

Atomic Computations at Four Hands ---

Dielectronic recombination studies for GSI/FAIR

Stephan Fritzsche, 8th October 2026



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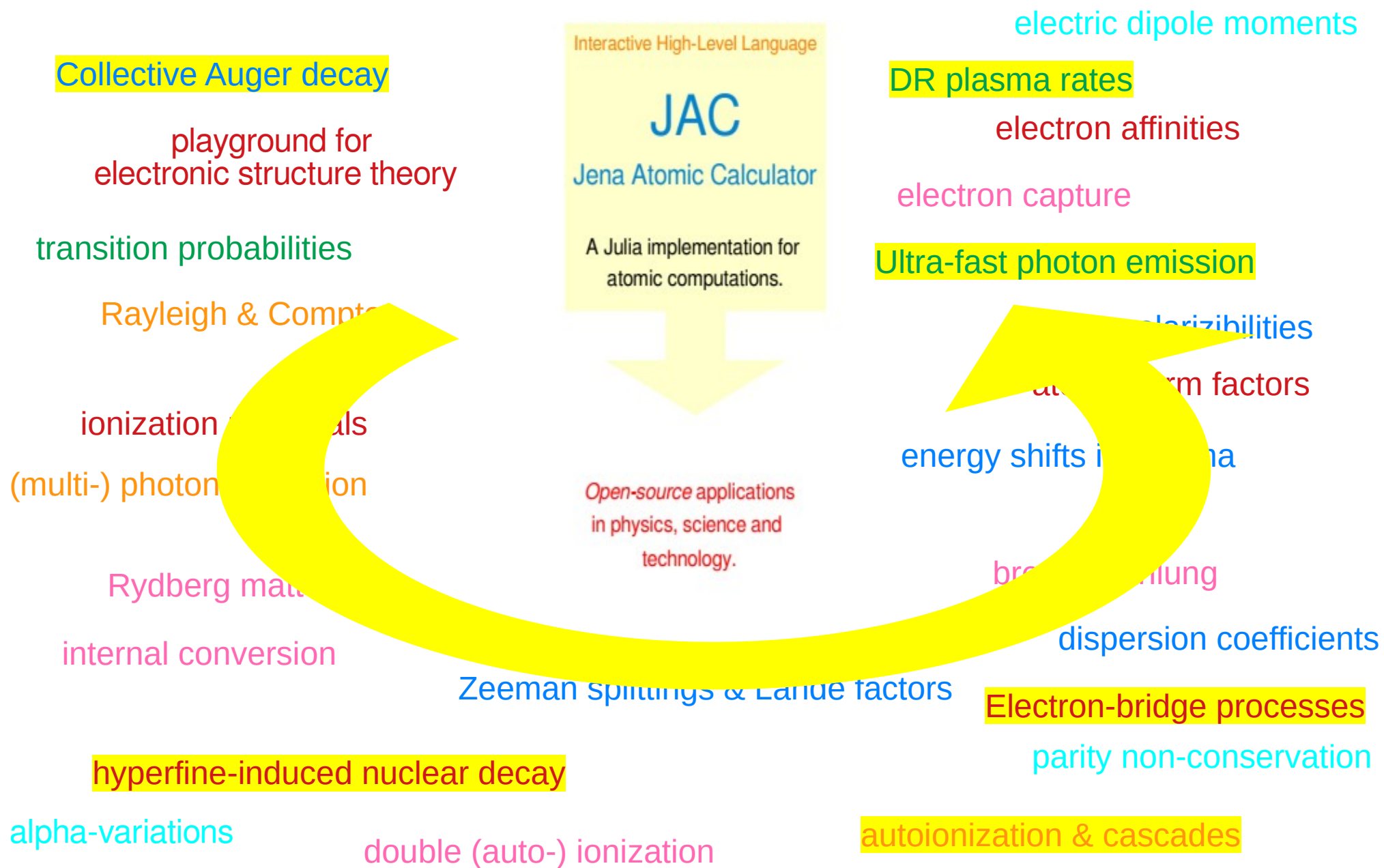
Jena Atomic Calculator

(Fully) relativistic atomic structure code
with focus upon continuum processes & cascades;
for (almost) all shell structures and elements;
user-friendly, open & features on demand.

- 🍷 Open, modular
- 🍷 Written from scratch in Julia
- 🍷 SF, CPC **240**, 1 (2019)
- 🍷 One person, one codebase,
roughly a decade
- 🍷 ...until four months ago



Community platform for atomic computations

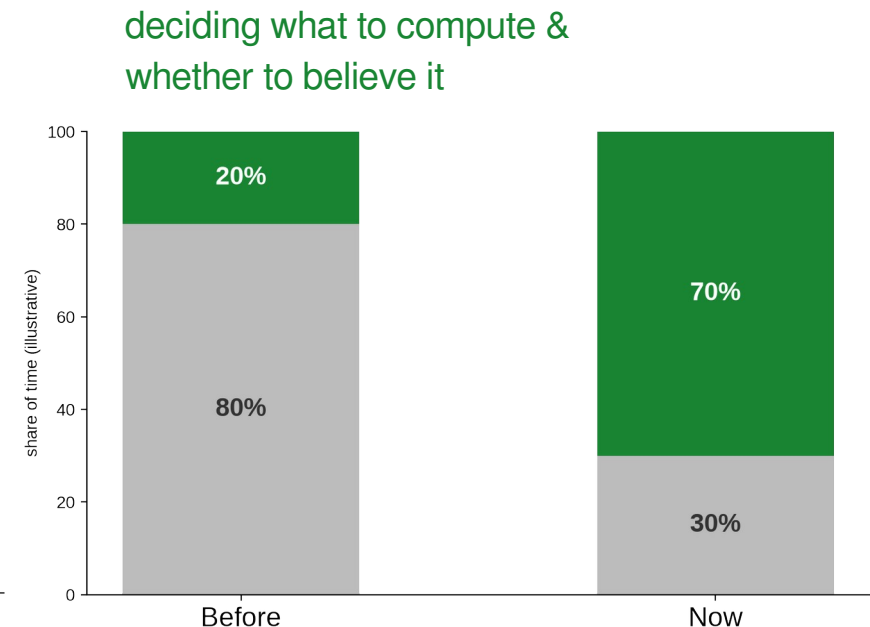
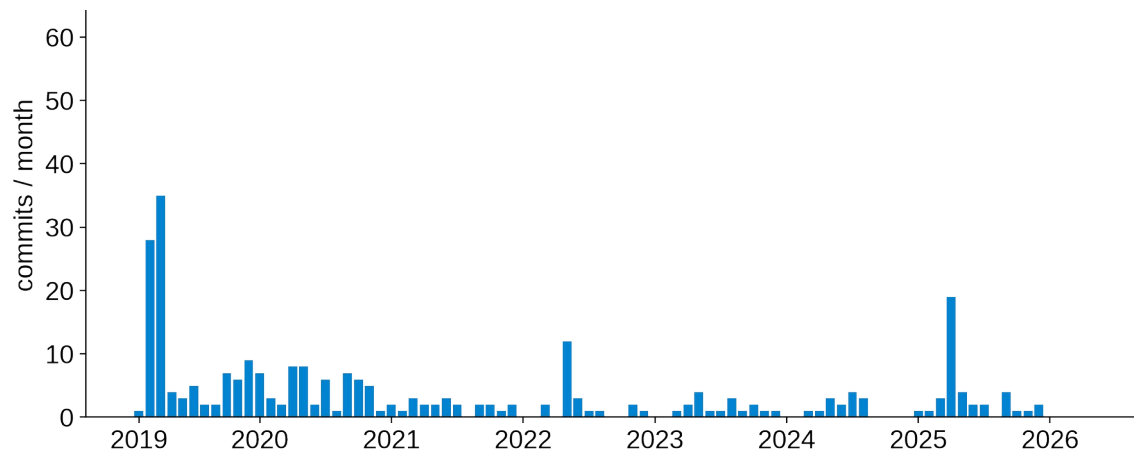


Ten years, one keyboard

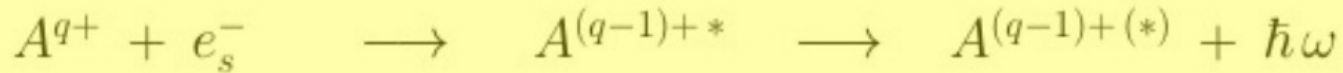
... now with a second pairs of hands by Claude

A co-worker at the same keyboard:

- Not asked for answers — asked to work alongside
- Code, yes — but also: re-deriving formulas from the literature
- Cross-checking independent routes, rebuilding regression tests
- Claude (Anthropic), used via Claude Code, 2025–2026
- Now: most hours go into deciding what's worth computing, and whether the answer is believable



Dielectronic recombination (DR) calculations



Example: Calculation of the **Pb⁷⁸⁺** (**Z=82**) **1s² 2s2p** [19lj] DR resonance strengths

```
> iConfigs = [Configuration("1s^2 2s^2")]
   eConfigs = [Configuration("1s^2 2s 2p")]
   fConfigs = [Configuration("1s^2 2s^2 2p")]
   addShells = Basics.generateShellList(19, 19, [l for l=0:18])
   toShells = Basics.generateShellList(2, 4, [0, 1, 2, 3, 4, 5, 6, 7])
   finalConfigs = Basics.generateConfigurations(fConfigs, [Shell("2s"), Shell("2p")], toShells)
   intermConfigs = Basics.generateConfigurationsWithAdditionalElectron(eConfigs, addShells)
   intermConfigs = Basics.merge(intermConfigs, finalConfigs)
   drSettings = DielectronicRecombination.Settings(..., multipoles = [E1], printBefore = true,
                                                    gauges = [UseBabushkin], electronEnergyShift = 1.2, calcOnlyPassages=true,
                                                    corrections = AbstractCorrections[HydrogenicCorrections(18,missing,missing),
                                                                 ResonanceWindowCorrection(0., 1.0)])

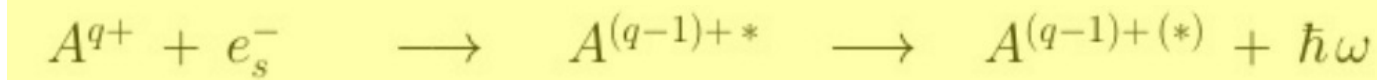
> comp = Atomic.Computation(..., name="Low-lying DR resonances for Pb^78+", grid=grid,
                             nuclearModel=Nuclear.Model(82.0),
                             initialConfigs = iConfigs, intermediateConfigs = intermConfigs, finalConfigs = finalConfigs,
                             processSettings = drSettings )

> results = perform(comp; output=true)
```

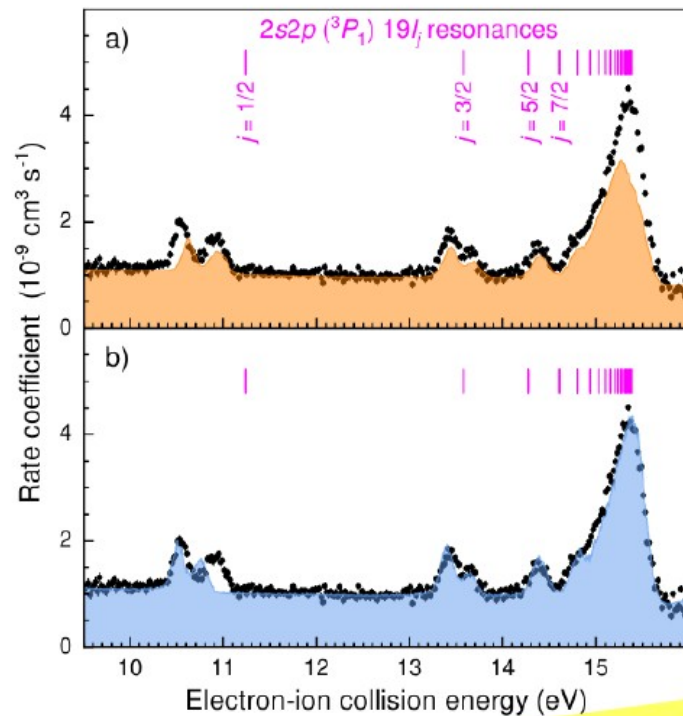


pre-AI

Dielectronic recombination (DR) calculations



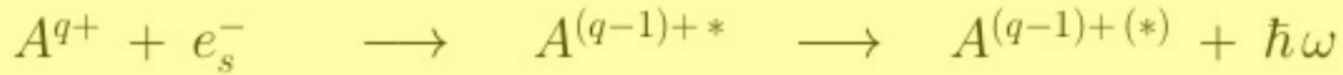
Example: Calculation of the Pb^{78+} ($Z=82$) $1s^2 2s2p$ [19]_lj DR resonance strengths



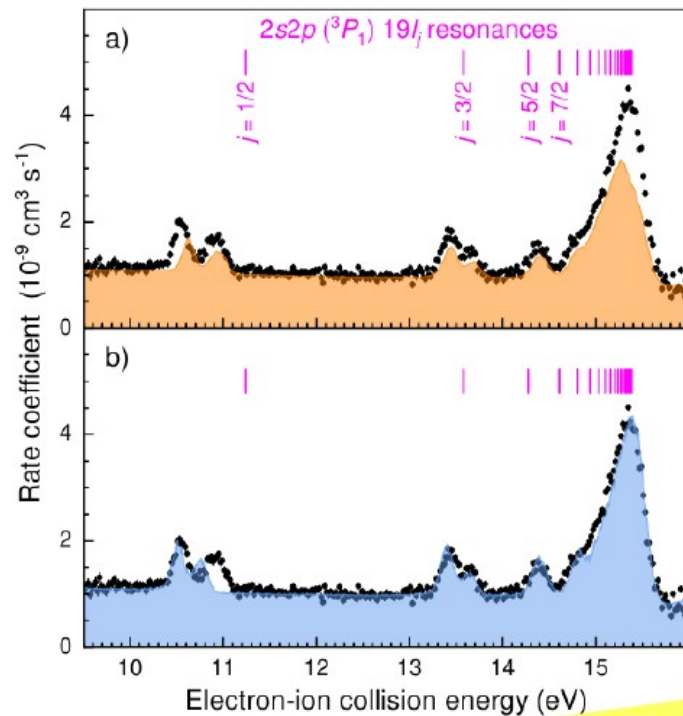
„autostructure“ calculations



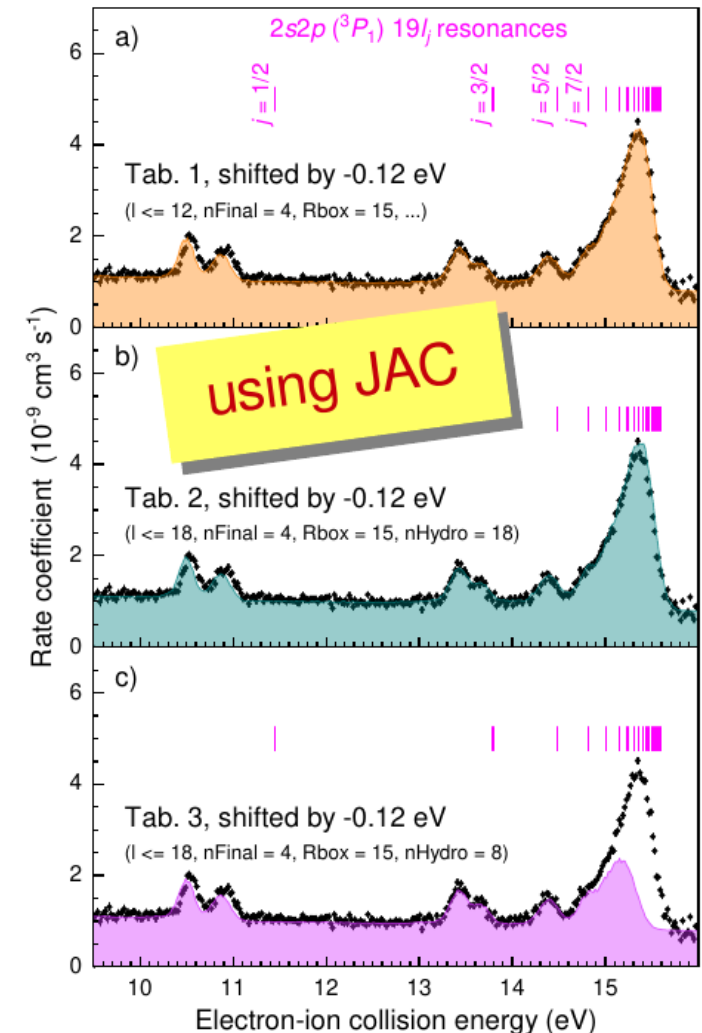
Dielectronic recombination (DR) calculations



Example: Calculation of the Pb^{78+} ($Z=82$) $1s^2 2s2p$ [19]_{*l*} DR resonance strengths



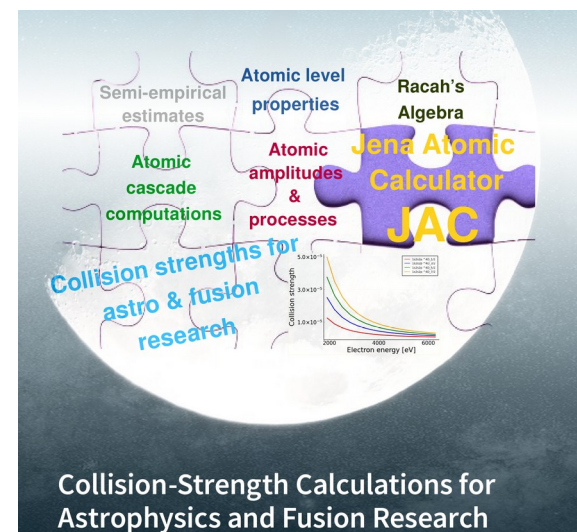
„autostructure“ calculations



Customer requests to atomic & collision physics

- **Astro physics:** Help in interpretation of optical and x-ray spectra
plasma rate coefficients of various kind (PI, RR, DR, EIE, EII, EIMI, ...)
Saha-Boltzmann equilibrium; neutron-star merger; non-LTE,
- **Plasma physics:** intensity ratios, plasma diagnostics, line shifts, ...
- **UV/EUV light sources:** lithography; cascade processes
- **Atomic clocks:** light shifts, magic frequencies, BBR, weak influences, ...
- **Nuclear physics:** Isotope shifts and hyperfine structures
- **Atomic spectroscopy:** (super-) heavy elements, actinides, transactinides
- **Inner-shell physics:** Nonradiative (inner-shell) transitions and autoionization
- **Ion recombination and photon emission**
- **Multi-photon & strong-field processes**
- ...
- „Complete experiments“
- Parity nonconservation (PNC)
- Search for electric dipole moments

*Remember:
e-p & e-e interactions!
nuclear moments ?*

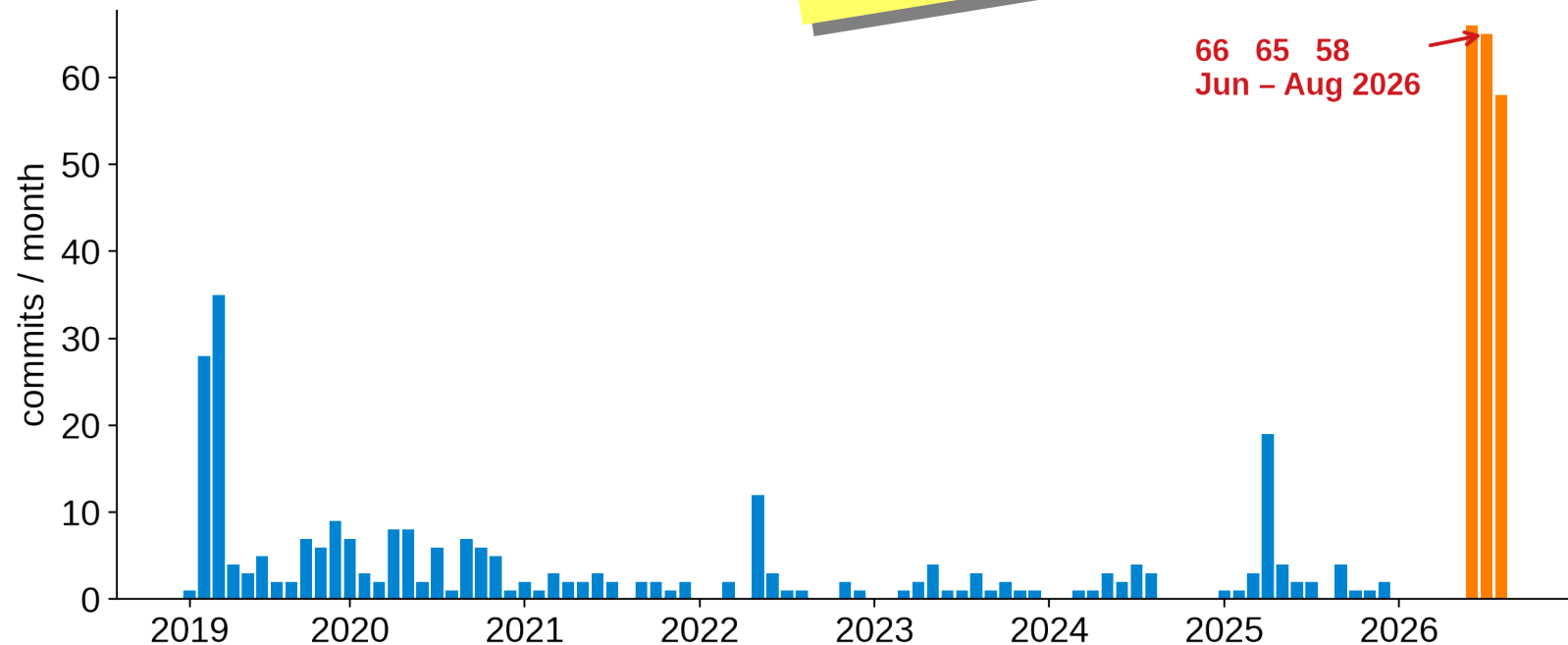


That a tireless co-worker is actually good at

... for a community that lives on its data

- Re-deriving a formula from the literature, start to finish, without cutting the derivation short.
- Running the same check across every module it touches, not just the one you asked about.
- Rebuilding a test suite instead of patching around a gap.

"tasks a human collaborator would consider tedious"



That a tireless co-worker is actually good at

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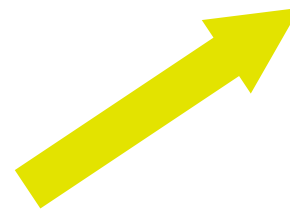
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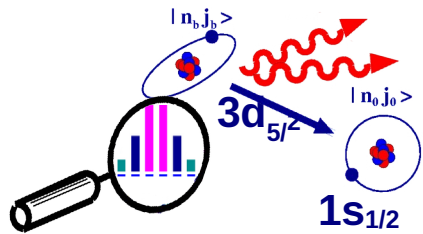
...

Atomic theory & computations

– research activities of our group

i) Structure and properties of atoms & HCl

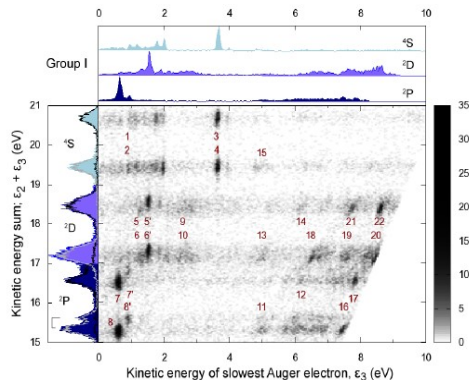
-- capture, excitation and ionization processes in strong static fields; accurate atomic calculations



PRA 109 (2024) 012815.
PRA 109 (2024) 022804.
JPB 57 (2024) 045202.
Phys. Plasma 31 (2024) 043301.
PRA 110 (2024) 012805.
PRA 110 (2024) 023105.
EPJD 78 (2024) 122.
PRA 110 (2024) 052812.
PRL 133 (2024) 163202.

ii) Auger cascades of light & medium elements

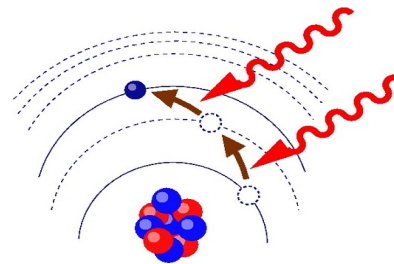
-- systematic treatment of shake-processes; multiple photo-detachment, electrons in plasma



Phys. Plasma 31 (2024) 042110.
EPJD 78 (2024) 69.
EPJD 78 (2024) 75.
PRA 109 (2024) 032817.
Plasma 7 (2024) 106.
EPJP 129 (2024) 986.

iii) Photoionization and photon scattering

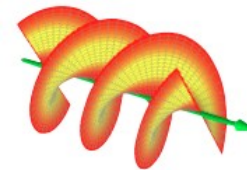
-- direct and sequential (multiple) ionization, strong-field ionization, HHG



PRA 109 (2024) 033103.
PRA 109 (2024) L041101.
PRA 109 (2024) 013118.
JPB 57 (2024) 225001.
PRL 133 (2024) 223001.

vi) Interactions with twisted light & electrons

-- photo-excitation, ionization, Compton scattering, Mott scattering and strong fields with Bessel & Laguerre Gaussian beams

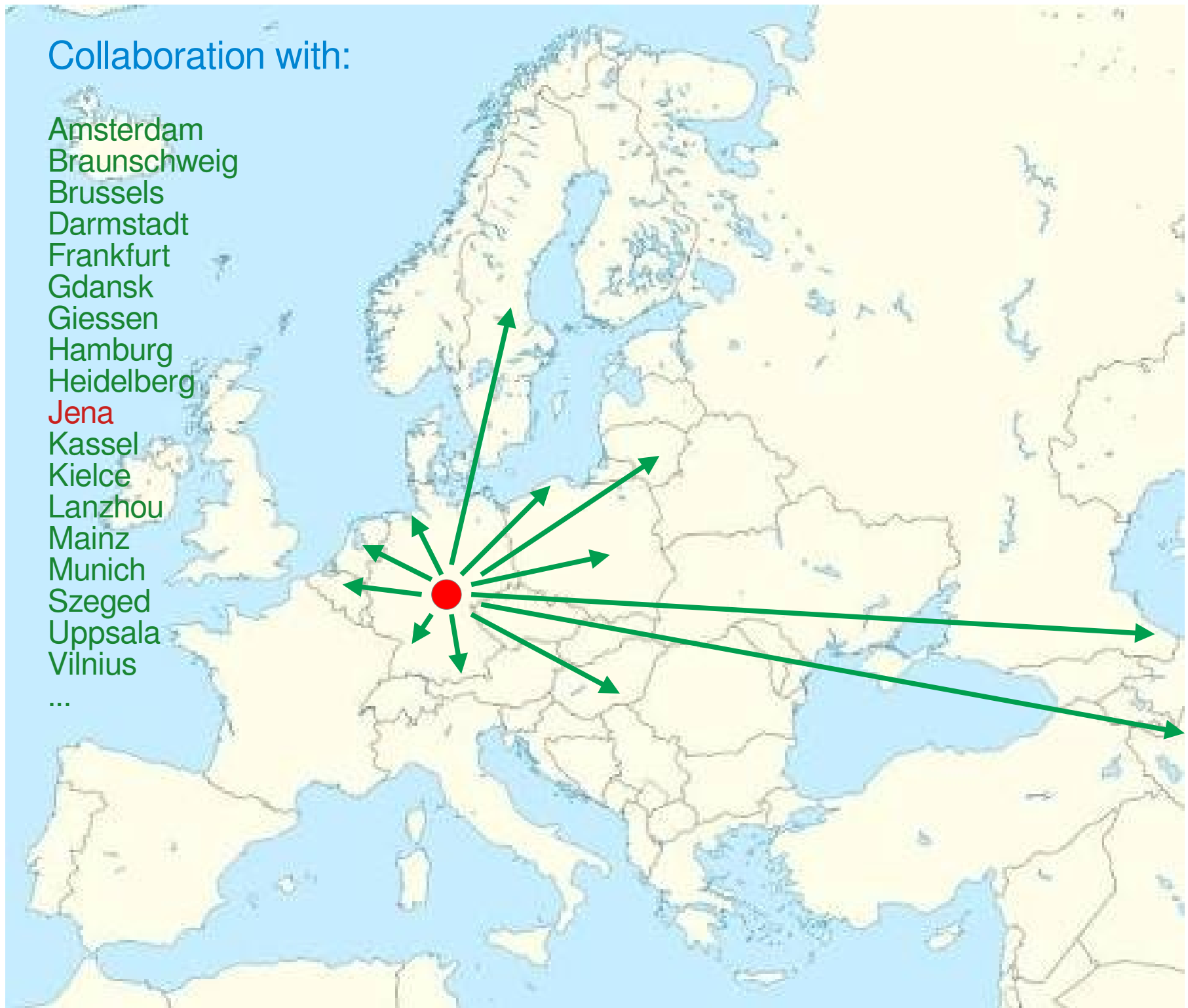


Ann. Phys. (2024) 2400048.
PRA 109 (2024) 023534.
NJP (2024) 093010.
PRA 110 (2024) 033718.
PRA 110 (2024) 043101.

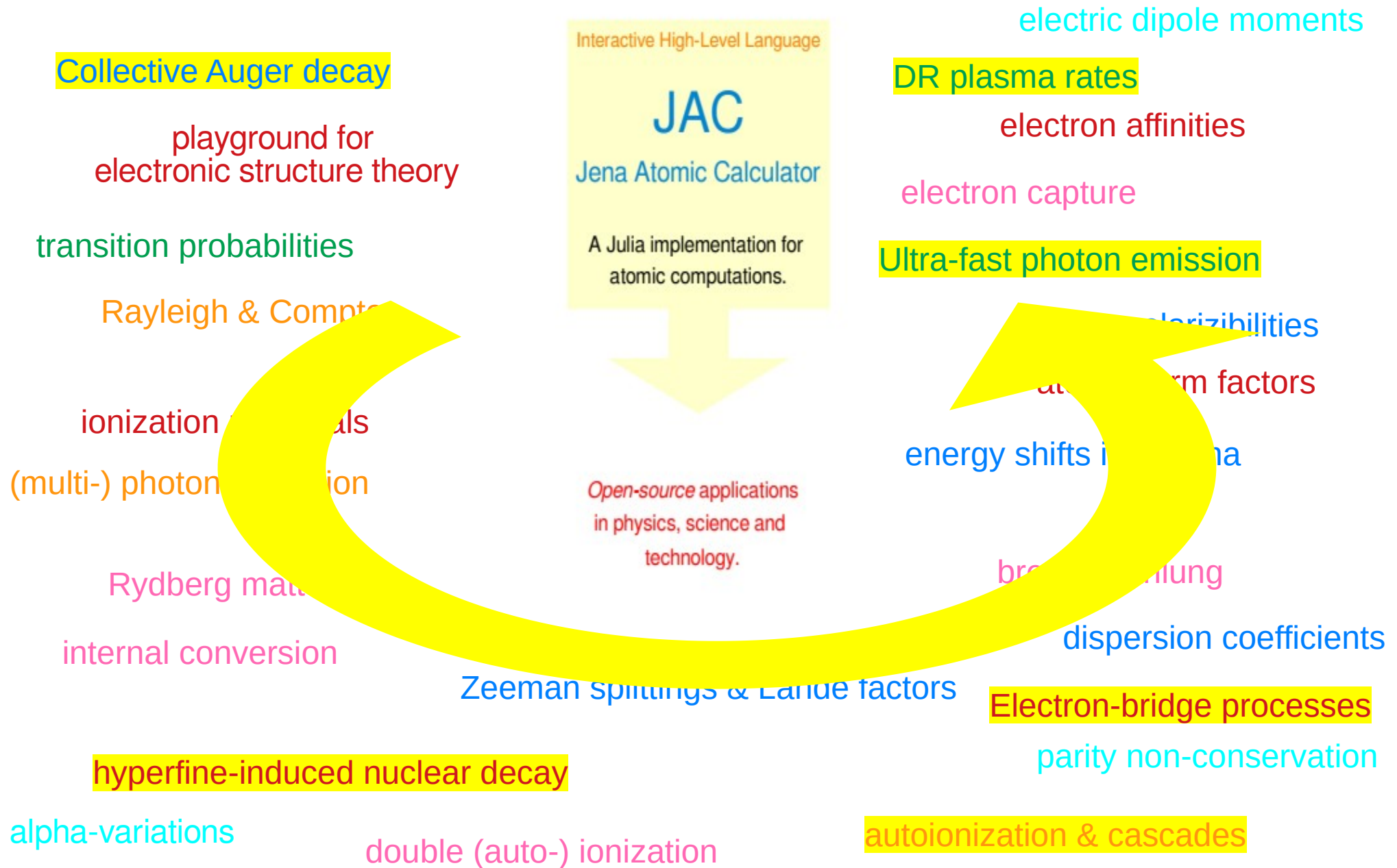
Collaboration with:

Amsterdam
Braunschweig
Brussels
Darmstadt
Frankfurt
Gdansk
Giessen
Hamburg
Heidelberg
Jena
Kassel
Kielce
Lanzhou
Mainz
Munich
Szeged
Uppsala
Vilnius

...



Summary: Community platform for atomic computations



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