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Photoionization And Resonant Ionization Data For K-shell in Highly Charged Iron Ions

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Introduction 1

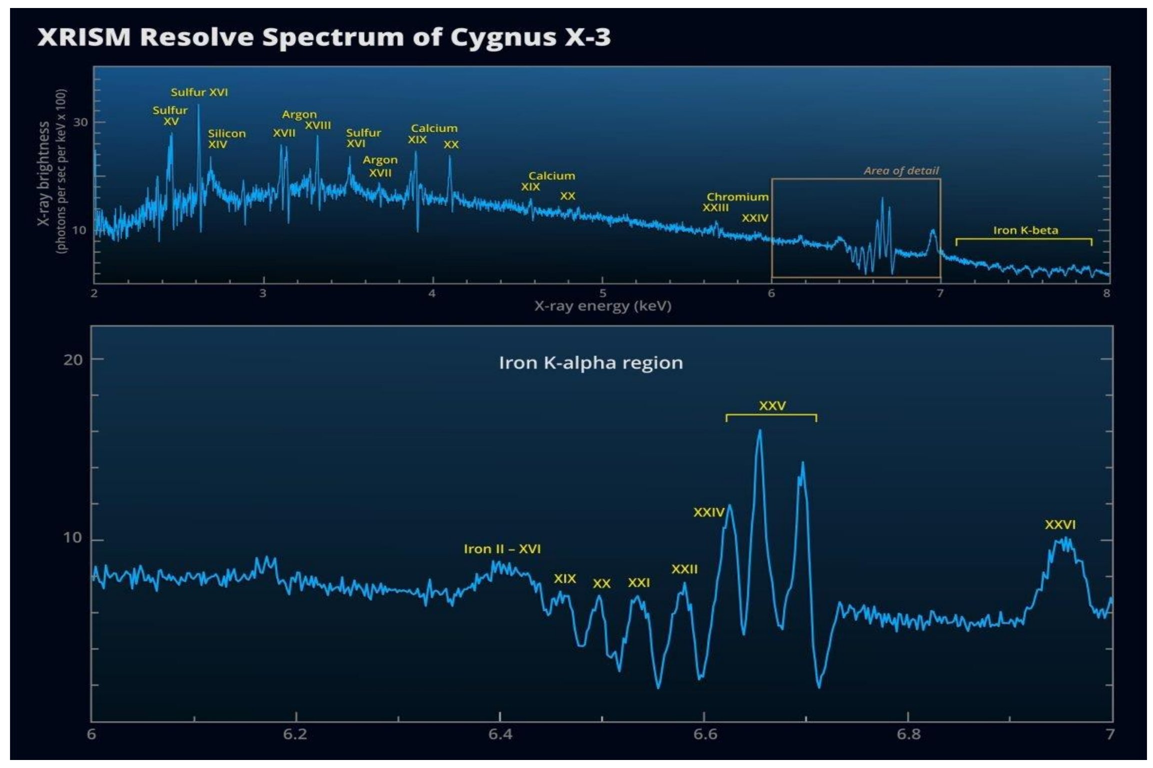
K-shell emission lines (Kα, Kβ, Kγ) are prominent features in astronomical X-ray spectra and serve as powerful diagnostics of plasma conditions and elemental abundances in sources such as AGN, X-ray binaries, and supernova remnants. Building on over 25 years of XSTAR development, this project focuses on improving K-shell spectral models for highly charged ions to meet the accuracy demands of current and future high-resolution missions like XRISM and NewAthena. Our primary emphasis is on iron K-shell transitions, with the long-term goal of extending calculations to all ions from H through Zn.

Objectives 3

- Compute resonance-resolved photoionization cross sections for Fe XVII–Fe XXVI
- Extend calculations to all ions from H to Zn
- Improve XSTAR models by separating background and resonant contributions
- Validate AUTOSTRUCTURE results against R-matrix data
- Support high-resolution X-ray missions: XRISM and NewAthena

Motivation 2

- XRISM resolves complex Fe K-line structures in Cygnus X-3
- Current K-line models are inadequate
- Athena will require higher-precision atomic data
- This project delivers improved cross sections in XSTAR



Credit: JAXA/NASA/XRISM Collaboration

Figure 1: *XRISM Resolve X-ray spectrum of Cygnus X-3.*

Methods 4

Calculations performed using AS, a relativistic distorted-wave code with configuration interaction (CI).

AS[5,6] is an extension of the **SUPERSTRUCTURE(SS)** program[7], designed to compute **fine-structure level energies, radiative rates, Auger rates, and photoionization cross-section** in a **Breit–Pauli (BP) relativistic framework.**

Single-electron orbitals $P_{nl}(r)$ are obtained by diagonalizing the non-relativistic Hamiltonian:

$$H_{nr} = -\frac{1}{2}\nabla^2 - \frac{Z}{r} + V(\lambda_{nl}, r)$$

within a statistical Thomas–Fermi–Dirac model potential $V(\lambda_{nl}, r)$[8].

The parameters λ_{nl} are **orbital scaling parameters**, adjusted to optimize agreement with the NIST database.

The **BP Hamiltonian** is included to account for relativistic effects:

$$H_{BP} = H_{nr} + H_{1b} + H_{2b}$$

where, H_{1b} includes one-body operators (mass correction, Darwin term, spin–orbit) and H_{2b} includes two-body Breit interactions.

Wavefunctions are expanded as:

$$\Psi = \sum_k c_k \Phi_k$$

capturing electron correlation through configuration mixing.

Conclusion 6

- Our calculations demonstrate that photoionization cross-sections and photo absorption cross-section, including resonance features critical for astrophysical modeling.
- The resulting datasets provide a significant upgrade to XSTAR, enabling more precise interpretation of current XRISM spectra and preparing for the next-generation NewAthena mission.
- This framework establishes a path toward comprehensive K-shell atomic data, beginning with iron and expanding to lighter and heavier ions.

Result and Discussion 5

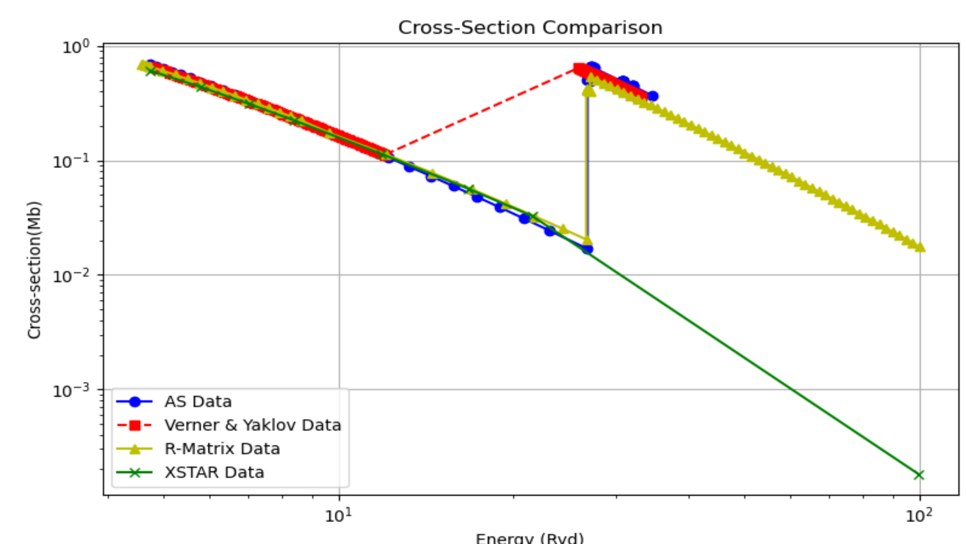


Figure 2. *Photoionization cross sections for Li-like carbon (C IV). AS results are compared with R-matrix (TOPbase), XSTAR, and Verner datasets.*

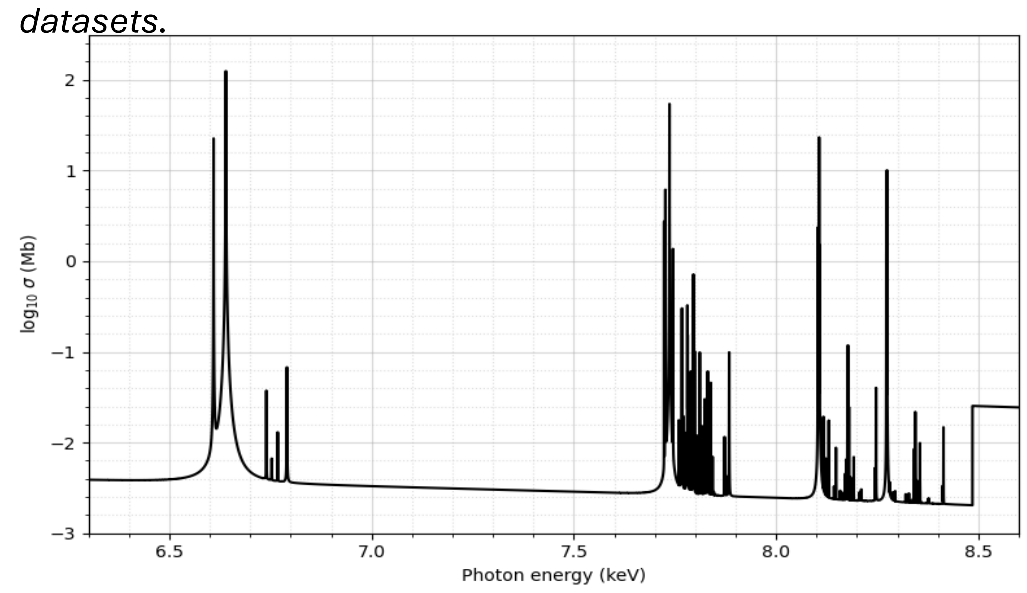


Figure 3. *Photoabsorption cross section of the ground state of Fe XXIII computed with AUTOSTRUCTURE assuming Lorentzian resonance profiles.*

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1. Serlemitsos, P. J., Boldt, E. A., Holt, S. S., et al. 1973, ApJ, 184, L1
2. Serlemitsos, P. J., Smith, B. W., Boldt, E. A., et al. 1977, ApJ, 211, L63
3. Sanford, P., Mason, K. O., & Ives, J. 1975, MNRAS, 173, 9P
4. Bautista, M.A.; Kallman, T.R., Astrophys. J. Suppl. Ser. 2001, 134, 139
5. Badnell, N. R. 1986, J. Phys. B, 19, 3827
6. Badnell, N. R. 1997, J. Phys. B, 30, 1
7. Eissner, W., Jones, M., & Nussbaumer, H. 1974, Comput. Phys. Commun., 8, 270
8. Eissner, W., & Nussbaumer, H. 1969, J. Phys. B, 2, 1028