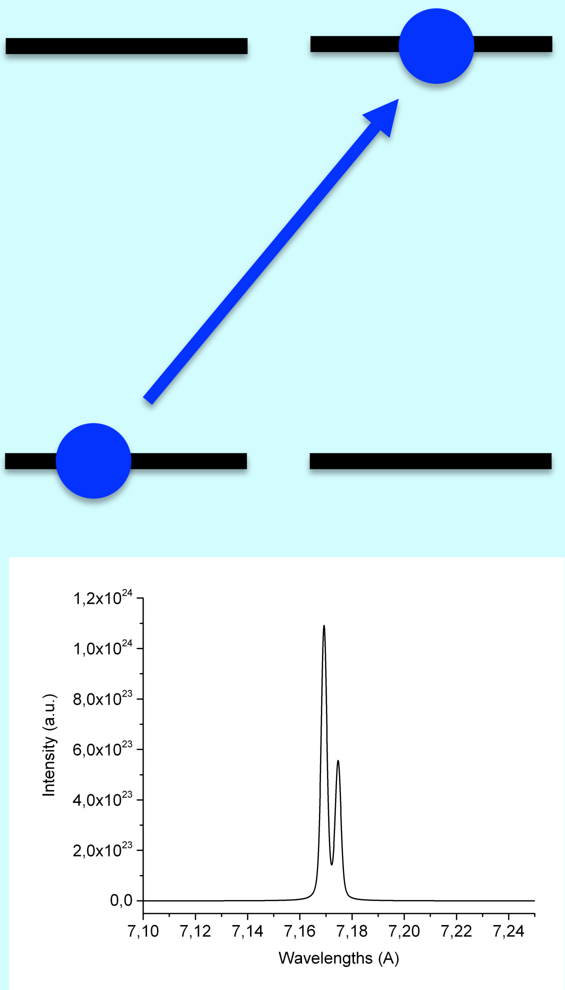


Simple and complex configurations

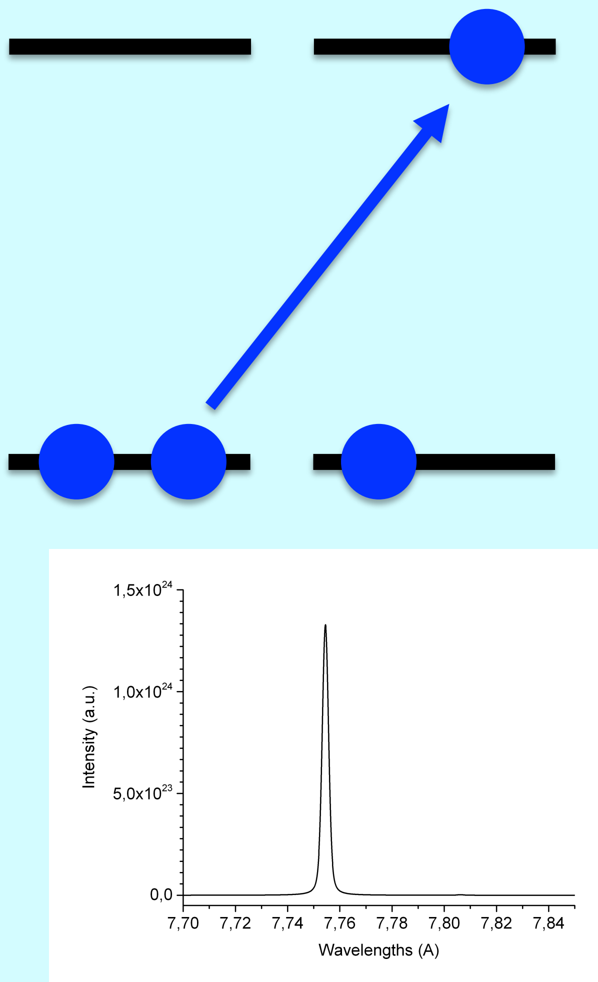


Simple and complex configurations

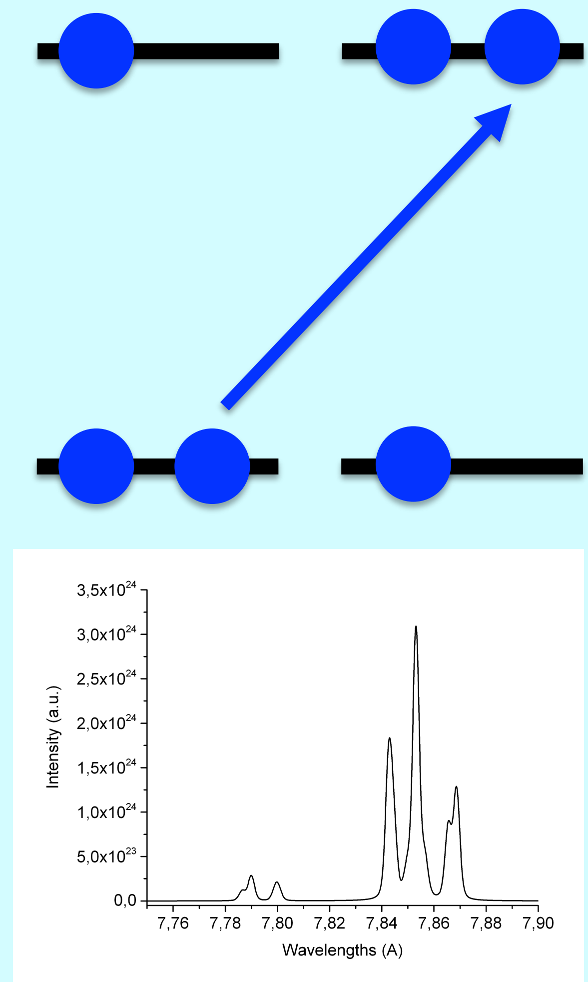
H-like



He-like

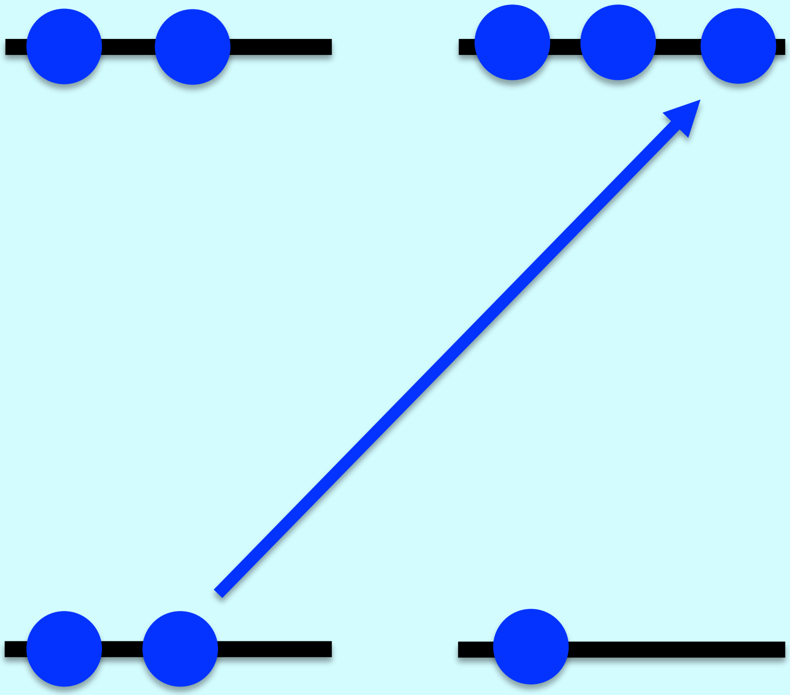


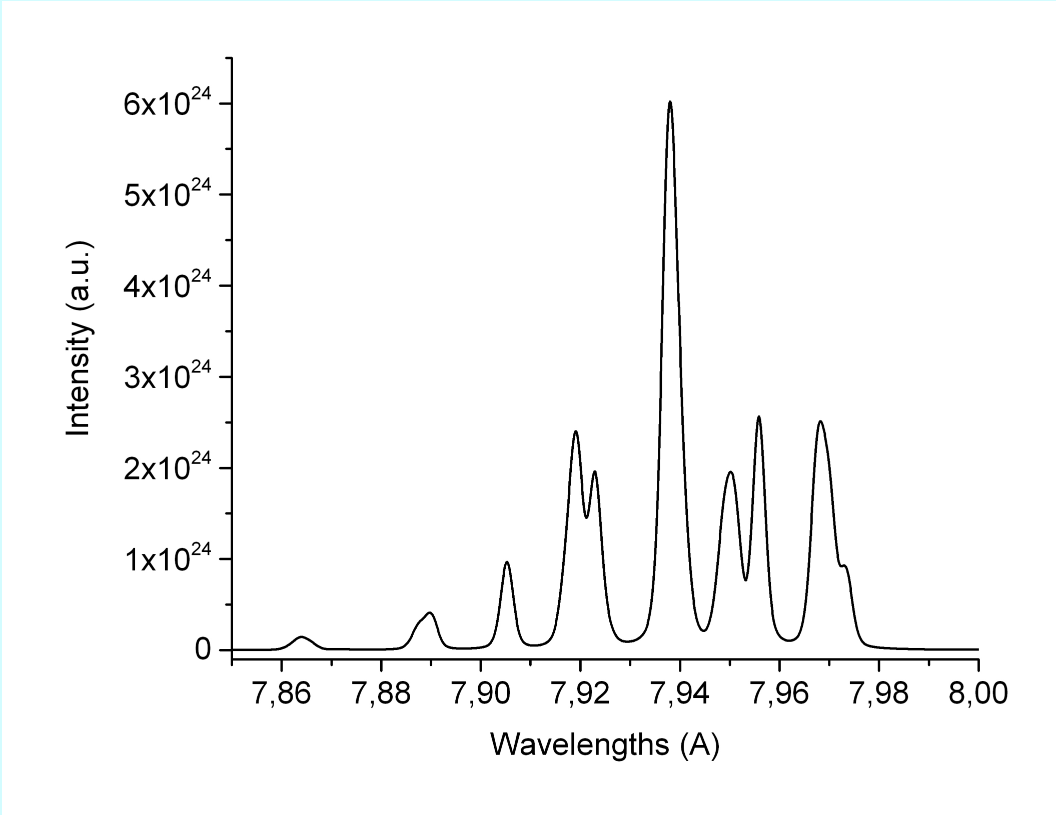
Li-like



Simple and complex configurations

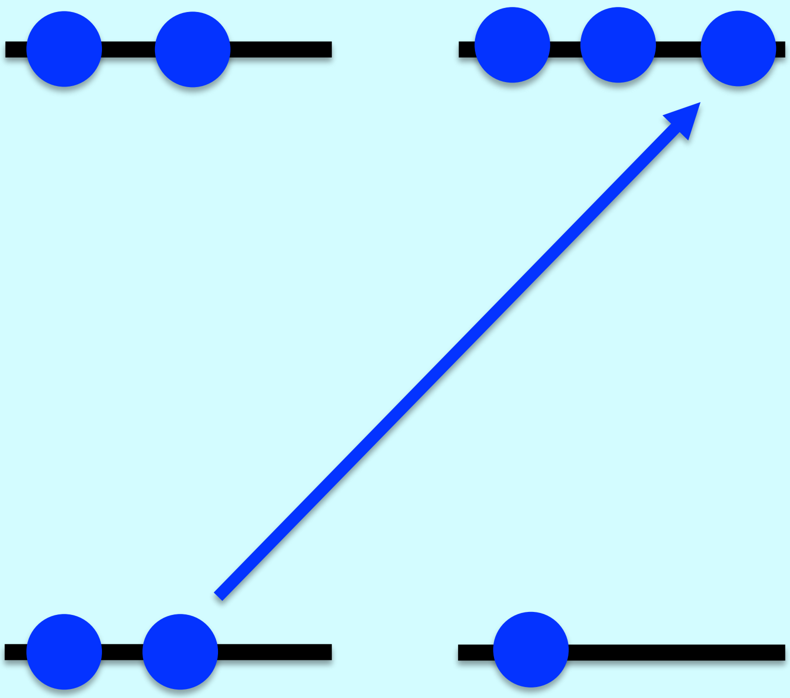
Be-like

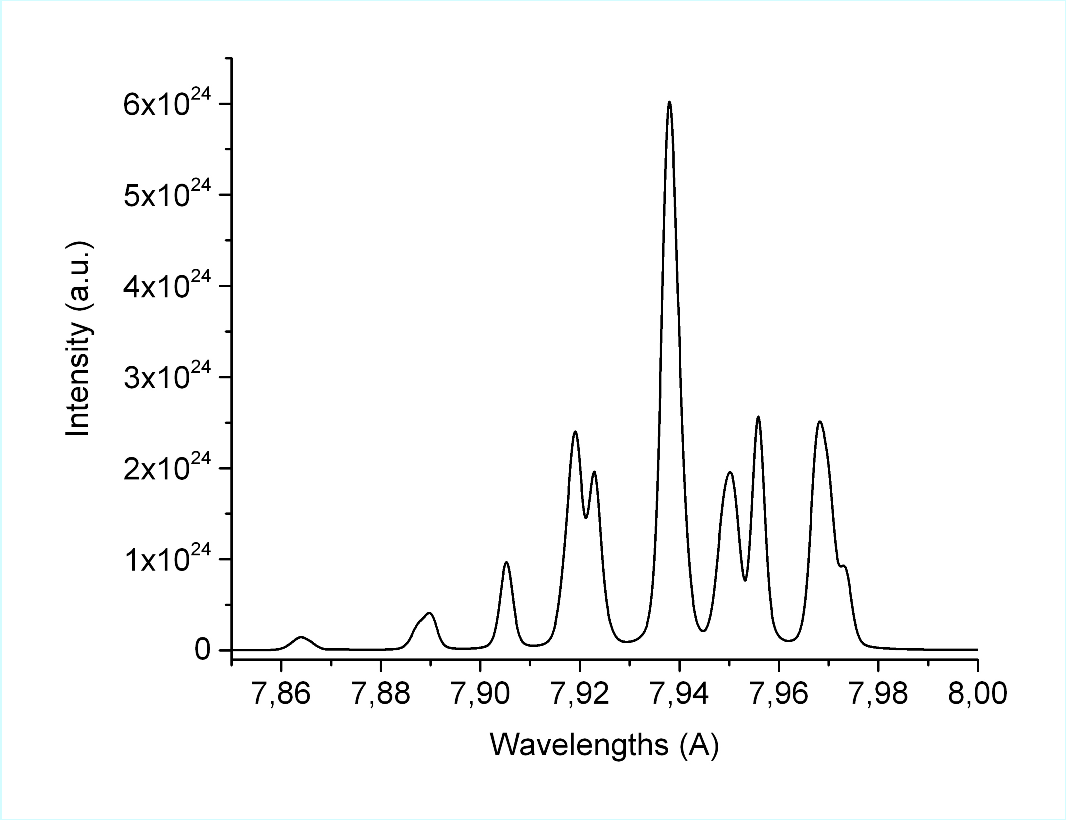




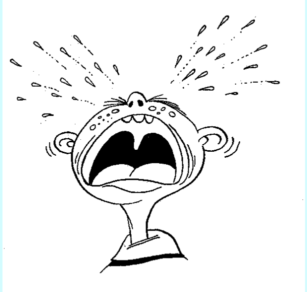
Simple and complex configurations

Be-like





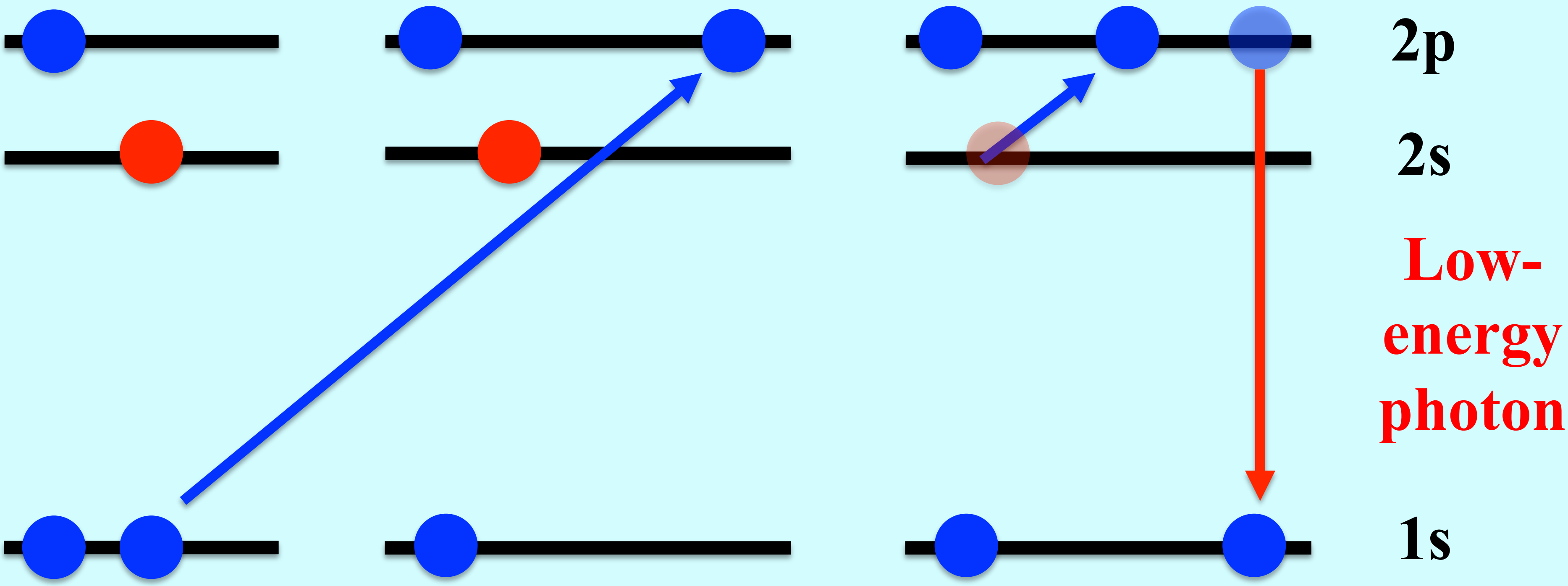
Too many and to close transitions for detailed studies



III. Two-electron transitions

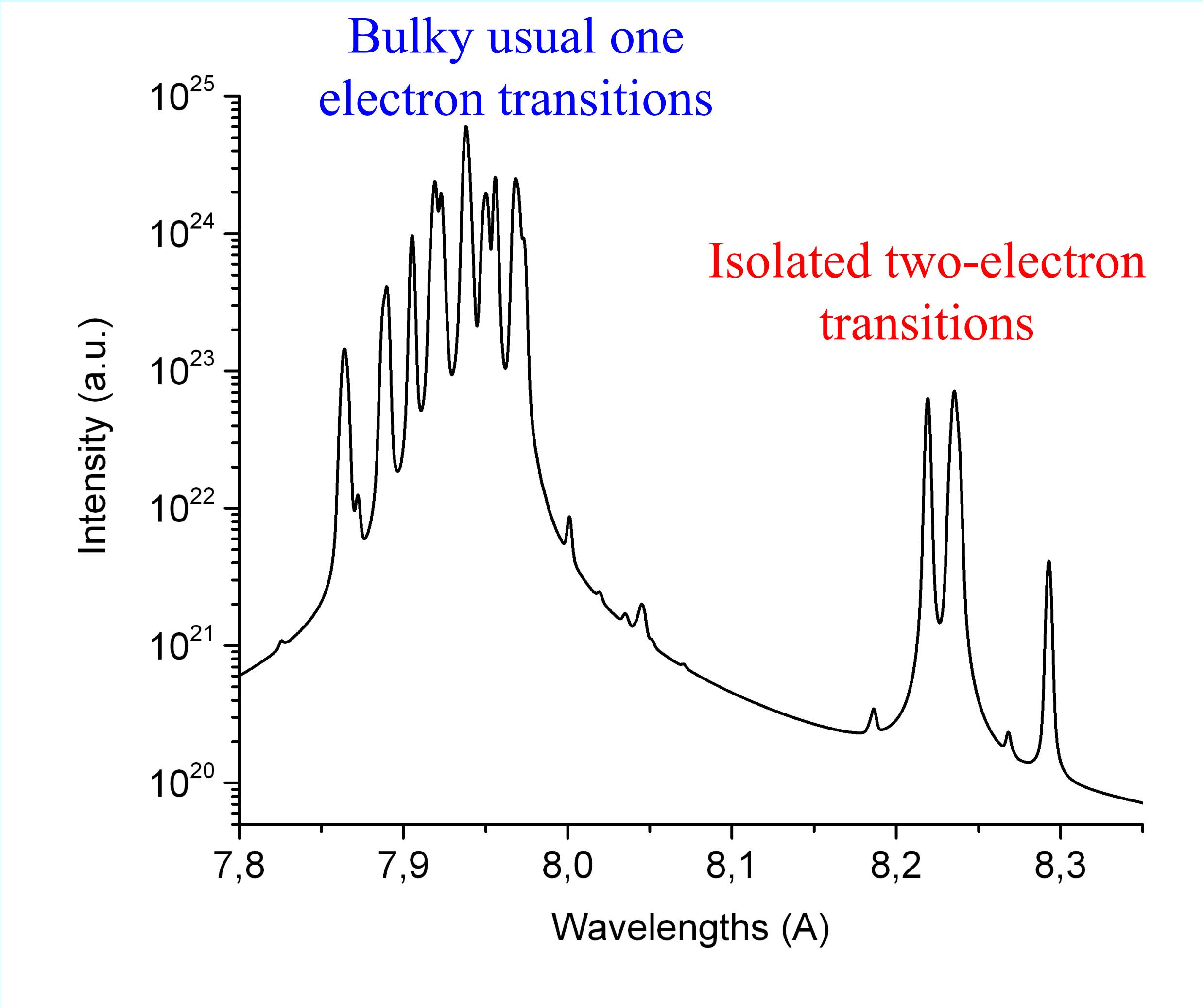
One photon + two-electron transitions

Be-like

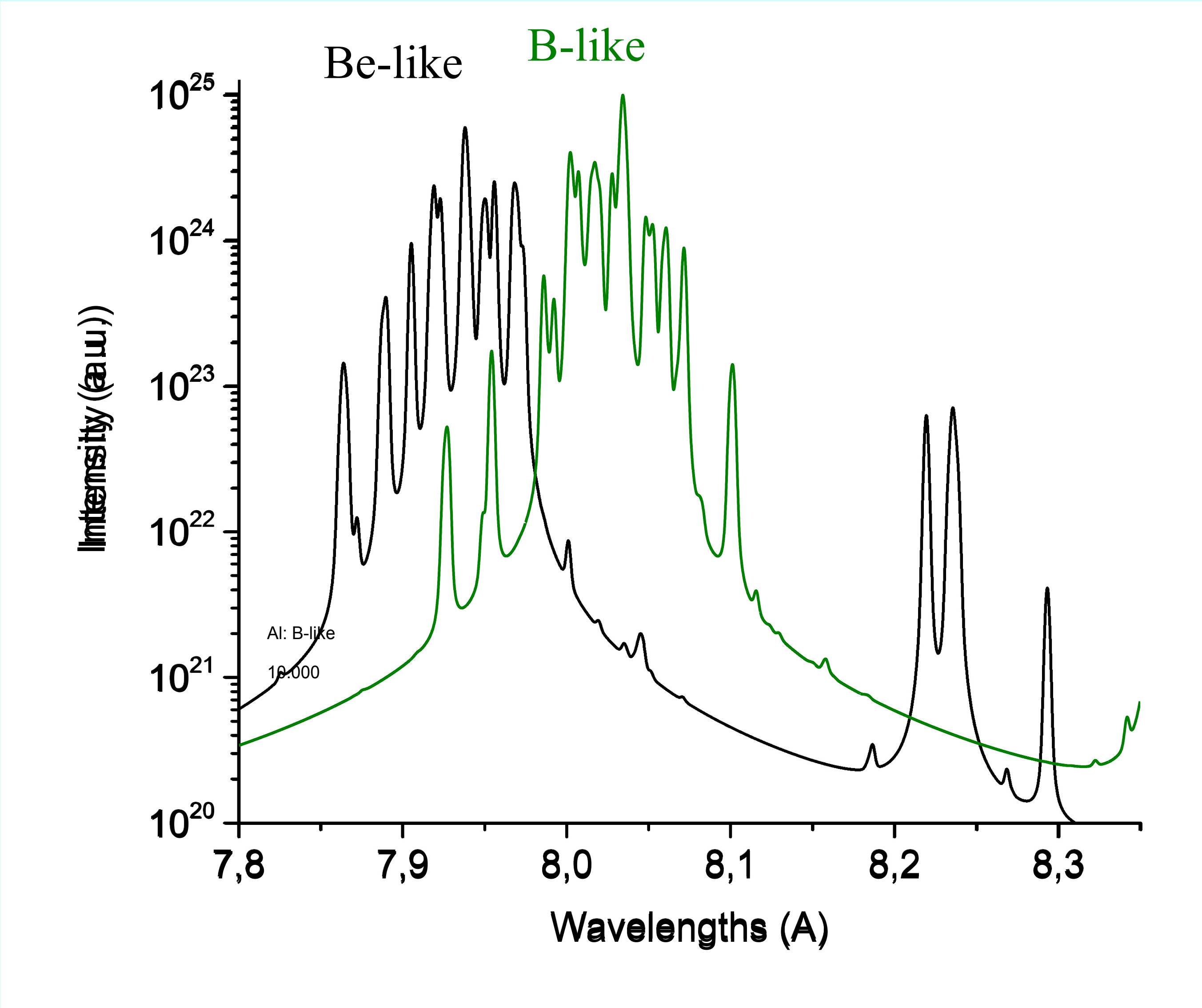


Low energy photon far away from "usual" one photon one electron transitions

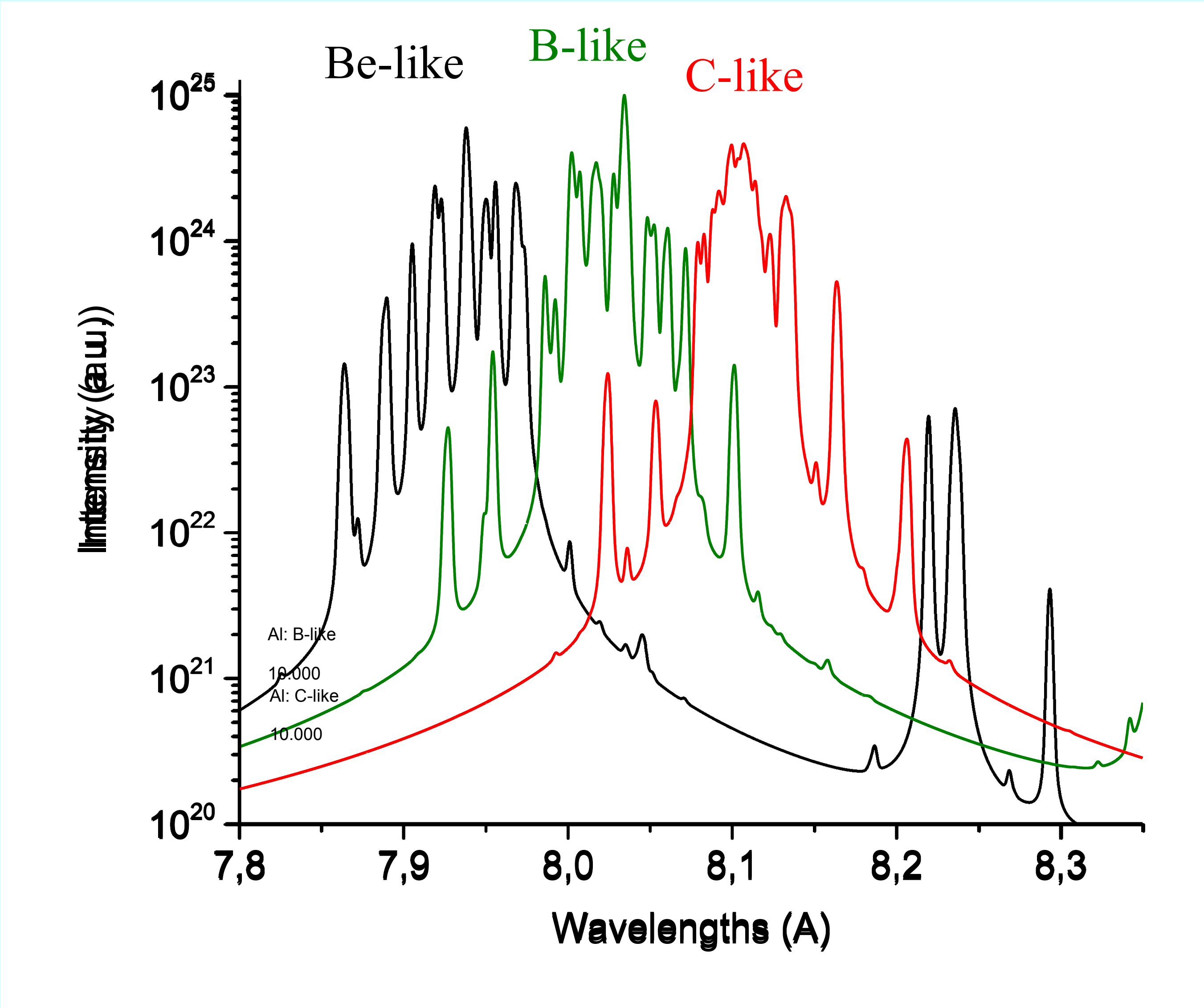
Be-like two-electron transitions



Overlap of transitions in hot dense plasmas



Overlap of transitions in hot dense plasmas



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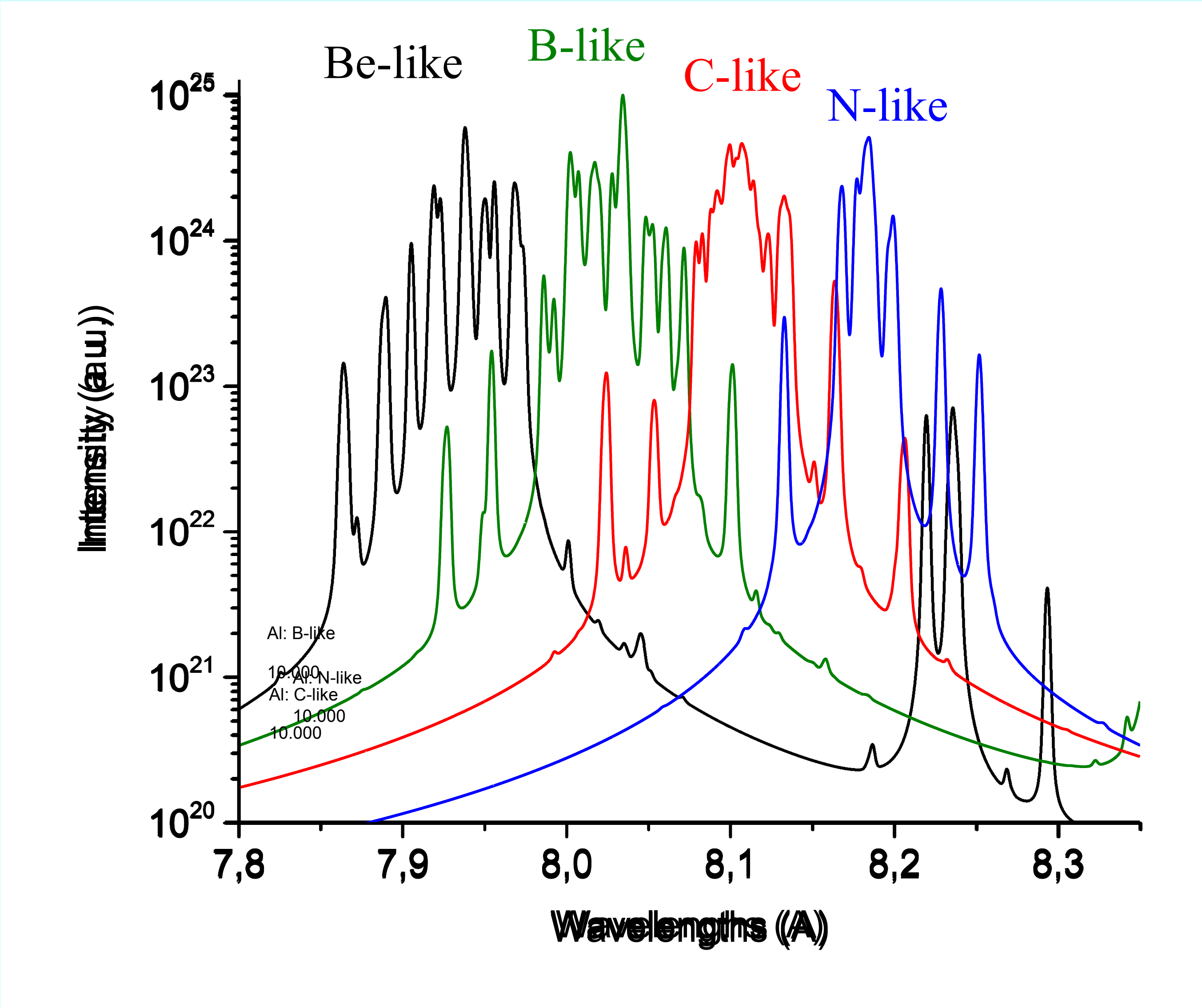

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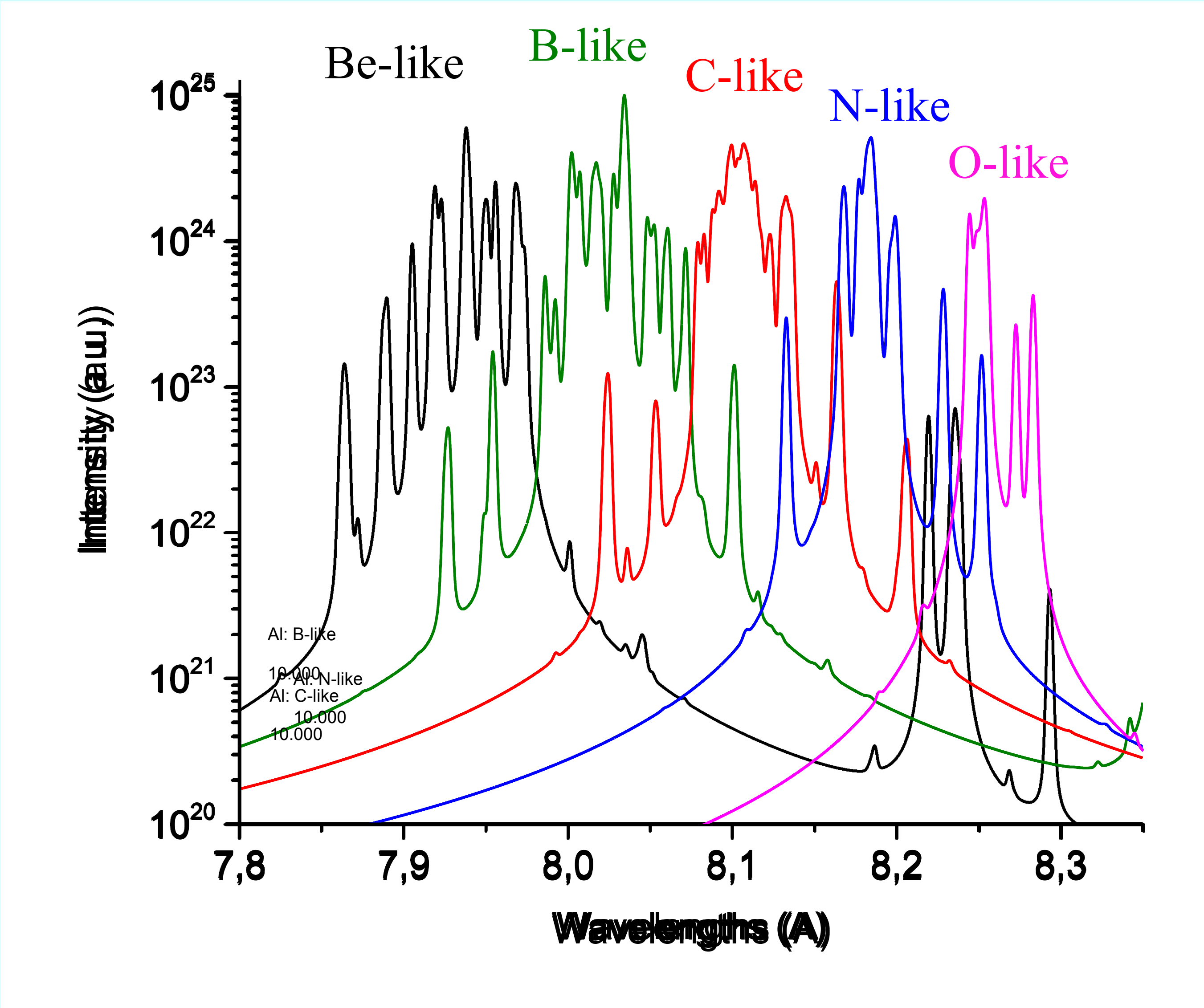

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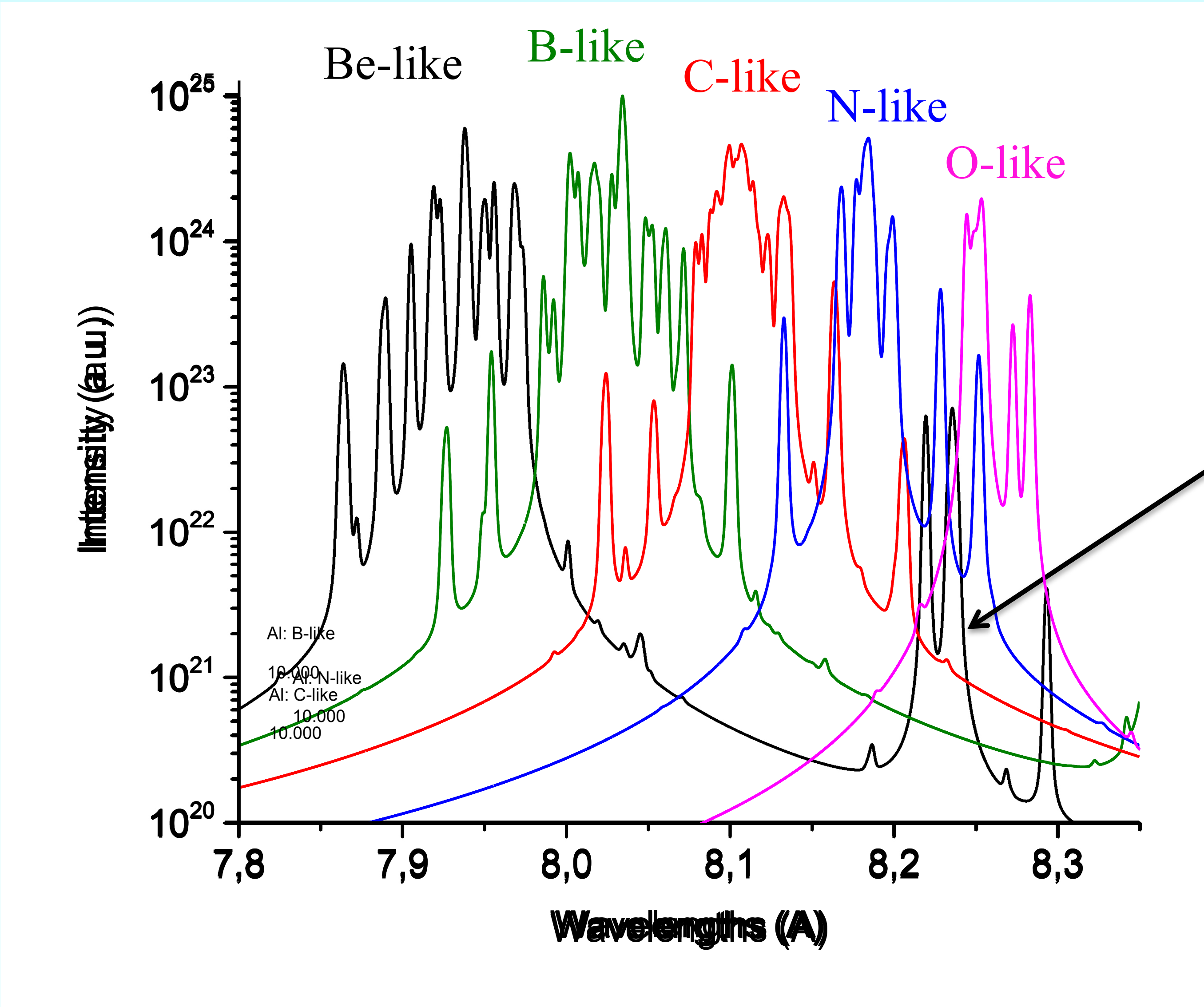
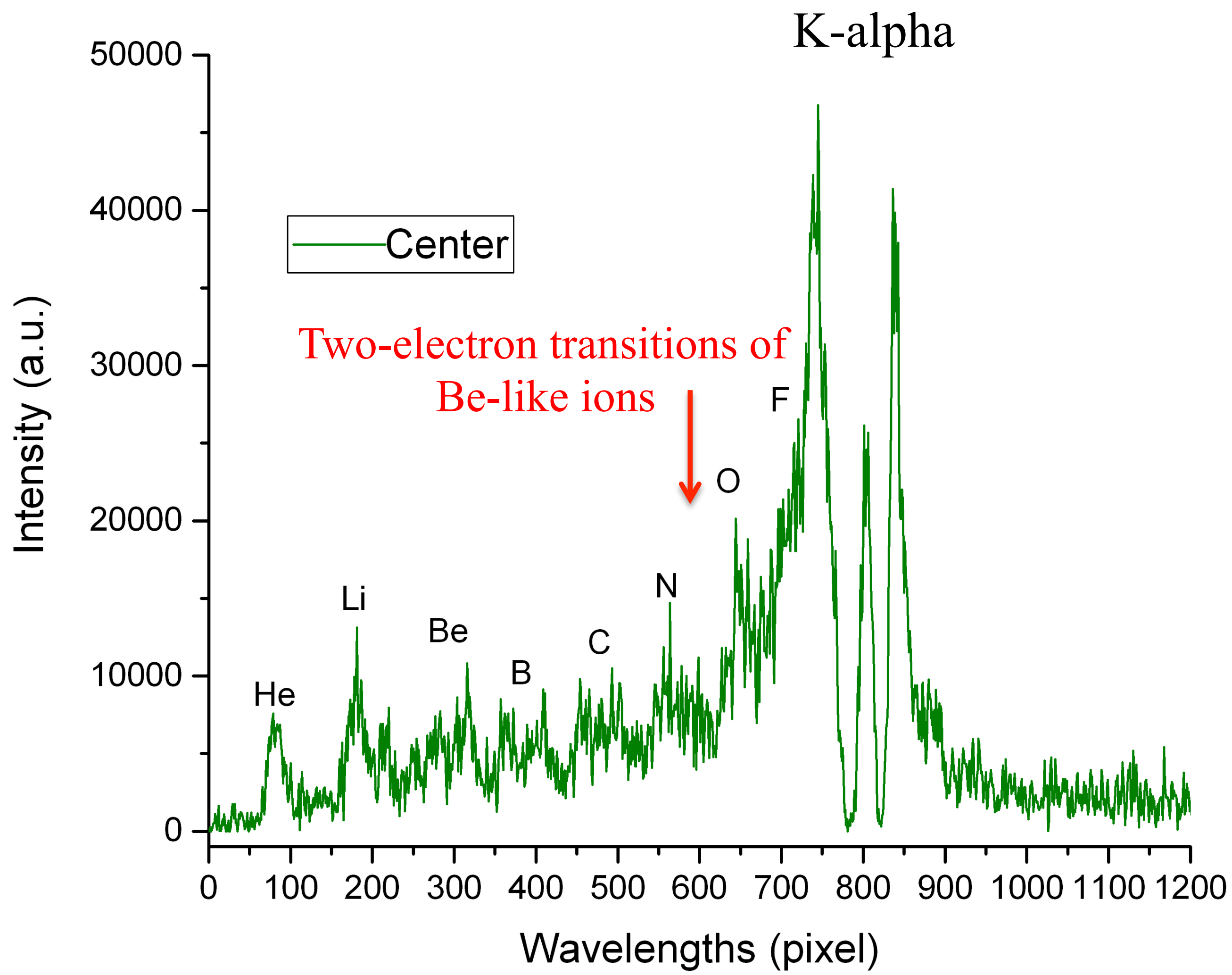


Two-electron transitions of Be-like ions overlap strongly with one electron transitions of N-like ions & O-like ions

Difficult to observe in dense plasma experiment

K-alpha series transitions in plasmas

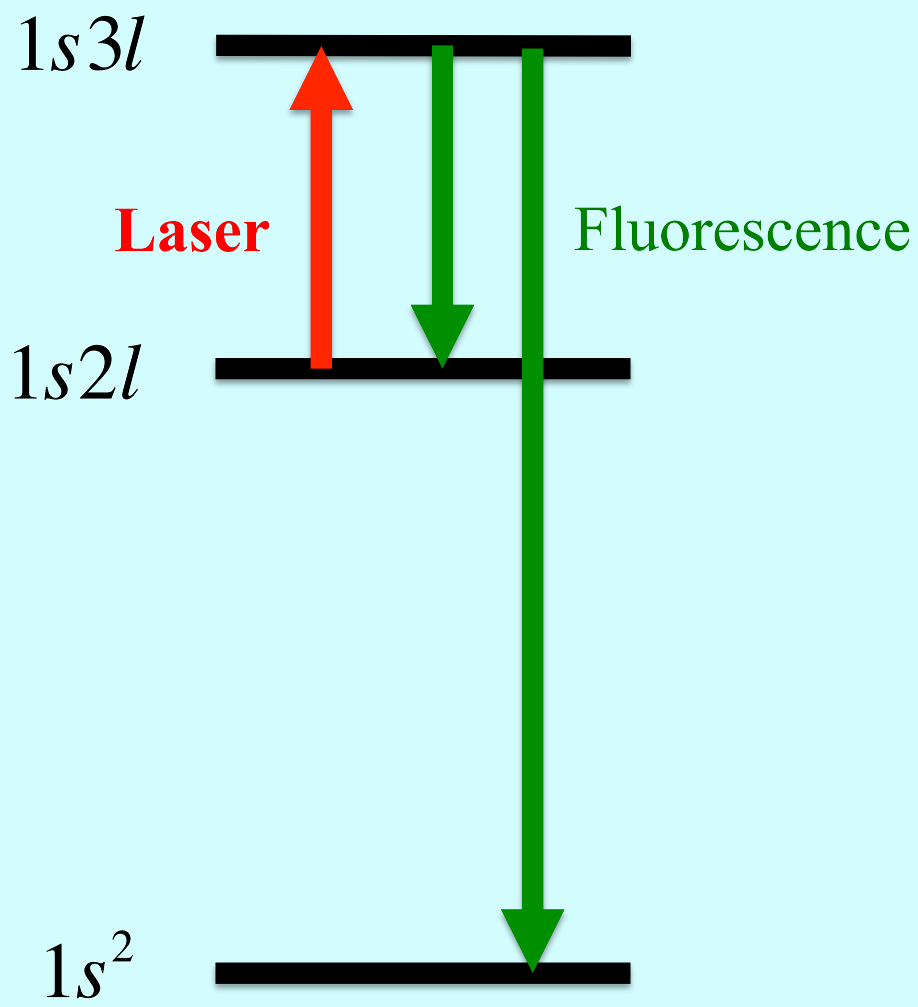


In plasmas, well separated two-electron transitions are usually masked by usual one-electron transitions from lower charge states

IV. Probing matter with XFEL: X-LIF

Laser induced fluorescence LIF in X-ray range: X-LIF

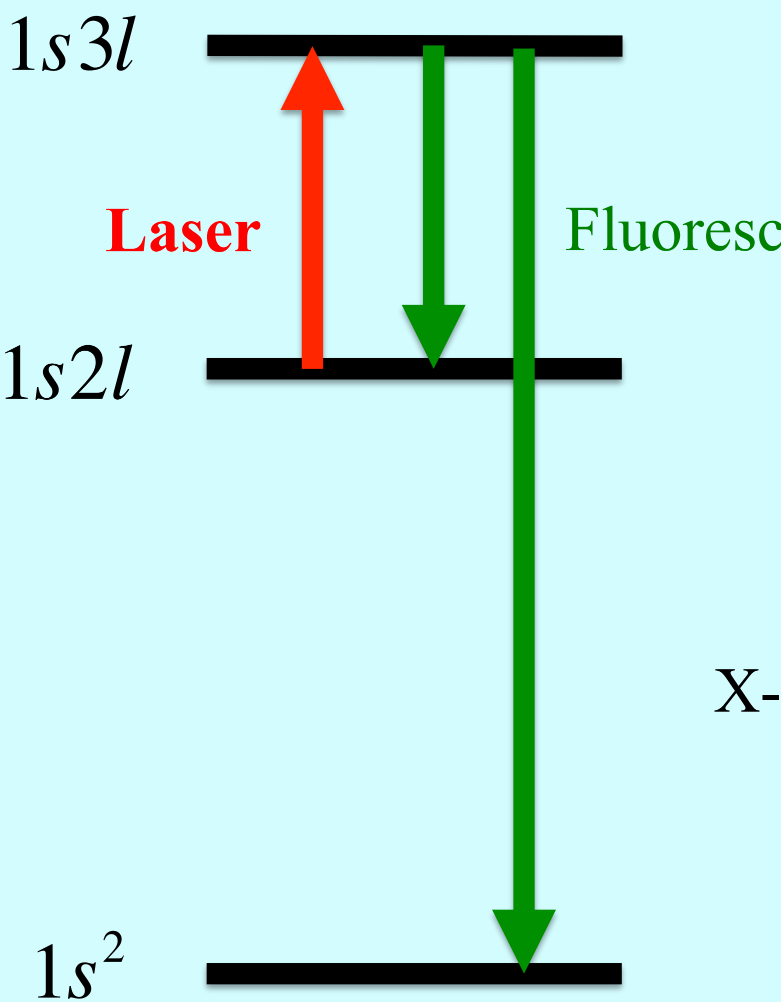
Laser induced fluorescence LIF lead to a "Revolution" in science and applications



- Study of electronic structure of atoms and molecules
- Detection of species
- Flow visualization
- Field effects
- …..

Laser induced fluorescence LIF in X-ray range: X-LIF

Laser induced fluorescence LIF lead to a "Revolution" in science and applications



- Study of electronic structure of atoms and molecules
- Detection of species
- Flow visualization
- Field effects
- …..

Optical lasers: energy interval very limited, few eV

X-ray range:

- All advantages of LIF

  &

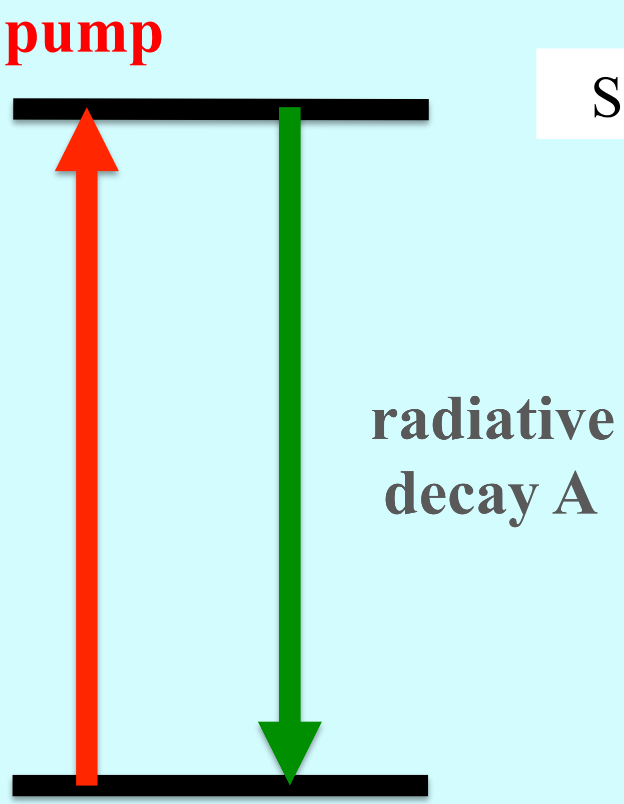
- Inner-shell phenomena
- Isoelectronic sequences
- Ionized atoms
- Matter heating

Why X-LIF is difficult ?

Photo excitation:

the pump must be more effective than spontaneous emission

$$pump\ rate > A$$



Scaling relations of energy and Einstein coefficients

$$I_{XFEL} \propto \Delta E^3$$

$$Energy \propto Z^2$$

$$I_{XFEL} \propto Z^6$$

Very large installations

10^{12} photons in 100 fs !

Synchrotrons will never make it !

X-rays: Synchrotrons & Free Electron X-ray Lasers

XFEL: $10^{13}\ X-ray\ \ photons\ \ in\ \ 10...100\ fs$

Intensities: up to 10^{18} W/cm^2, sub-micrometer focusing

Photon density: $$\tilde{N}_0 \approx \frac{N_{tot,\tau}}{0.76 \cdot A \cdot c \cdot \tau} \approx 6x10^{22}\ \frac{Photons}{cm^3}$$

"solid" photon density

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XFEL brilliance*: 10 orders of magnitude higher than synchrotrons*

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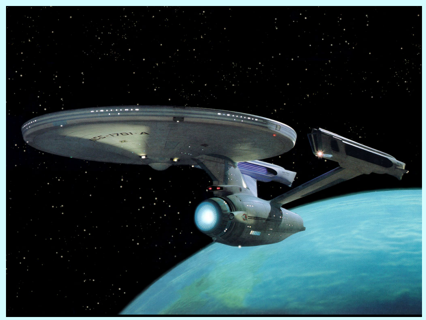
"solid" photon density

***XFEL brilliance**: 10 orders of magnitude higher than synchrotrons*

10 orders of magnitude in velocity



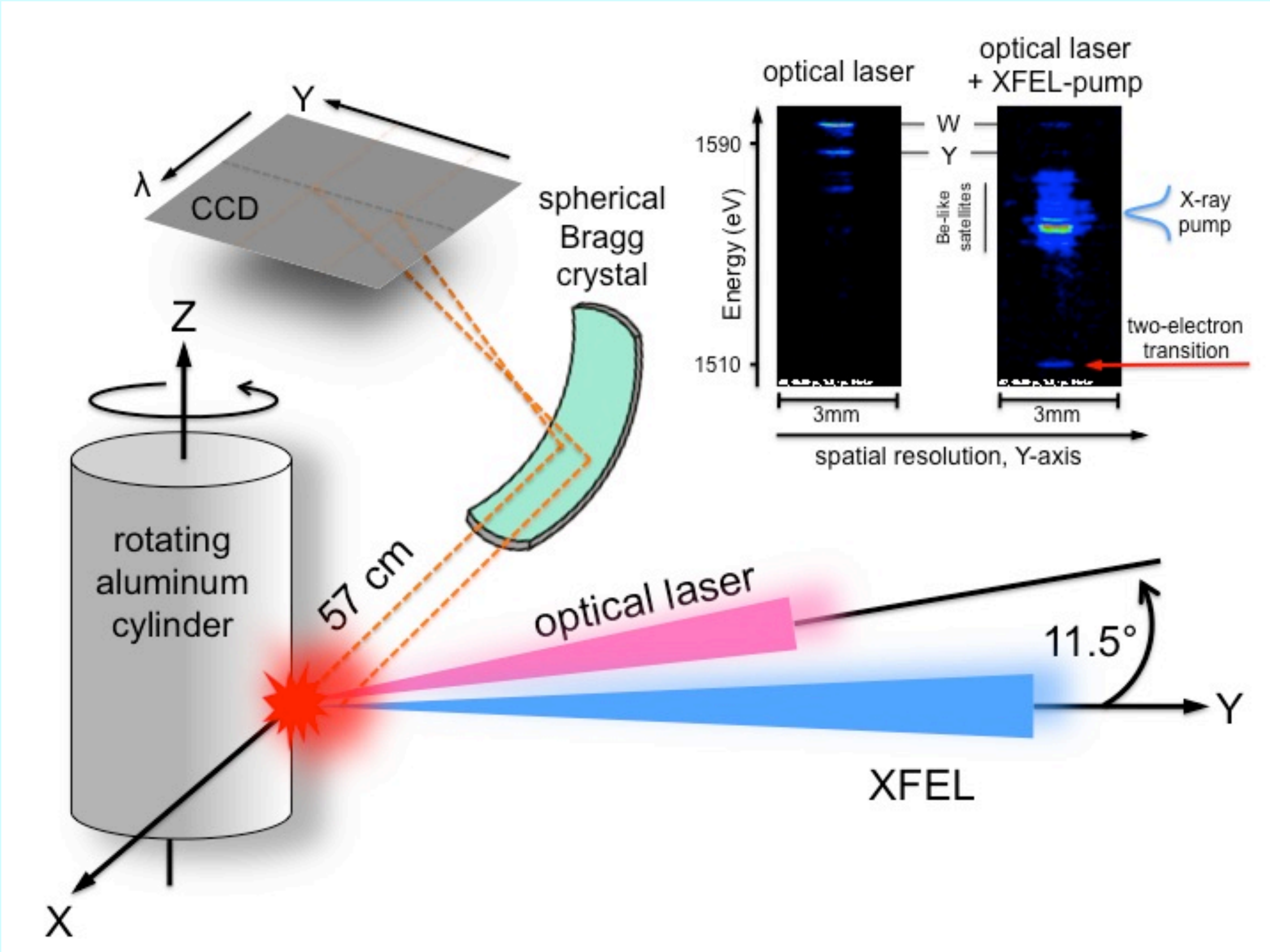
Not just more quick ...but completely different

Synchrotrons: rare "atomic" perturbations...

XFEL: Every atom is concerned New kind of matter samples !

V. Experiment

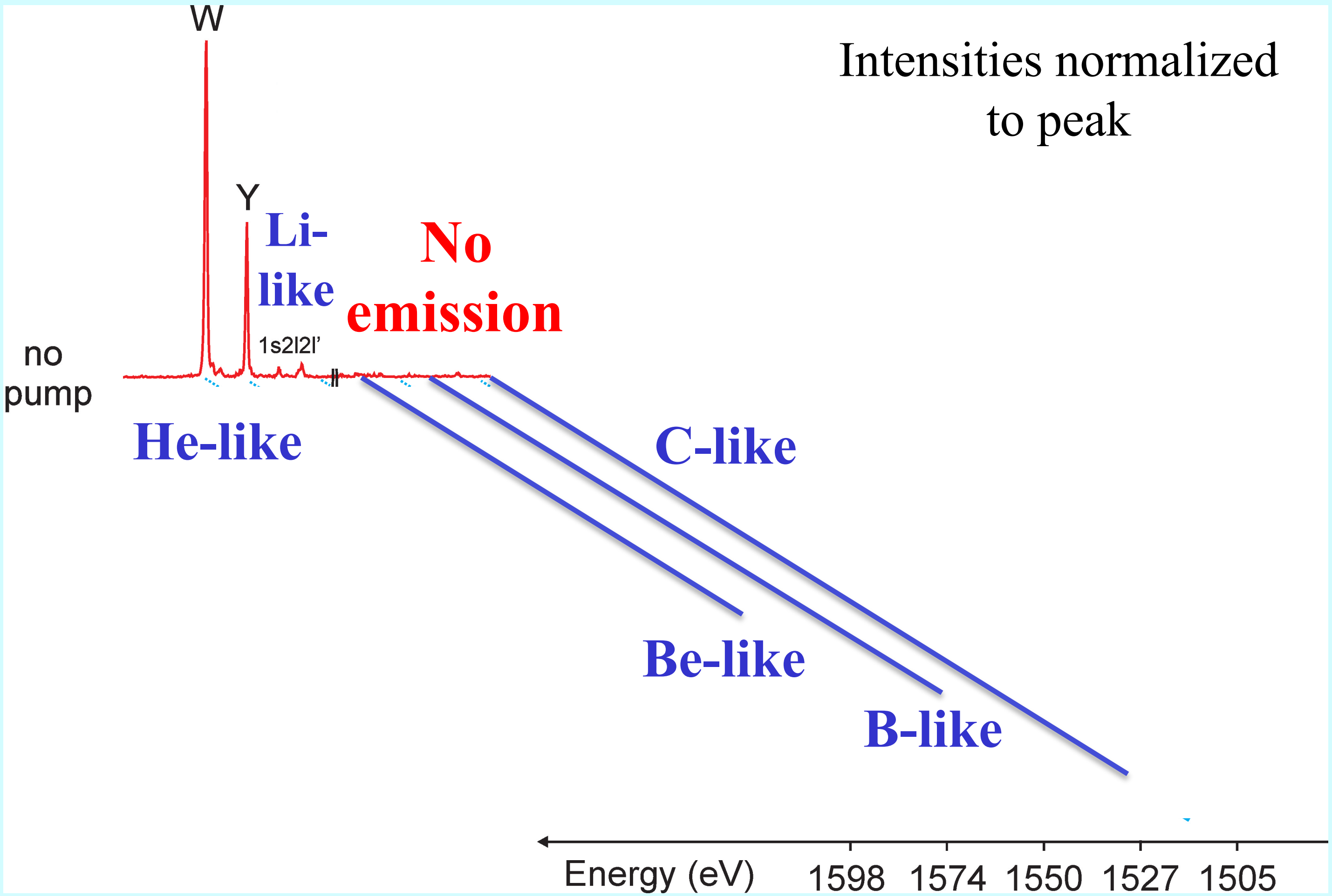
First X-LIF experiment to pump dense plasmas



F.B. Rosmej et al., *Plasma Atomic Physics, Springer 2021*.

Resonance pumping of dense Al-plasma with XFEL

Optical laser only:
No emission from
Be-like,
B-like,
C-like ions



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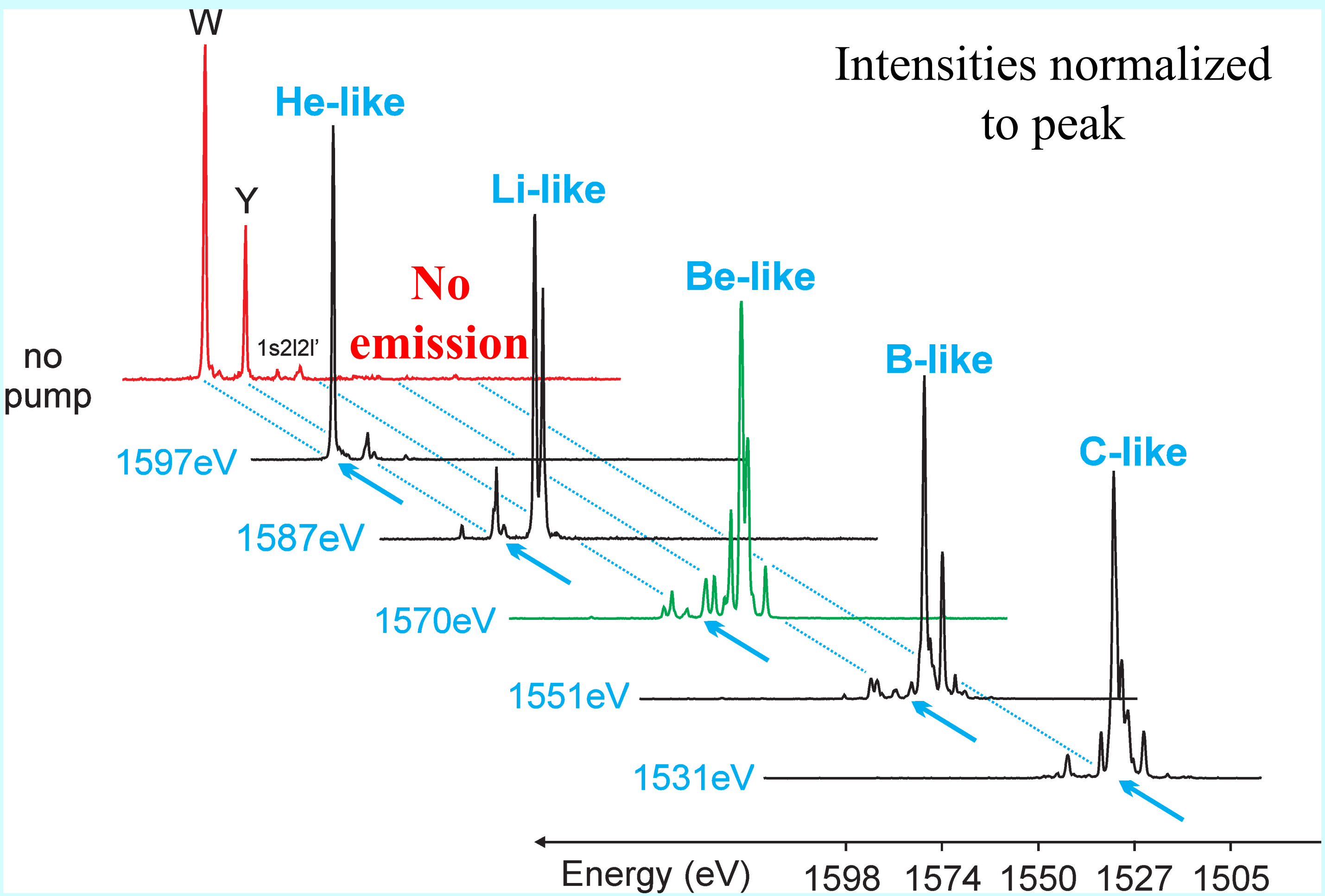
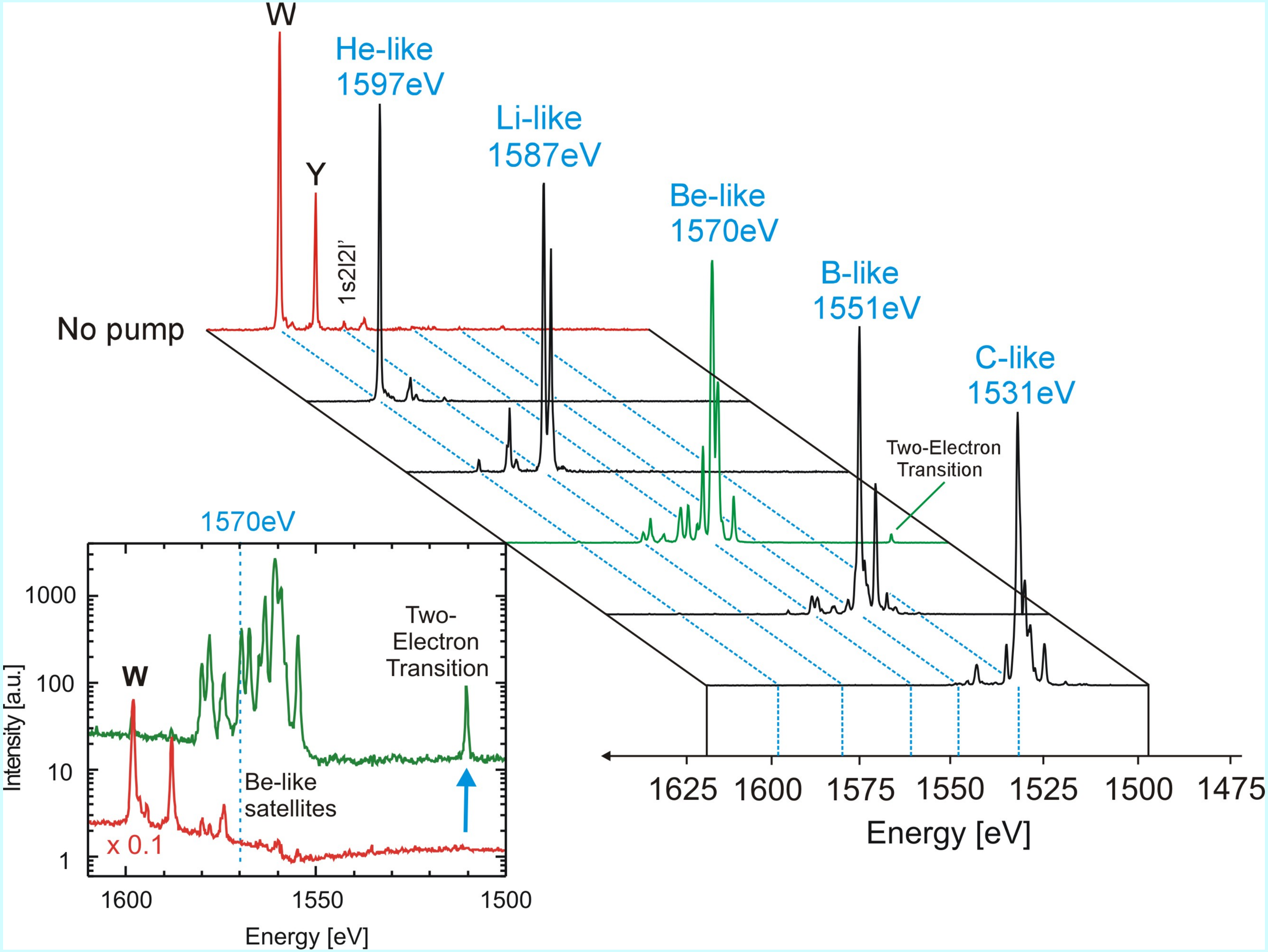


With XFEL pump:
At definite energies
He-like….C-like ions
are pumped and emit
X-ray fluorescence

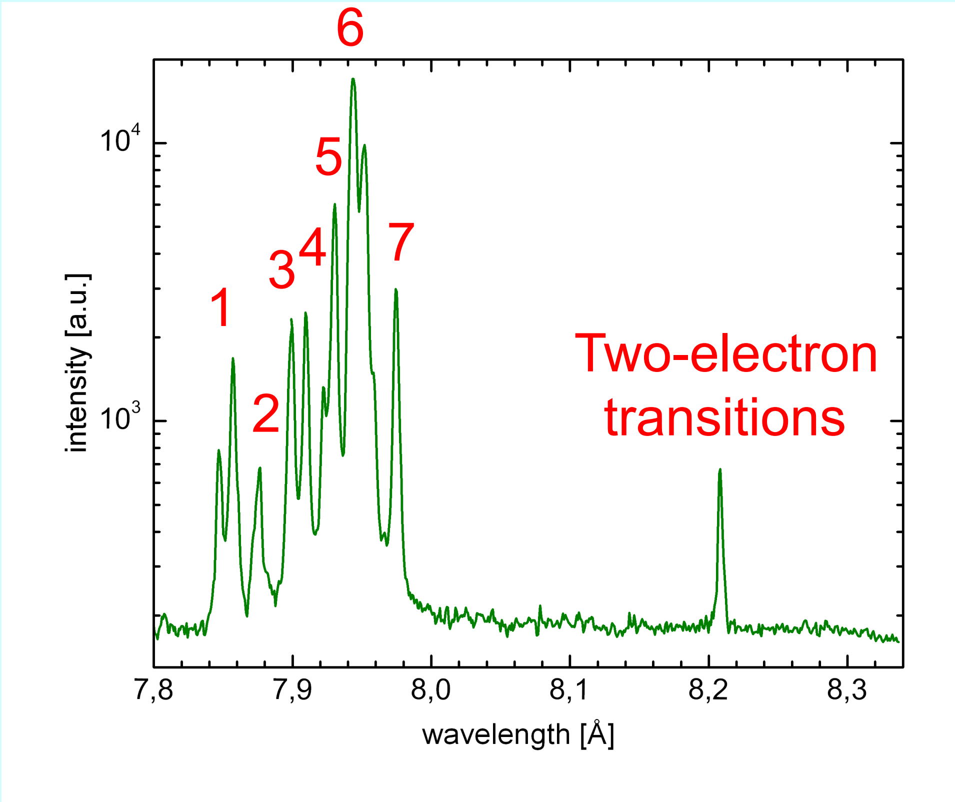
First demonstration of X-LIF at LCLS

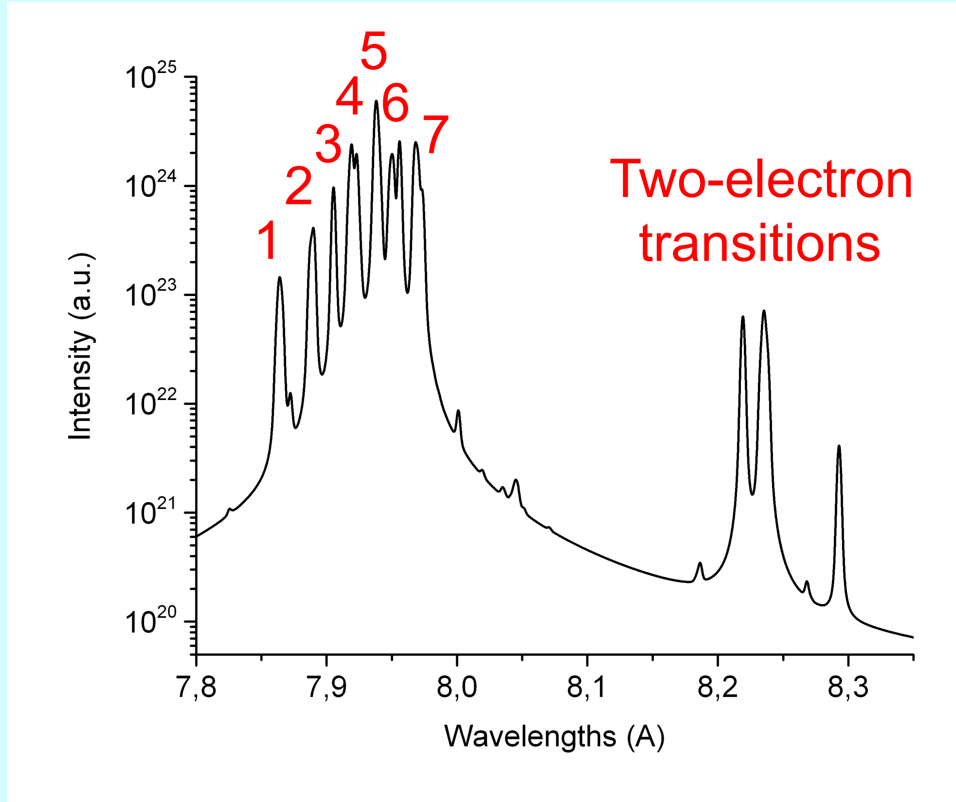
X-LIF: atomic physics studies



VI. First data analysis

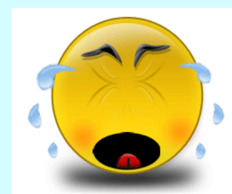
Experiment versus simulation



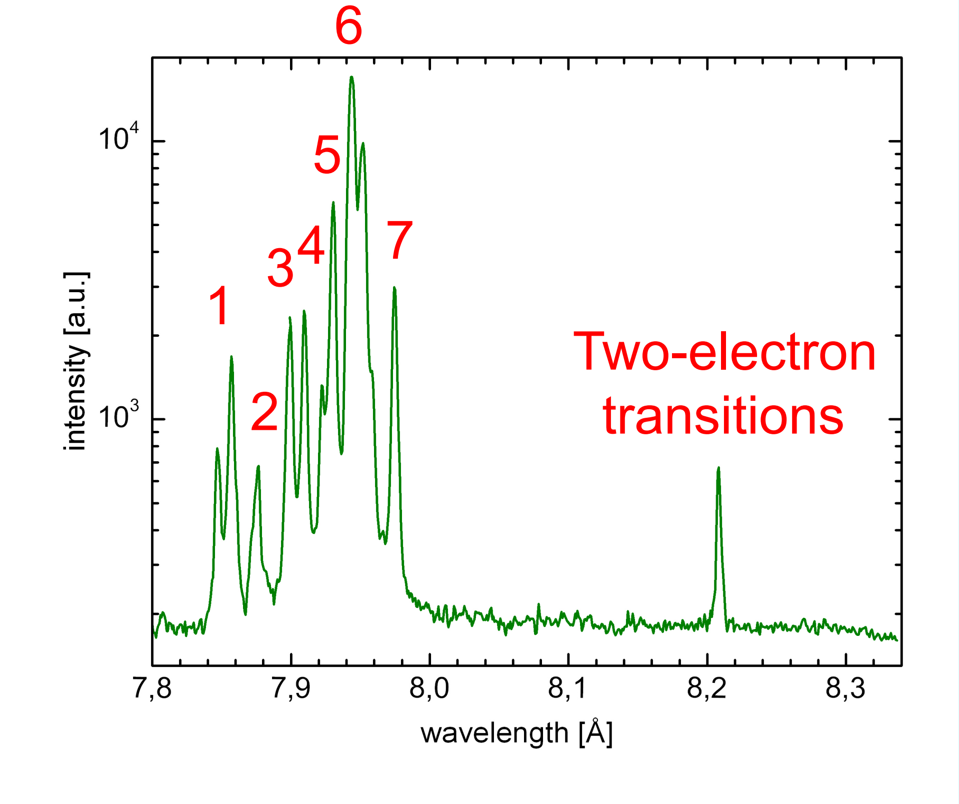


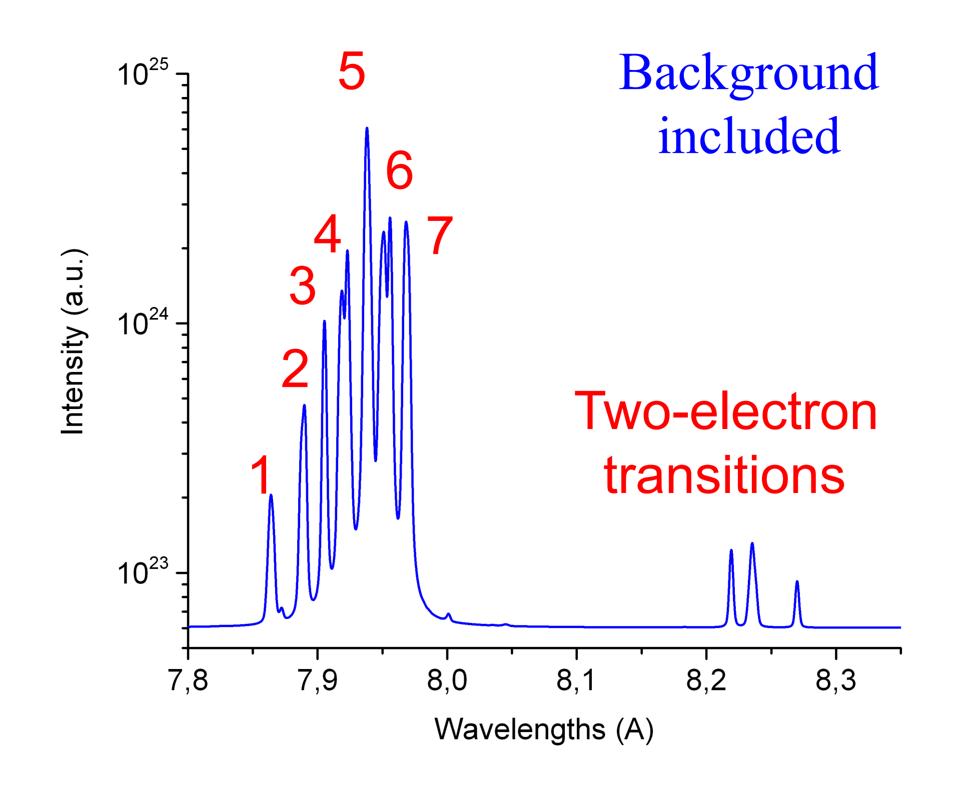
Usual one electron transitions (groups 1-7) in good agreement

Two-electron transitions in bad agreement



Line shapes measured over 2 orders of magnitude





Line shapes measured over 2 orders of magnitude in intensity in dense plasmas

Two-electron transitions in bad agreement

Configuration analysis

Theory: rel. HF with intermediate coupling + configuration interaction

$$1s^2 2p^2\ ^3P_2 \rightarrow 1s^1 2s^2 2p^1\ ^3P_2 : 8.2352\,A$$

$$1s^2 2p^2\ ^1D_2 \rightarrow 1s^1 2s^2 2p^1\ ^1P_1 : 8.2191\,A$$

Experiment: high-resolution X-ray spectroscopy+reference lines

$$1s^2 2p^2\ LSJ \rightarrow 1s^1 2s^2 2p^1\ LSJ : \left(8.208 \pm 0.0005\right) A$$

Complex calibration procedure: O. Renner

Very bad agreement in wavelengths and number of transitions !

Comparison with different methods

MCDF:

$$1s^2 2p^2 \ {}^1D_2 \rightarrow 1s^1 2s^2 2p^1 \ {}^1P_1 : 8.2298\,A$$

FAC:

$$1s^2 2p^2 \ {}^1D_2 \rightarrow 1s^1 2s^2 2p^1 \ {}^1P_1 : 8.2280\,A$$

MZ:

$$1s^2 2p^2 \ {}^1D_2 \rightarrow 1s^1 2s^2 2p^1 \ {}^1P_1 : 8.2205\,A$$

Experiment: high-resolution X-ray spectroscopy + reference lines

$$1s^2 2p^2 \ LSJ \rightarrow 1s^1 2s^2 2p^1 \ LSJ : \left(8.208 \pm 0.0005\right) A$$

VII. Conclusion and Outlook

• Line profiles from complex configurations are of interest for energy transport that involves all bound and free states of atoms/ions

• Many overlapping transitions make analysis of single transitions from complex configurations difficult

• Two-electron transitions are located well outside the bunch of usual transitions; the number of transitions turns out to be rather small

• In usual plasmas, two-electron transitions are masked by “usual” transitions from lower charge states

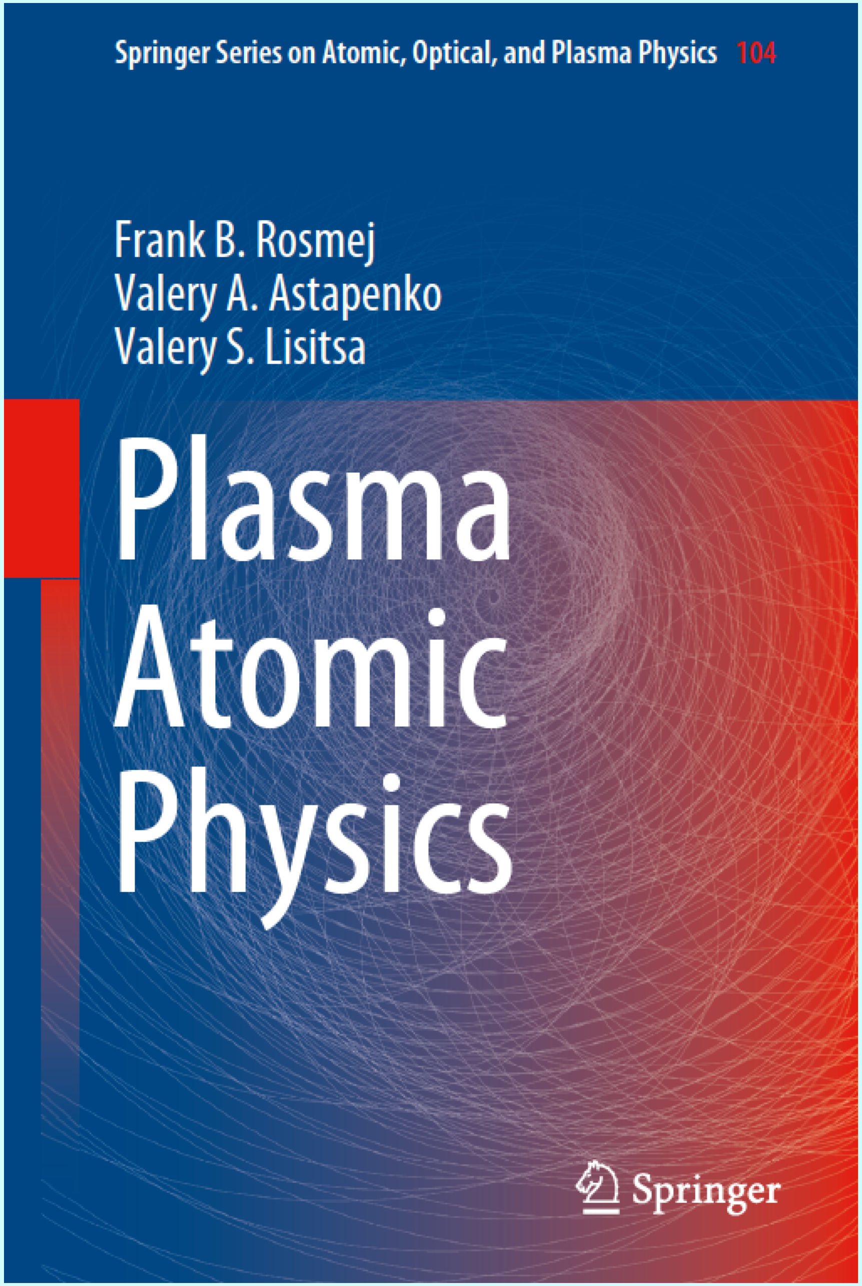
• LIF in X-ray spectral range may select transitions of complex configurations in plasmas from one charge state only

• Successful demonstrations of X-LIF in dense plasmas

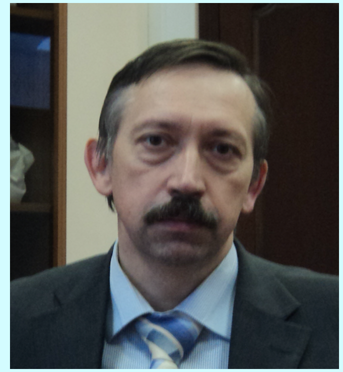
• Line shapes are measured over 2 orders of magnitude in intensity with excellent signal/noise ratio in dense plasmas

• Two-electron transitions are in bad agreement with theory

.... spectroscopy...



Frank Rosmej



Valery Astapenko

Valery Lisitsa

ISBN 978-3-030-05966-8, Heidelberg (2021)

Configuration interaction

No radiative decay from $1s^1 2s^2 \; {}^2S_{1/2} \rightarrow \ldots.$

Configuration interaction:

$$\Psi\left(1s^1 2s^2\right) = \alpha \cdot \Psi^{pure}\left(1s^1 2s^2\right) + \beta \cdot \Psi^{pure}\left(1s^1 2p^2\right)$$

Radiative decay:

$$A\left(1s^1 2s^2 \rightarrow 1s^2 2p\right) \propto \beta^2 \cdot \left|\left\langle \Psi^{pure}\left(1s^1 2p^2\right) \middle| r \middle| \Psi^{pure}\left(1s^2 2p^1\right)\right\rangle\right|^2$$

Mixed wavefunctions

$1s^2 2p^2 \ {}^1D_2 \rightarrow 1s^1 2s^2 2p^1 \ {}^1P_1 :$

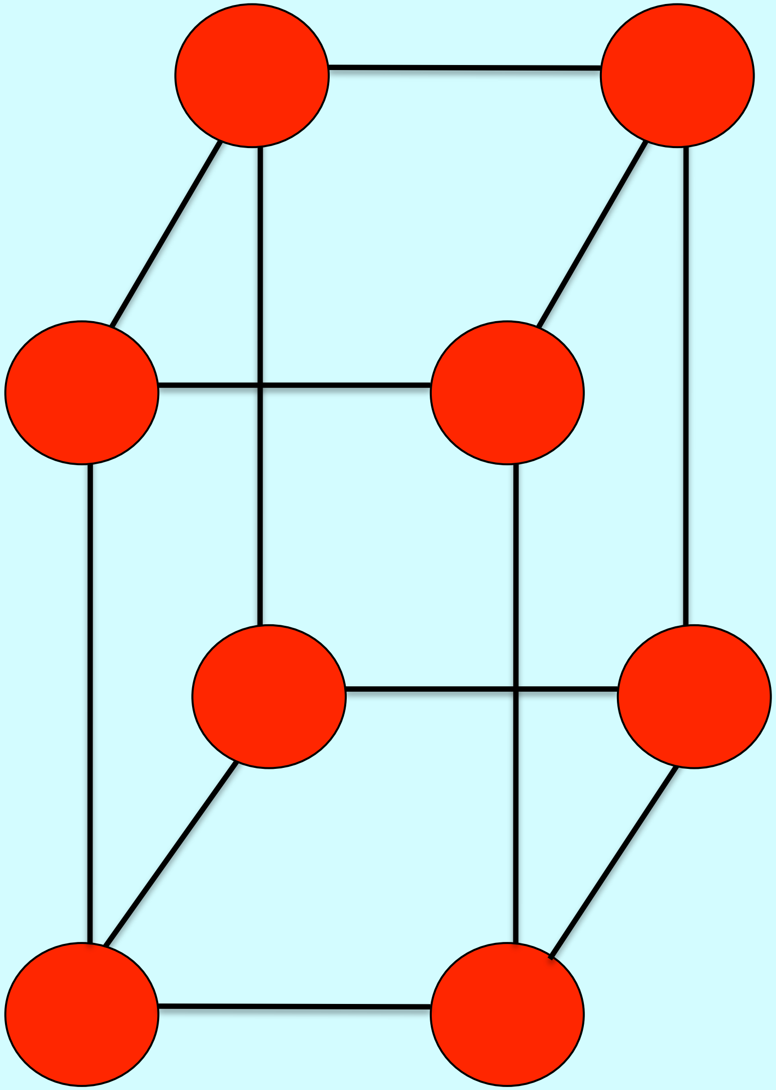
$$\Psi\left(1s^1 2s^2 2p^1 \ {}^1P_1\right) \approx 0.97064 \cdot \Psi^{pure}\left(1s^1 2s^2 2p^1 \ {}^1P_1\right) +$$
$$0.23671 \cdot \Psi^{pure}\left(1s^1 2p^3 \ {}^1P_1\right) + ...$$

$$\Psi\left(1s^2 2p^2 \ {}^1D_2\right) \approx 0.999865 \cdot \Psi^{pure}\left(1s^2 2p^2 \ {}^1D_2\right) +$$
$$0.00683 \cdot \Psi^{pure}\left(1s^2 2p^2 \ {}^3P_2\right) + ...$$

Info configuration interaction $2s^2$+$2p^2$:

$$\Psi\left(1s^2 2p^2 \ {}^1S_0\right) \approx 0.96972 \cdot \Psi^{pure}\left(1s^2 2p^2 \ {}^1S_0\right) +$$
$$0.24246 \cdot \Psi^{pure}\left(1s^2 2s^2 \ {}^1S_0\right) + ...$$

XFEL interaction with matter



XFEL

volumetric photoionization
of internal shells

$$K^2L^8M^3 + \hbar\omega_{XFEL} \rightarrow K^1L^8M^3 + e_{photo}$$

Heating

More than 1 photon per atom !

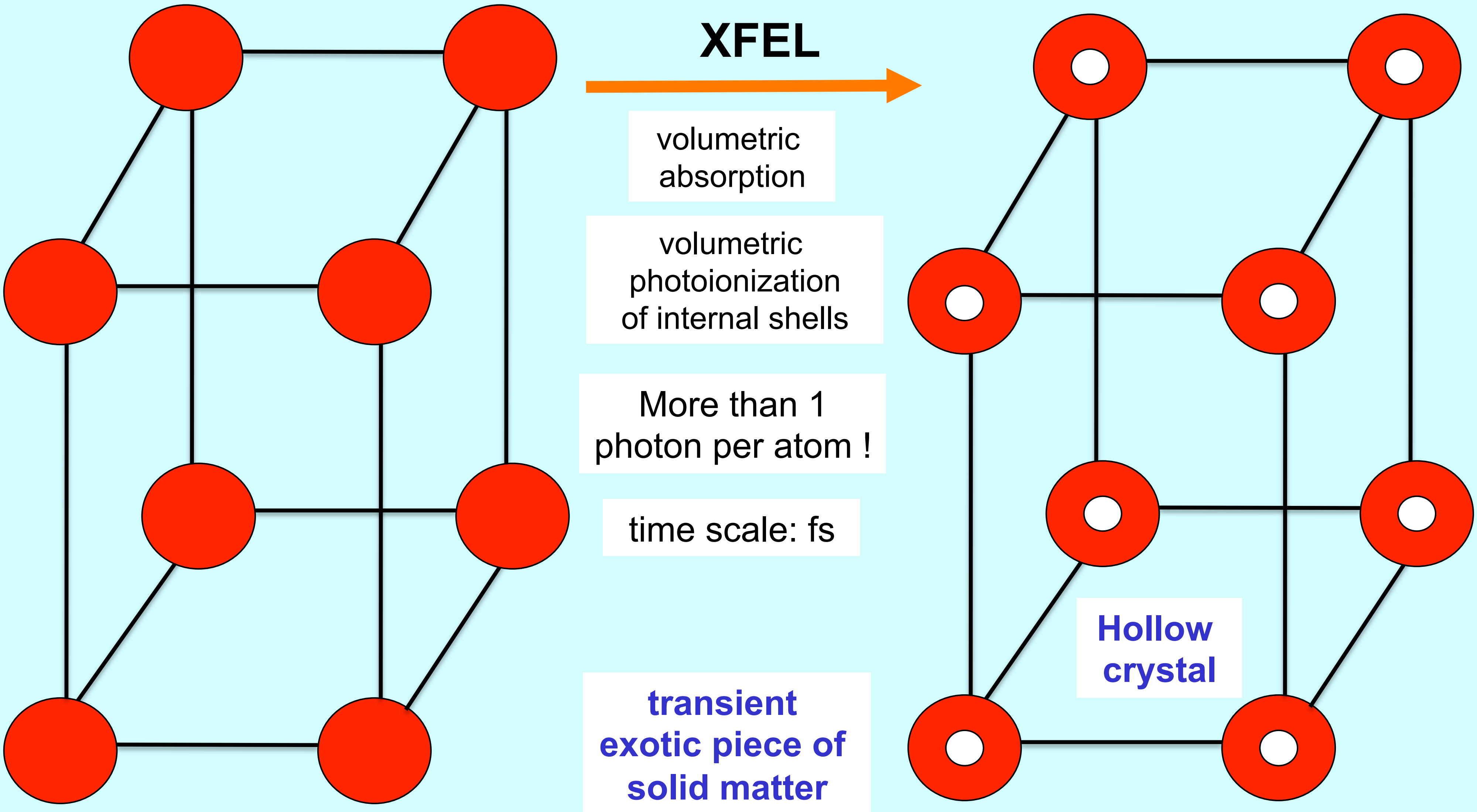
$$E_{photo} = E_{XFEL} - E_K = 0 \ldots\ldots keV$$

Time scale

Auger effect, some 10 fs

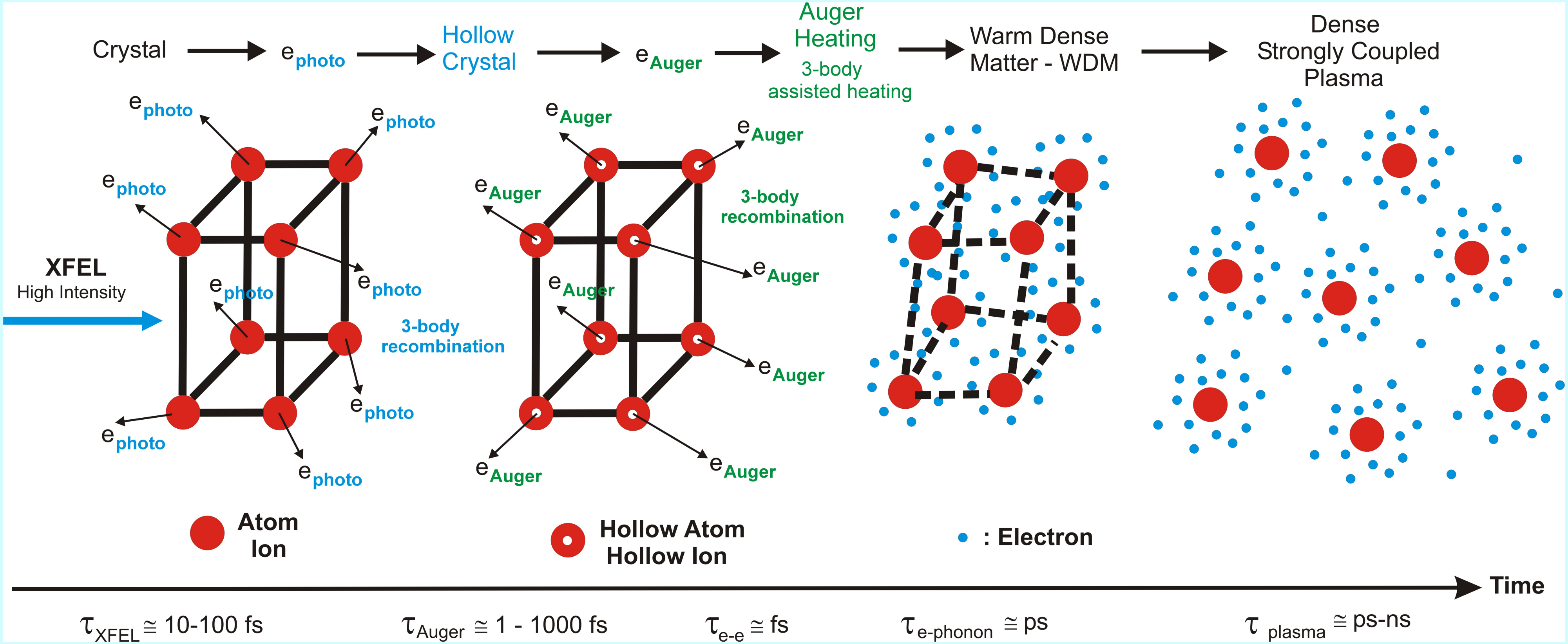
$$K^1L^8M^3 \rightarrow K^2L^6M^3 + e_{Auger}$$

XFEL interaction with matter



F.B. Rosmej et al., *Plasma Atomic Physics*, Springer 2021

The cartoon of XFEL interaction with matter



F.B. Rosmej, V.A. Astapenko, V.S. Lisitsa, *Plasma Atomic Physics,* Springer 2021

Release of potential energy

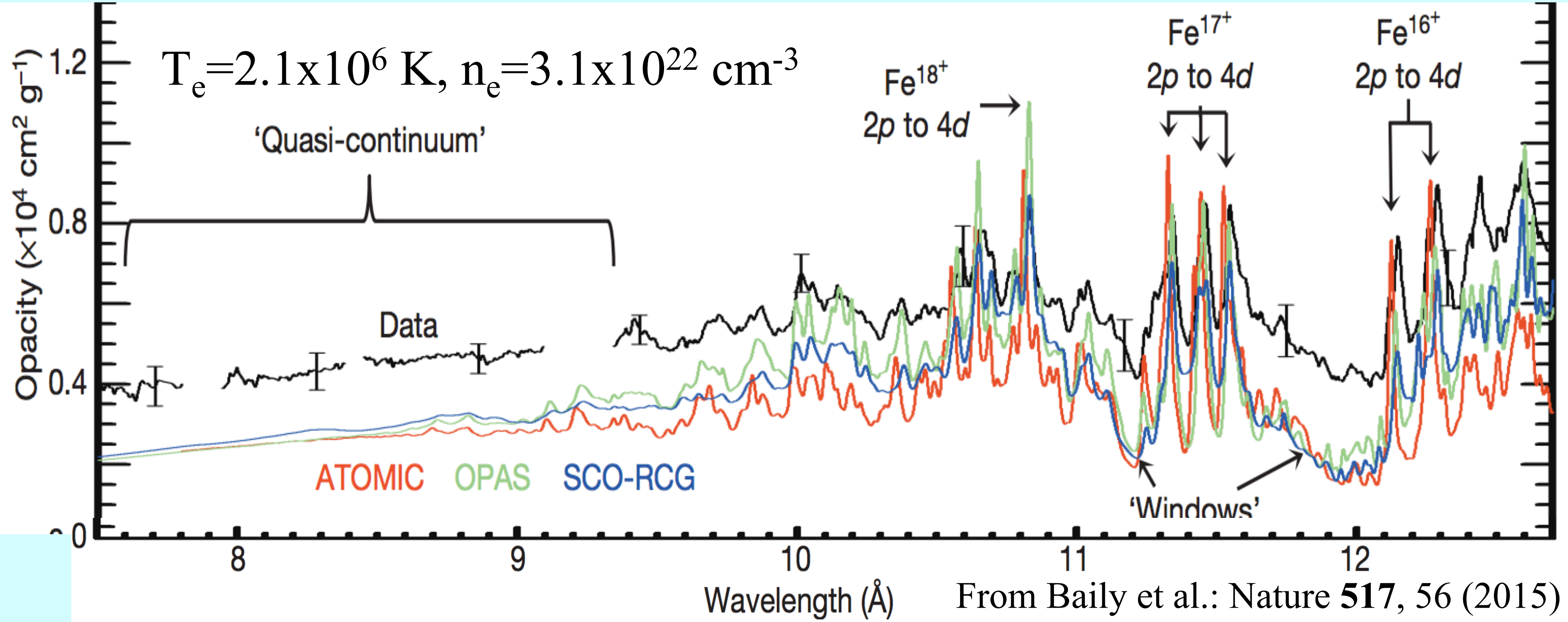
Time dependent evolution......

Equivalence: The XFEL removes so much and so *quick* "matter" that the whole structure becomes instable and is destroyed *after* a certain time

Annex

Laboratory measurements: Solar opacity has a problem ?

Fe accounts for about 1/4 of the solar opacity



From Baily et al.: Nature **517**, 56 (2015)

Observed continuum stronger than predicted

Spectral windows more filled

Bound-bound emission less pronounced

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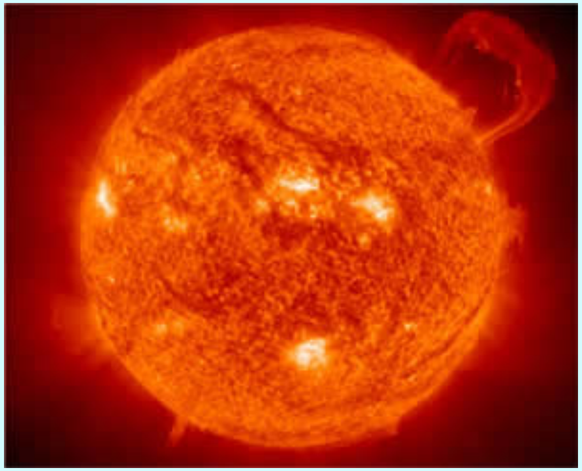
Solar opacity problem



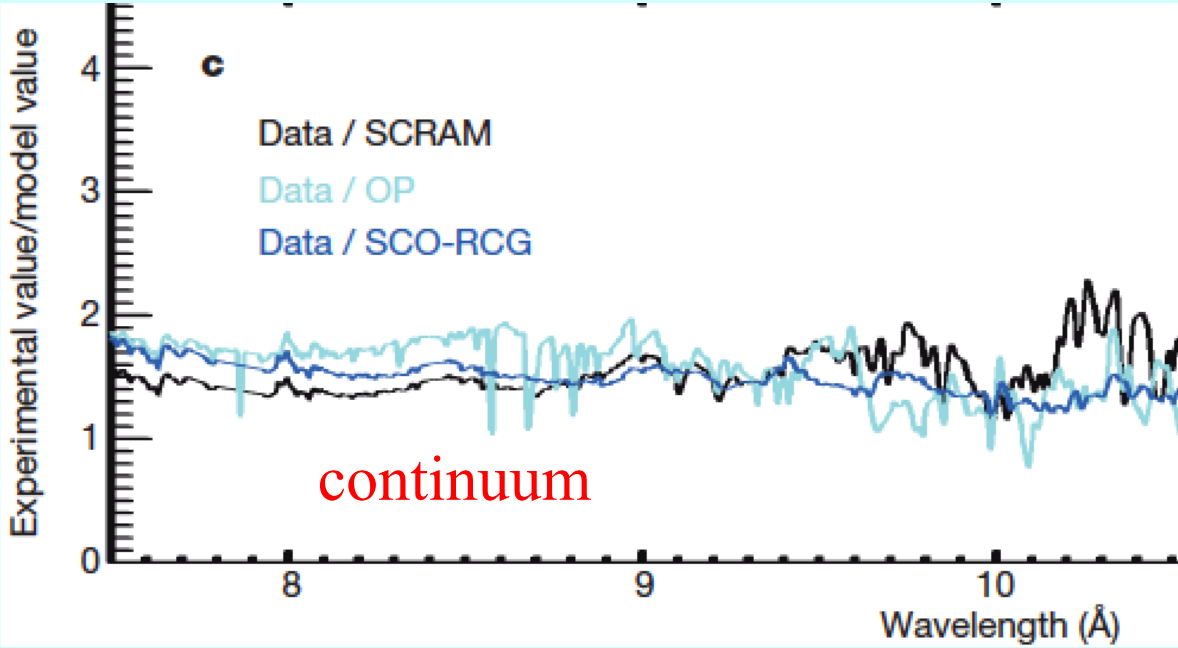
Photosphere spectral analysis:
revised element abundances of C, N, O

Revised abundances disagree with helioseismic observations (e.g. sun quake), that determine the internal solar structure using acoustic oscillations

This problem *could* be resolved, if the true mean opacity would be higher by about 15 %

Measurements of the opacity in a laboratory experiment of Bailey et al. [Nature **517**, 56 (2015)] indicate opacities up to 4 times higher than predicted …..but no consistent explanation/theory could be given…..

Opacity data / simulations



From Baily et al.: Nature **517**, 56 (2015)

Observed continuum stronger than predicted

Spectral windows more filled

Is our general understanding of opacity incomplete ?