JAC: Jena Atomic Calculator

— User Guide, Compendium & Theoretical Background —

https://github.com/OpenJAC/JAC.jl

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Atomic representations

- Configuration-based expansions
- Restricted active spaces (layer-by-layer)
- CI+perturbation theory; Gamov states
- Approximate Green functions, ...

Processes & properties

- Transition probabilities
- Excitation, ionization & recombination
- Auger, DR, Rayleigh-Compton, multi-y
- Hyperfine & Zeeman splitting; plasma
- Isotope shifts, Lande & form factors

Atomic cascades

- Average singe-configuration approach
- Multiple-configuration approach
- Incorporation of shake-up & shake-off
- Ion & electron distributions, ...

Symbolic Racah algebra

- Wigner symbols, special values
- Symmetries & recursions
- Symbolic sum rule evaluation
- Spherical harmonics & tensors

Interactive High-Level Language

JAC

Jena Atomic Calculator

A Julia implementation for atomic computations.

Open-source applications in physics, science and technology.

Atomic responses

- Field-induced processes & ionization
- High-harmonic generation
- Particle-impact processes
- Charge exchange

Time evolution

- Liouville equation for statistical tensors
 & atomic density matrices
- Atoms in intense light pulses
- Angle & polarization-dep. observables

Atomic descriptors

- Feature transform. & machine learning
- Bi-spectra of electronic densities
- Subshell & coupling descriptors
- Atomic fragments & effective charges

Semi-empirical estimates

- Weak-field ionization rates
- Asymptotic behaviour & formulas
- Stopping powers
- Plasma Stark broadening, ...

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