Improving Theoretical Charge Exchange Cross Sections for Astrophysical X-ray Emission Modeling: Limitations and Future of Kronos

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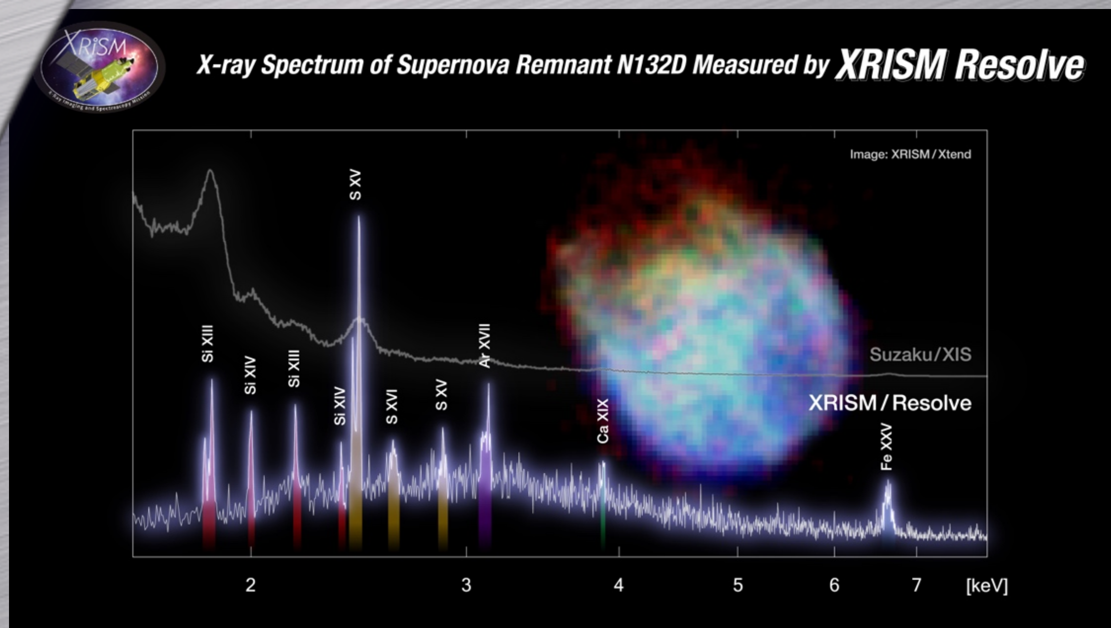

Collaborators

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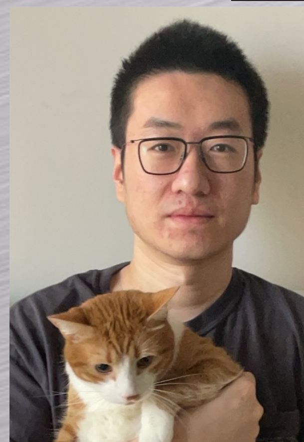

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Outline

- Introduction
- CX Theoretical Methods Overview
- The Kronos Database/Spectra Model
- Other CX Databases
- Examples - importance of Double Capture
- Summary
- The Future

CX Cross Section Theory

- *n*-, *l*-, *L*-, and *S*-resolved cross sections are needed for ~10 eV/u to ~10 MeV/u
- Various methods used:
  - Lattice time-dependent Schroedinger equation (LTSE)
  - Quantum molecular-orbital close-coupling (QMOCC)
  - Atomic-orbital close-coupling (AOCC)
  - Classical-trajectory Monte Carlo (CTMC)
  - Multichannel Landau-Zener (MCLZ)

Accuracy

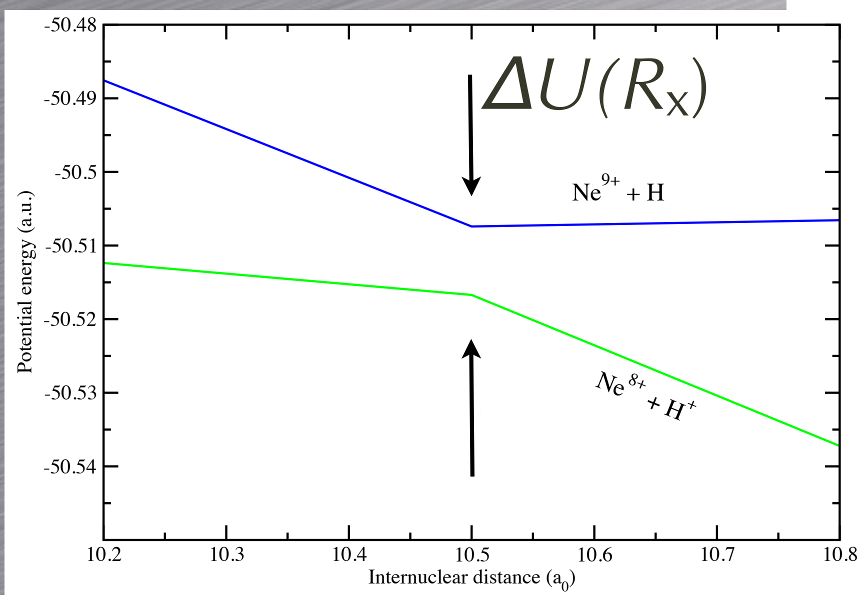
Computational Effort

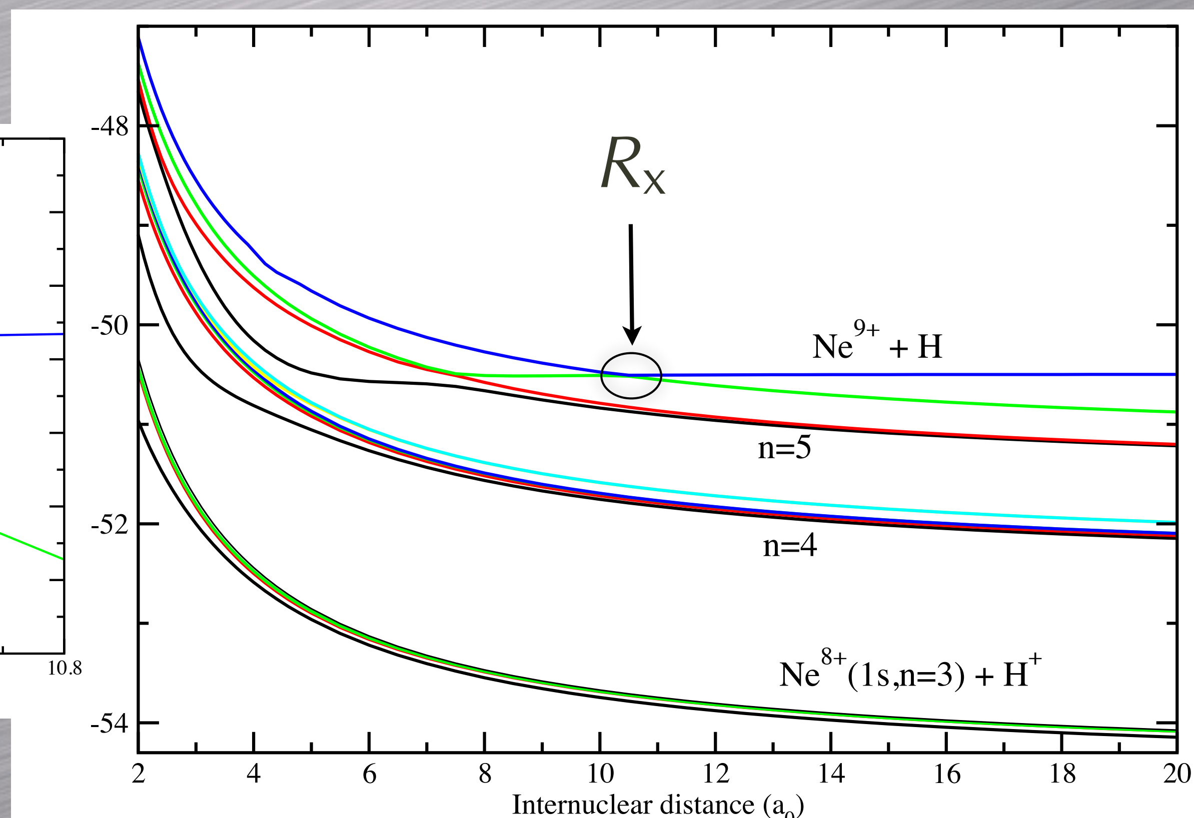
Multichannel Landau-Zener

- Janev, McDowell, & Bransden (1983); Butler & Dalgarno (1980); Gershstein (1963)
- N-channels — almost unlimited
- LZ parameters: 1) avoided-crossing distances (R_x), 2) potential energy difference at R_x [$\Delta U(R_x)$], and 3) the difference in diabatic potential slopes at R_x [$F(R_x)$]
- R_x - from asymptotic atomic energies (NIST) and IPs
- $F(R_x)$ - model potential functions w/polarizabilities
- Problem: bare-ion cases give only <u>*n*-resolved cross sections</u> → *l*-distribution functions must be used

Multichannel Landau-Zener

- Largest uncertainty from $\Delta U(R_x)$
- Various models for $\Delta U(R_x)$: one-electron (Olson-Salop 1977), multi-electron (Tauljberg 1986), low-charge (Butler-Dalgarno 1980)





l-distributions from CX

- Model *l*-distribution functions often used:
  - 1. Low-energy (Landau-Zener) (< 1 keV/u?) ➞ $$\frac{(2l+1)(n-1)!}{(n+l)!(n-l-1)!}$$
  - 2. Low-energy II (< 1 keV/u?)
  - 3. Separable (< 1keV/u?)
  - 4. Flat (even) (1-10 keV/u?) - all *l* cross sections equal
  - 5. Statistical (>10 keV/u?) ➞ $$\frac{(2l+1)}{n^2}$$
- *Required for bare-ion MCLZ calculations only* (H-like emission)

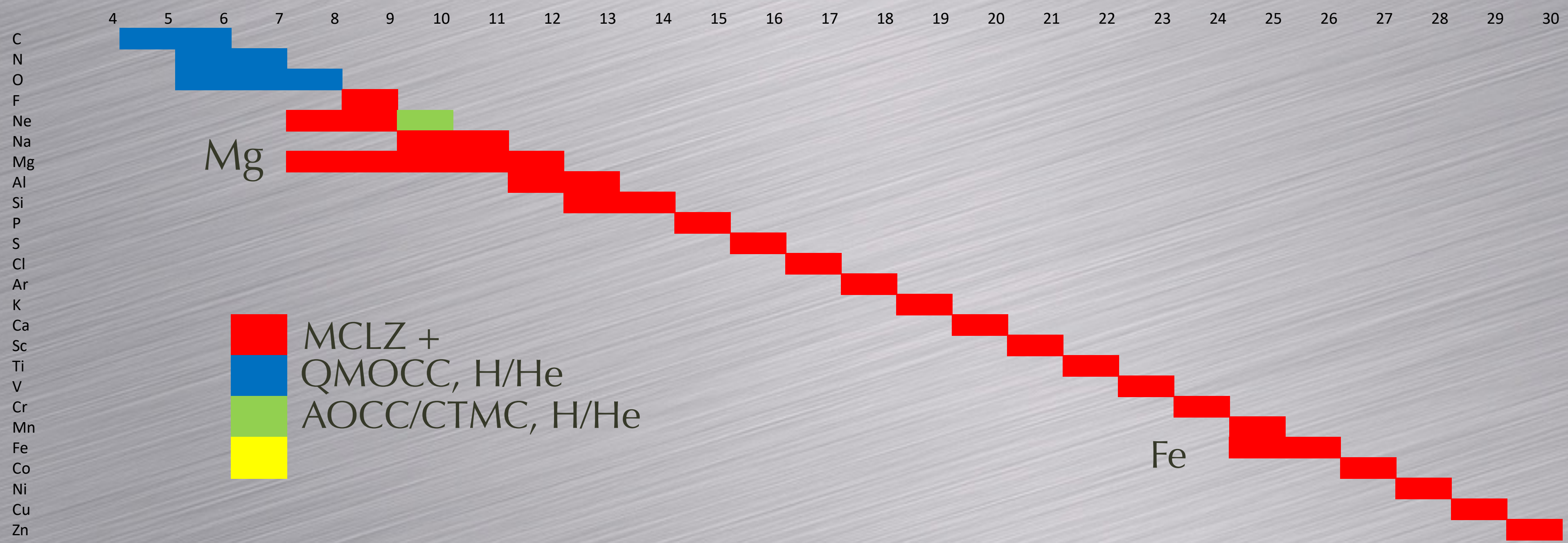
The Kronos CX Database

(sites.physast.uga.edu/ugacxdb)

- **First version (2017-2019):**
  - Database of *Single Electron Capture* (SEC) cross sections, ion energies and A-values (NIST, analytical, and Autostructure), and cascade/X-ray spectrum model
  - Mostly MCLZ results, but also QMOCC, AOCC, CTMC, "recommended"
  - Ions: H-like C-Zn, He-like C-Si
  - Neutral targets: H, He, H_2, N_2, H_2O, CO, CO_2, some cross sections for O, OH, Kr

Mullen et al. 2016, ApJS, 224, 31; 2017, ApJ, 844, 7
Cumbee et al. 2019, ApJ 852, 7

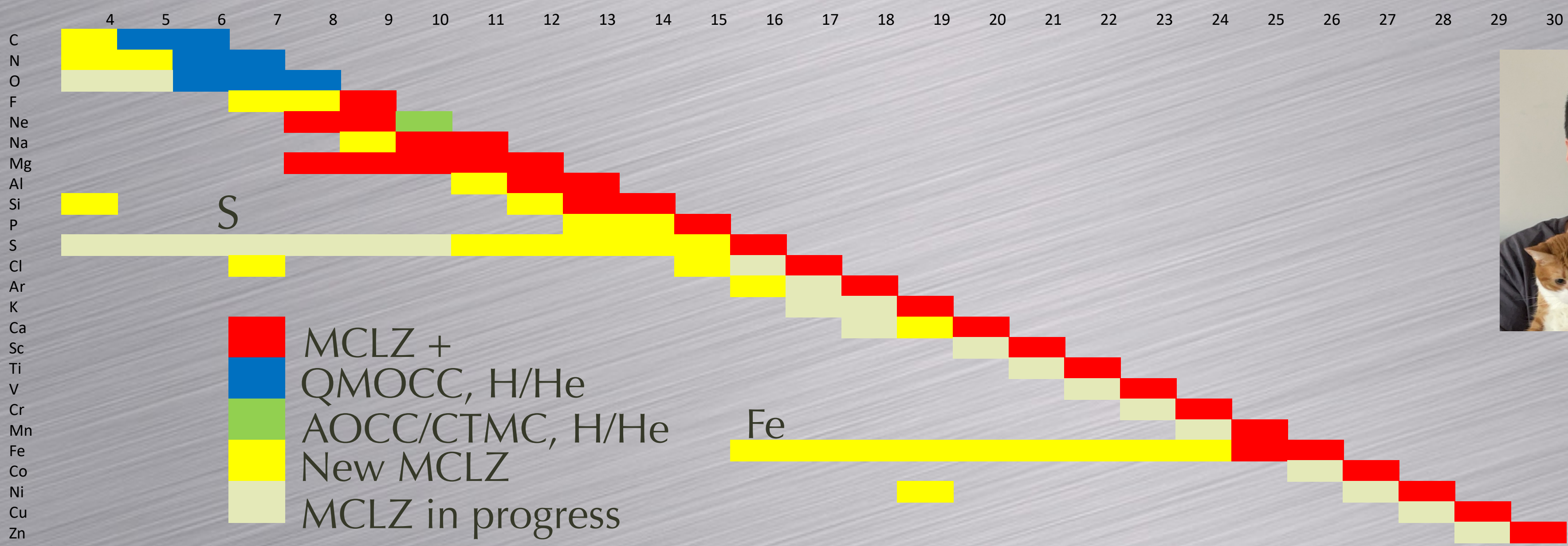
Current Kronos (v3.1)

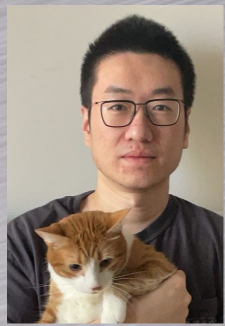


The Kronos CX Database

- **New version (Fall 2024):**
  - He-like ions (P-Zn)
  - All Li-like ions (C-Zn)
  - Additional targets: CH_4, NH_3
  - Multielectron ions: C, O, Ne, S, Mg, and Fe
  - Complex atomic structure: *n, l, L, 2S+1*, seniority
  - GUI
  - More literature data
  - Data provenance

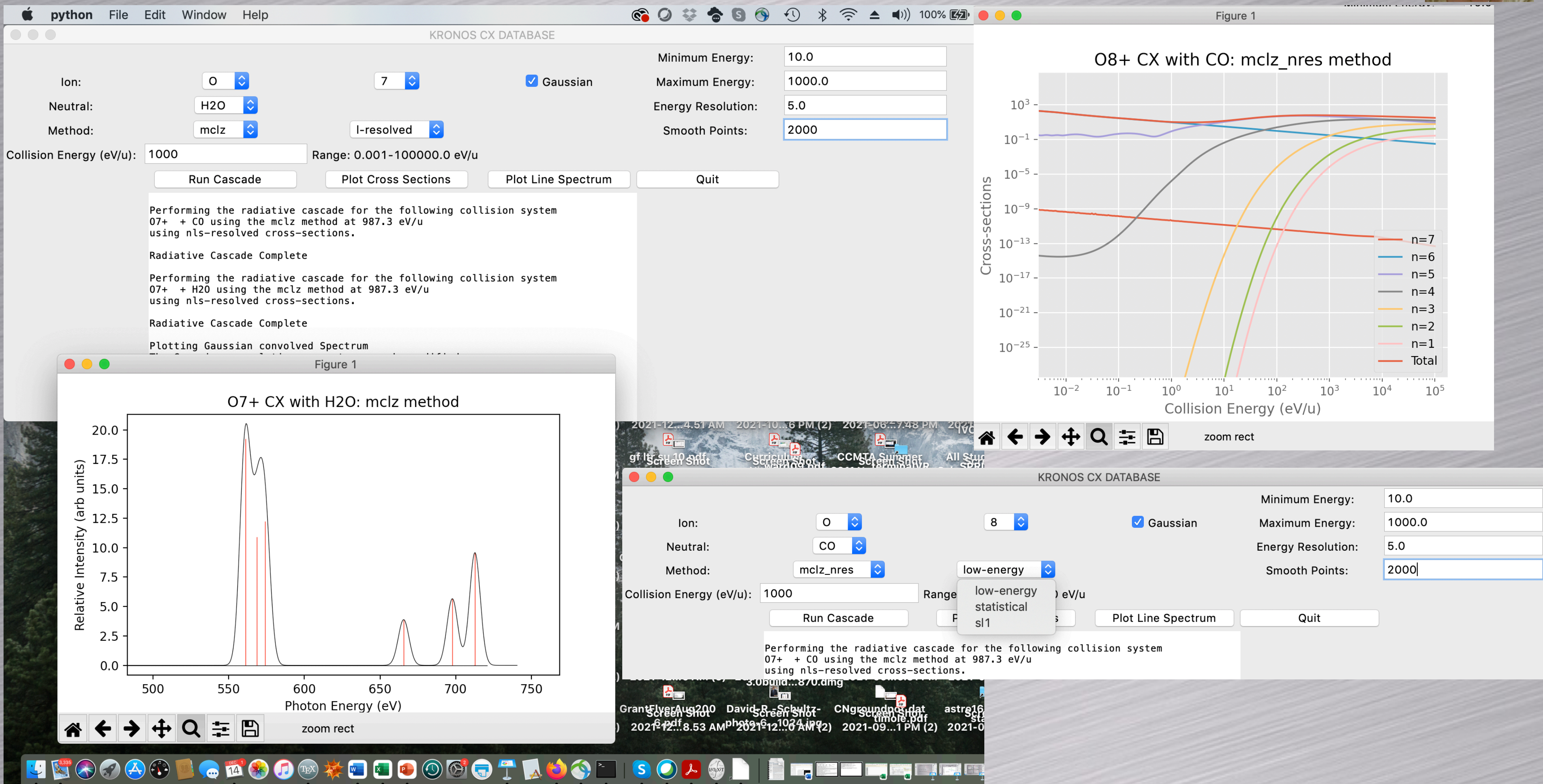
Next Kronos





Not pictured:
Lior Shefler
Sean McIlvane

Kronos GUI



- Beta testing in progress
- Jupyter notebooks in progress - comparison to ACX, SPEX, NIST thermal spectra

Kronos Details

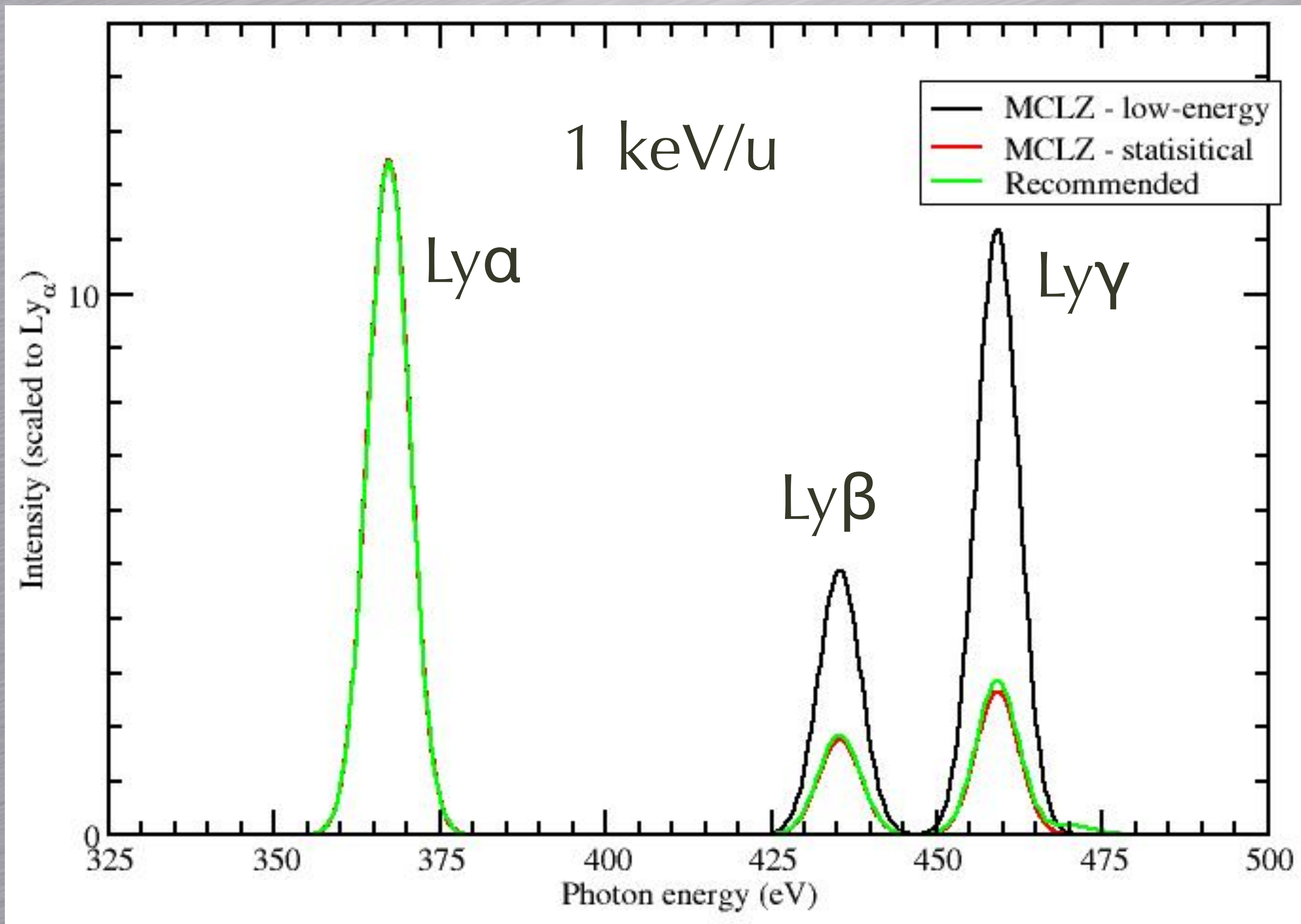
- **What Kronos does:**
  - MCLZ: *l*-distribution models for H-like ions only
  - 2+ electrons, no *l*-distribution needed
  - MCLZ, QMOCC: no assumed triplet-singlet ratio
- **What Kronos doesn't do:**
  - Fine-structure-resolved cross sections (*coming soon*)
  - Multiple electron capture (*only single electron capture*)
- **Coming soon (2 NASA APRA grants):**
  - QMOCC pipeline calculations (nearly exact 1-electron)
  - Two-electron AOCC code
  - Benchmarking to EBIT and other measurements
  - Machine learning optimization to improve MCLZ

CX Databases

- **AtomDB: AtomDB Charge Exchange** (ACX v1) model:
  - Classical over-the-barrier (COB) model, 2 parameters: *q*, IP of neutral
  - Predicts total CX cross section, dominant *n*; no velocity dependence
  - *l*-distribution models, triplet-singlet ratio = 3
  - ACX v2: ingested *Kronos* data, ACX v1 for systems not in Kronos
- **SPEX:**
  - Fits of existing experimental data
  - Ingested *Kronos* data
- **Flexible Atomic Code (FAC)**
  - Ingested *Kronos* data
- Also **xstar and Cloudy ->** mostly total rate coefficients

Examples

X-ray Spectra for C^{6+} + H comparison

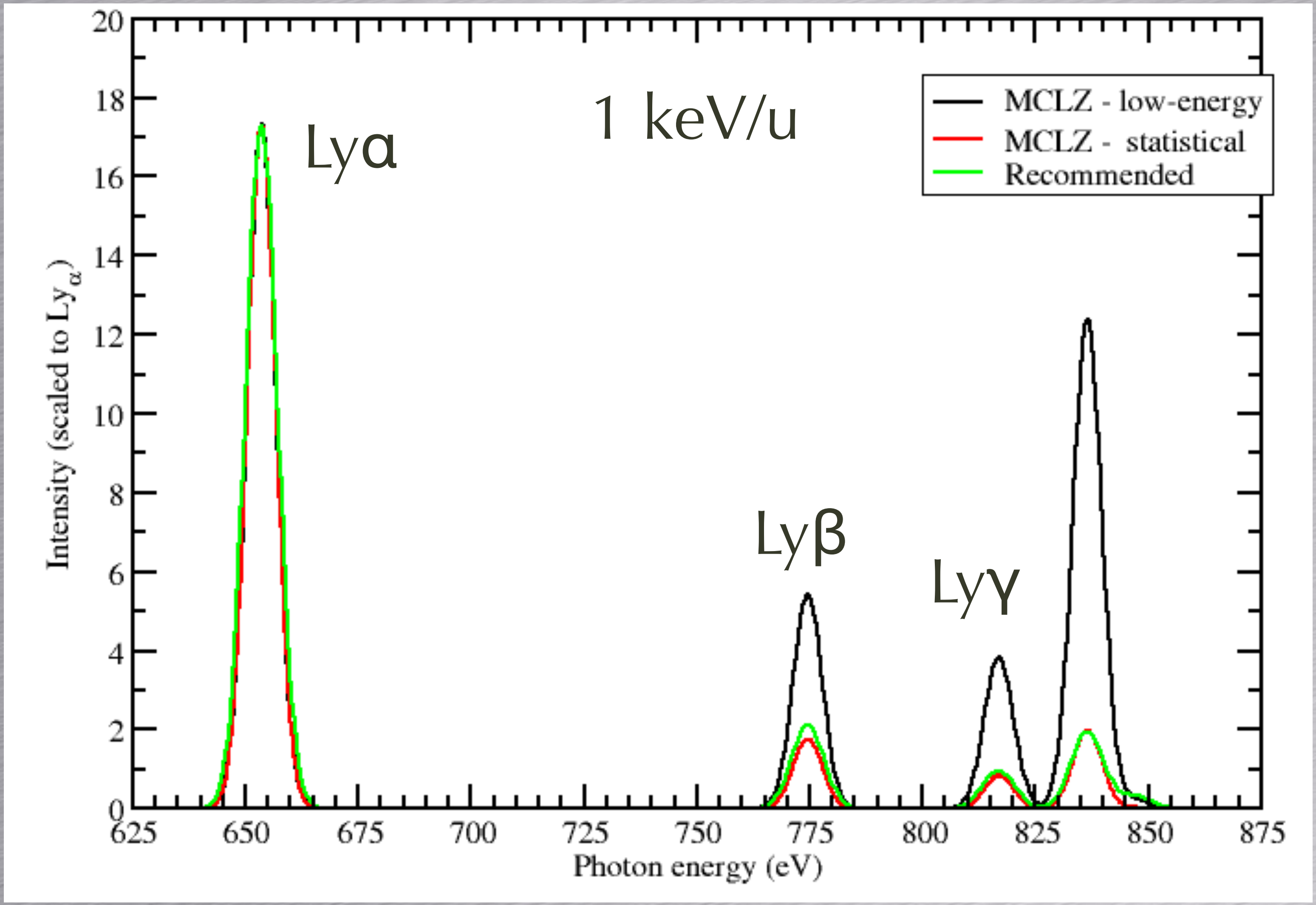


4.5 eV resolution

Cumbee et al. (2019)

Recommended: Janev et al. 1993, ADNDT, 55, 201

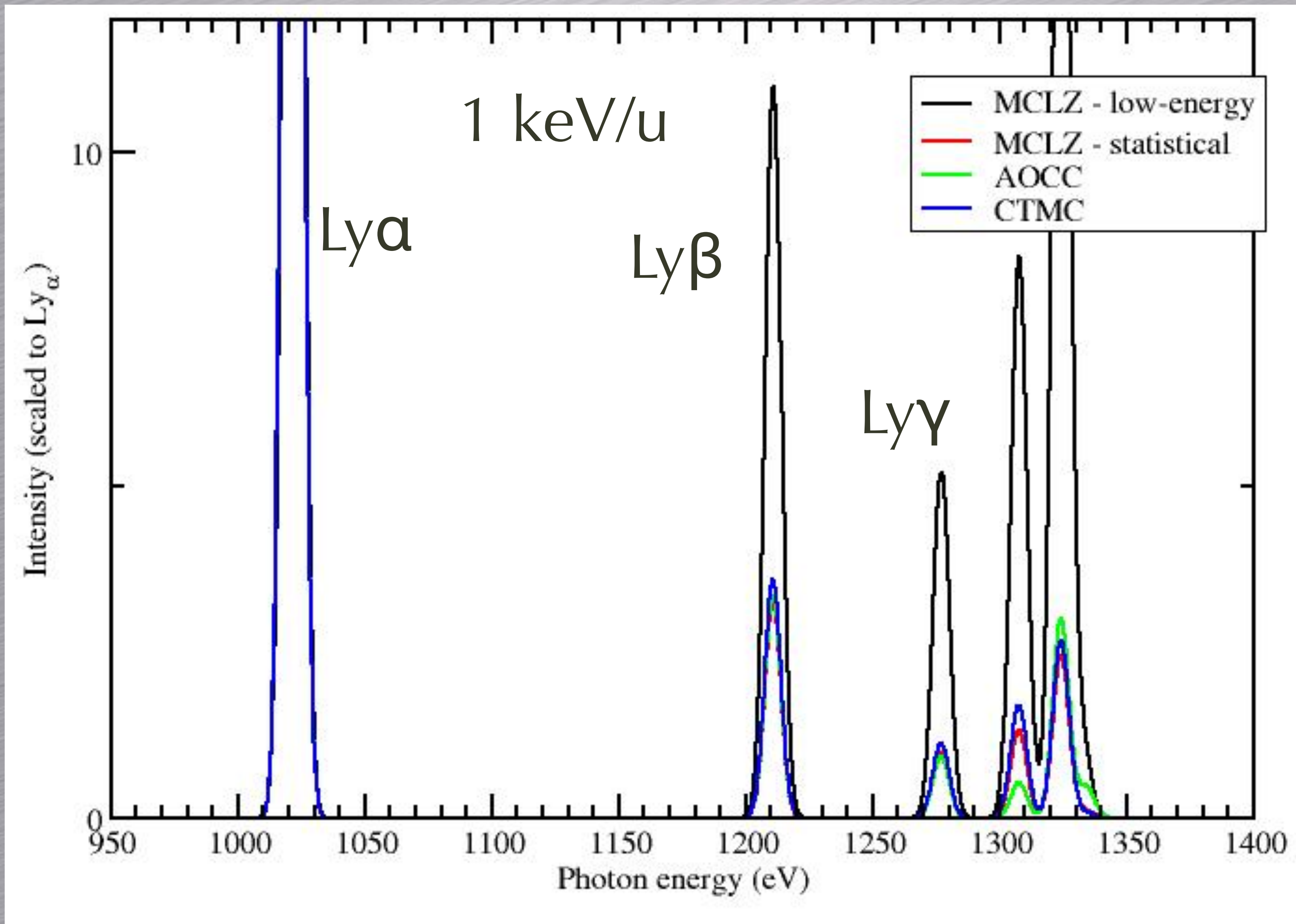
X-ray Spectra for O^{8+} + H comparison



4.5 eV resolution

Cumbee et al. (2019)

X-ray Spectra for Ne^{10+} + H comparison

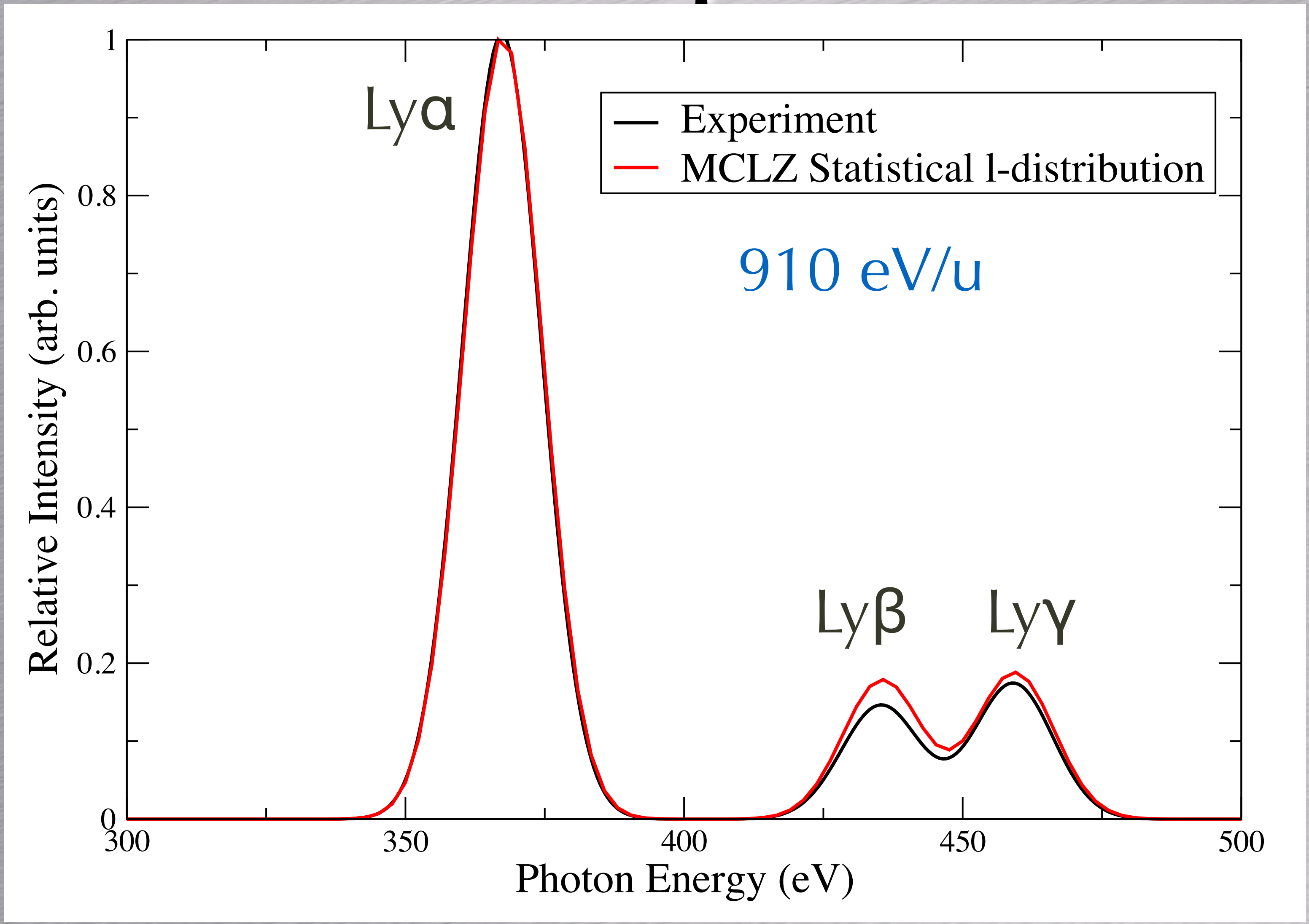


4.5 eV resolution

Lyons et al. (2016)
Cumbee et al. (2016)

CTMC: Schultz & Krstic (1997); AOCC: Cumbee et al. (2016)

X-ray Spectra for $C^{6+} + H_2$ compared to experiment

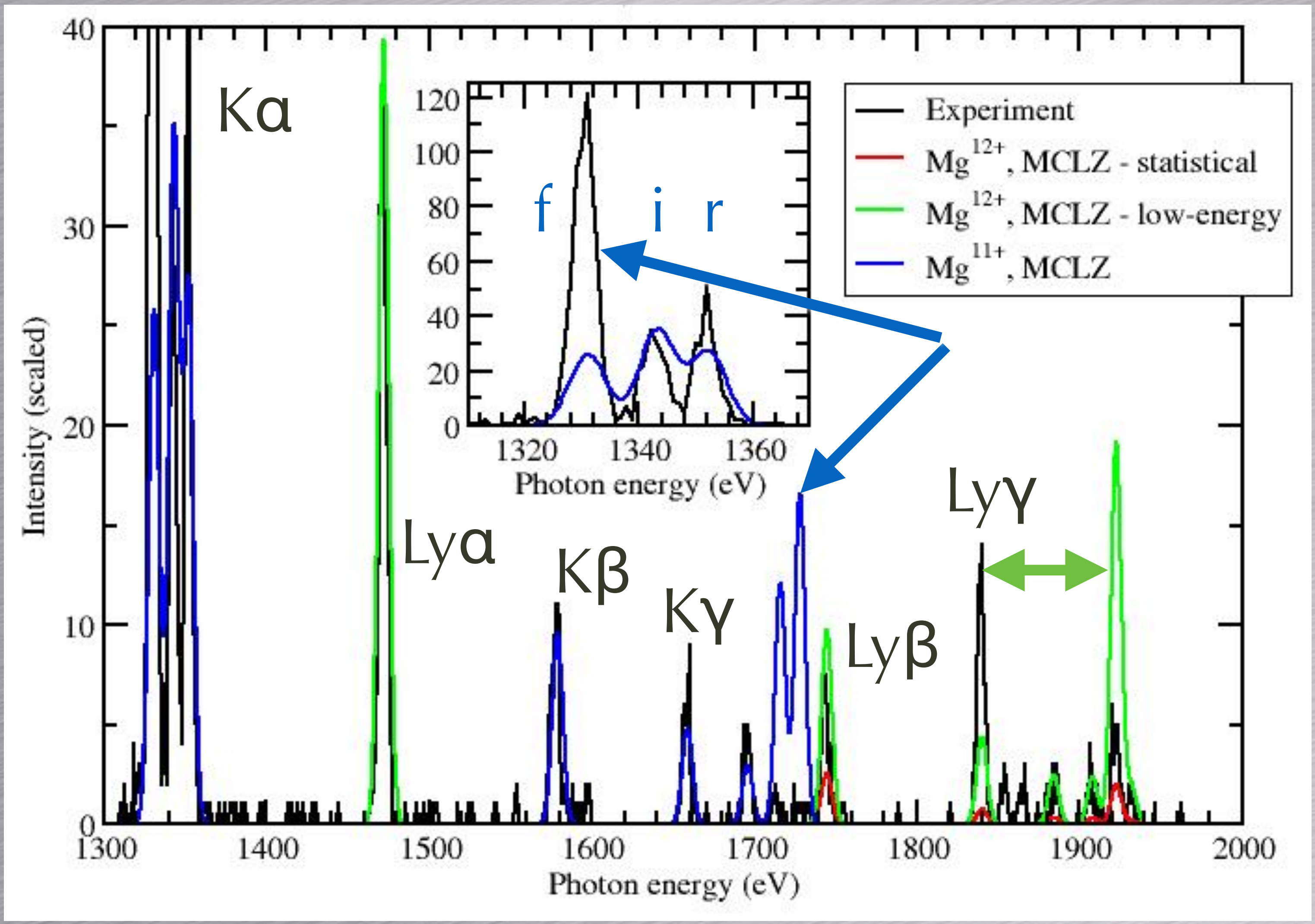


10 eV resolution

Cumbee et al. (2019)

Experiment: Fogle et al. 2014, PRA, 89, 042705

X-ray Spectra for Mg^{12+} and $Mg^{11+} + H_2$ compared to experiment



25 eV/u

4.5 eV resolution

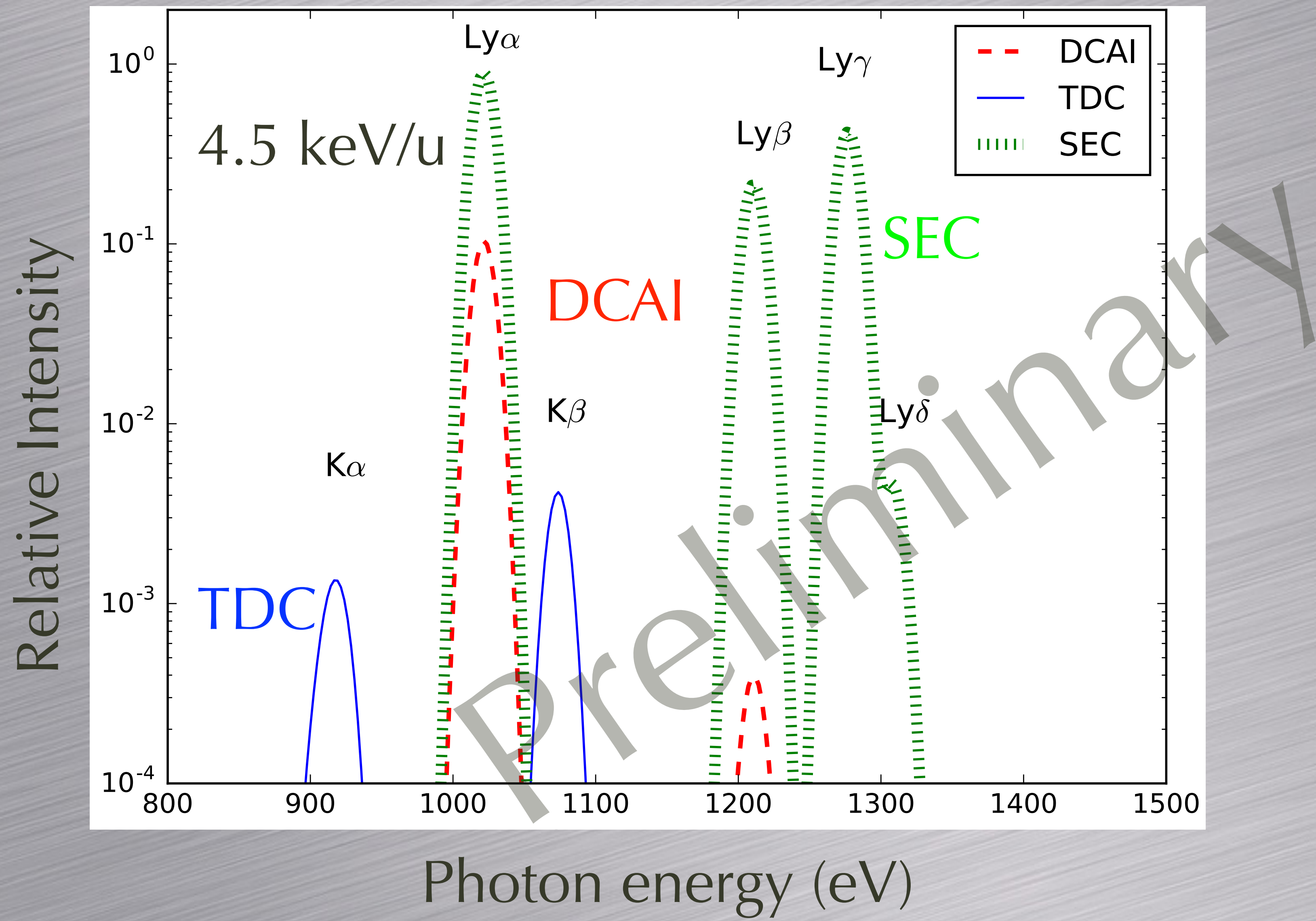
Cumbee et al. (2019)

Experiment: Betancourt-Martinez et al. 2014, PRA, 90, 052723

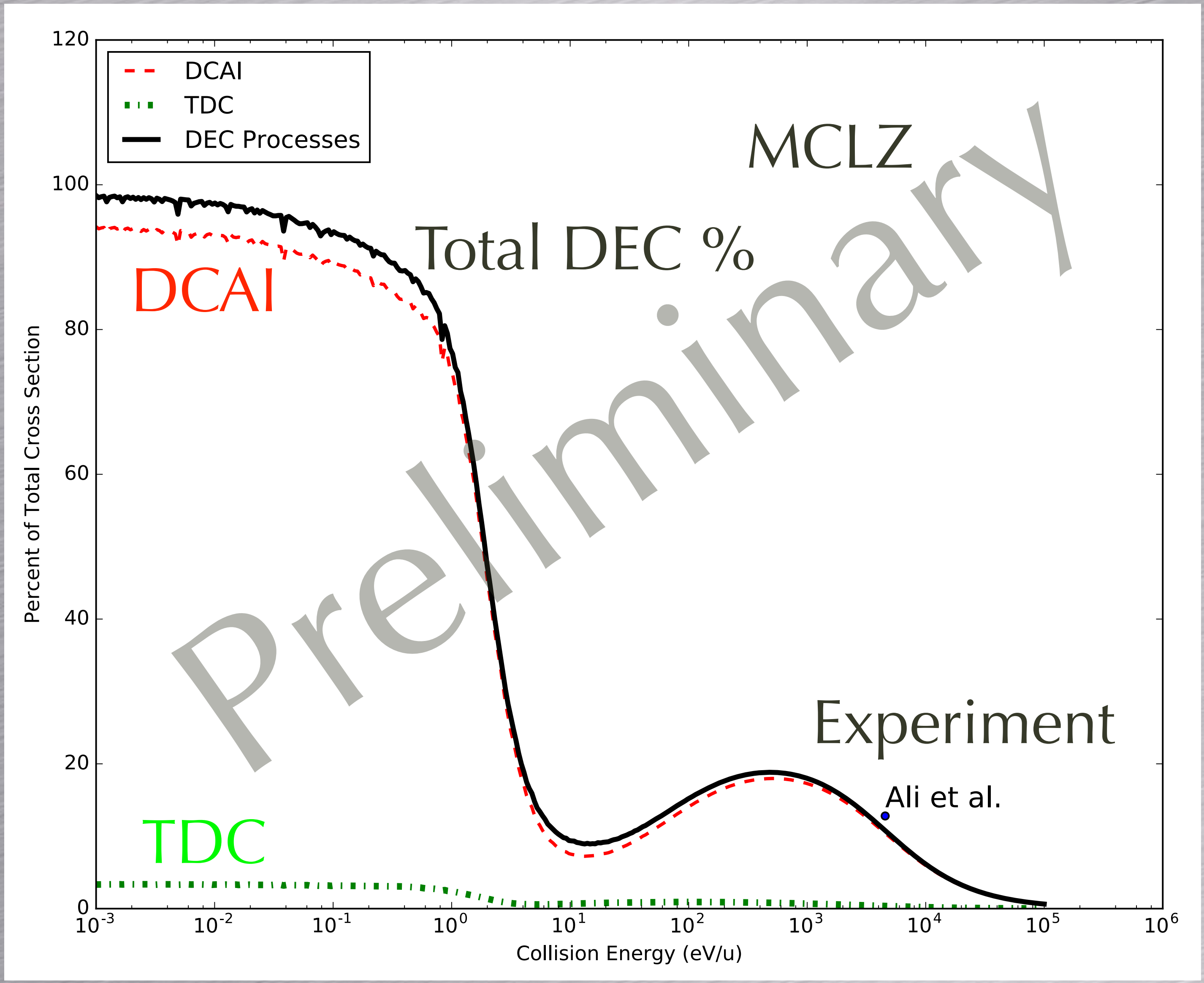
Double Electron Capture?

- Single Electron Capture (SEC)
- $$\mathrm{Mg}^{12+} + \mathrm{H}_2(1s^2) \rightarrow \mathrm{Mg}^{11+}(n\ell) + \mathrm{H}_2^+(1s)$$
- Double Electron Capture (DEC)
$$\mathrm{Mg}^{12+} + \mathrm{H}_2(1s^2) \rightarrow \mathrm{Mg}^{10+}(n'\ell', n''\ell'') + 2\mathrm{H}^+$$
- Double Capture Autoionization (DCAI) or True DC (TDC)
$$\rightarrow \mathrm{Mg}^{11+}(n\ell) + e^- \qquad \rightarrow \mathrm{Mg}^{10+}(n'\ell', n'''\ell''') + h\nu$$
- SEC + DCAI = q,q-1
- Measurement is of q,q-1
- Need Autoionization and Radiative Decay rates to determine branching ratios

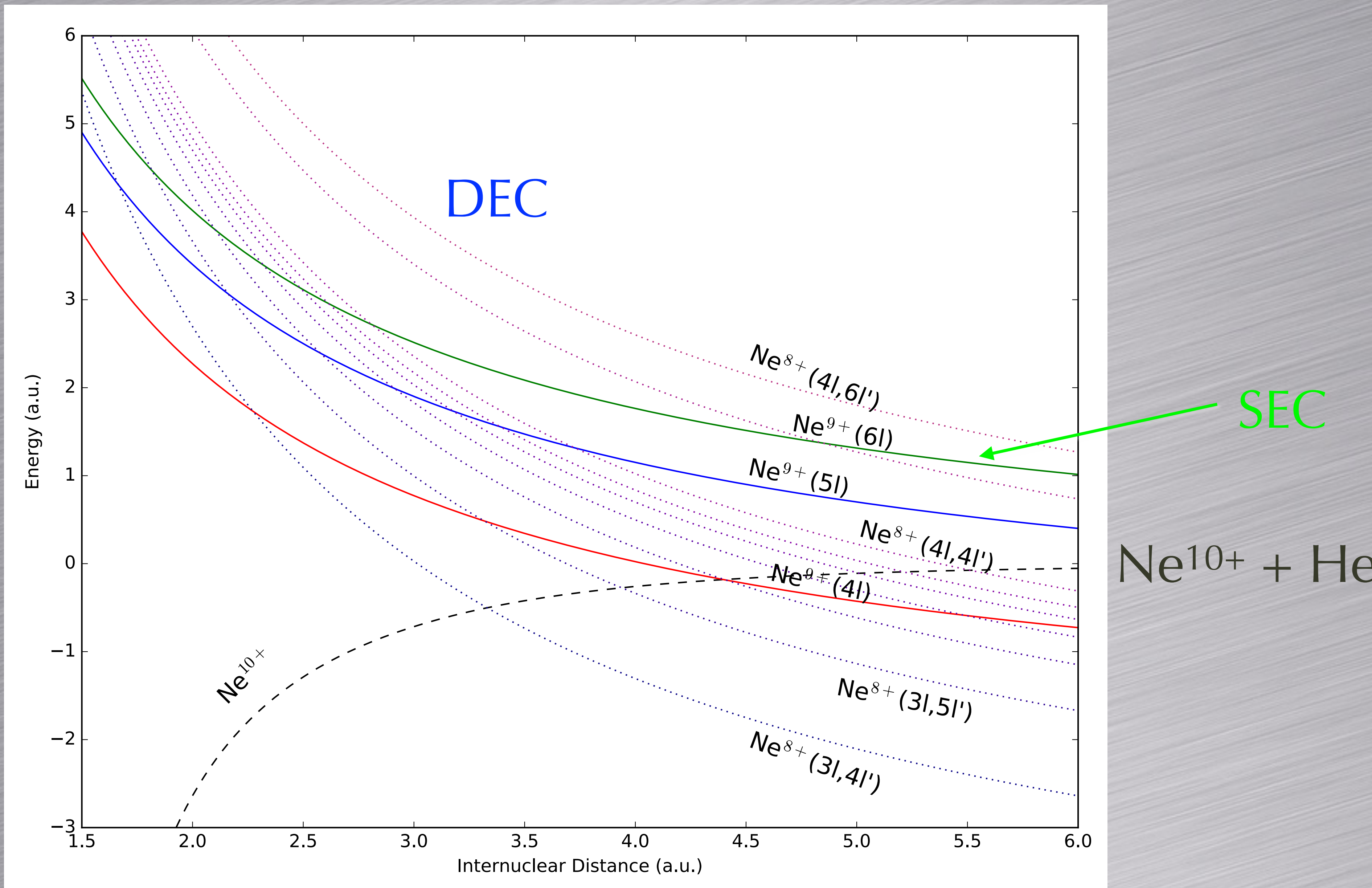
Ne^{10+} + He
Spectrum Contributions



Ne^{10+} + He Double Capture Processes



Ne^{10+} + He
Empirical Potentials

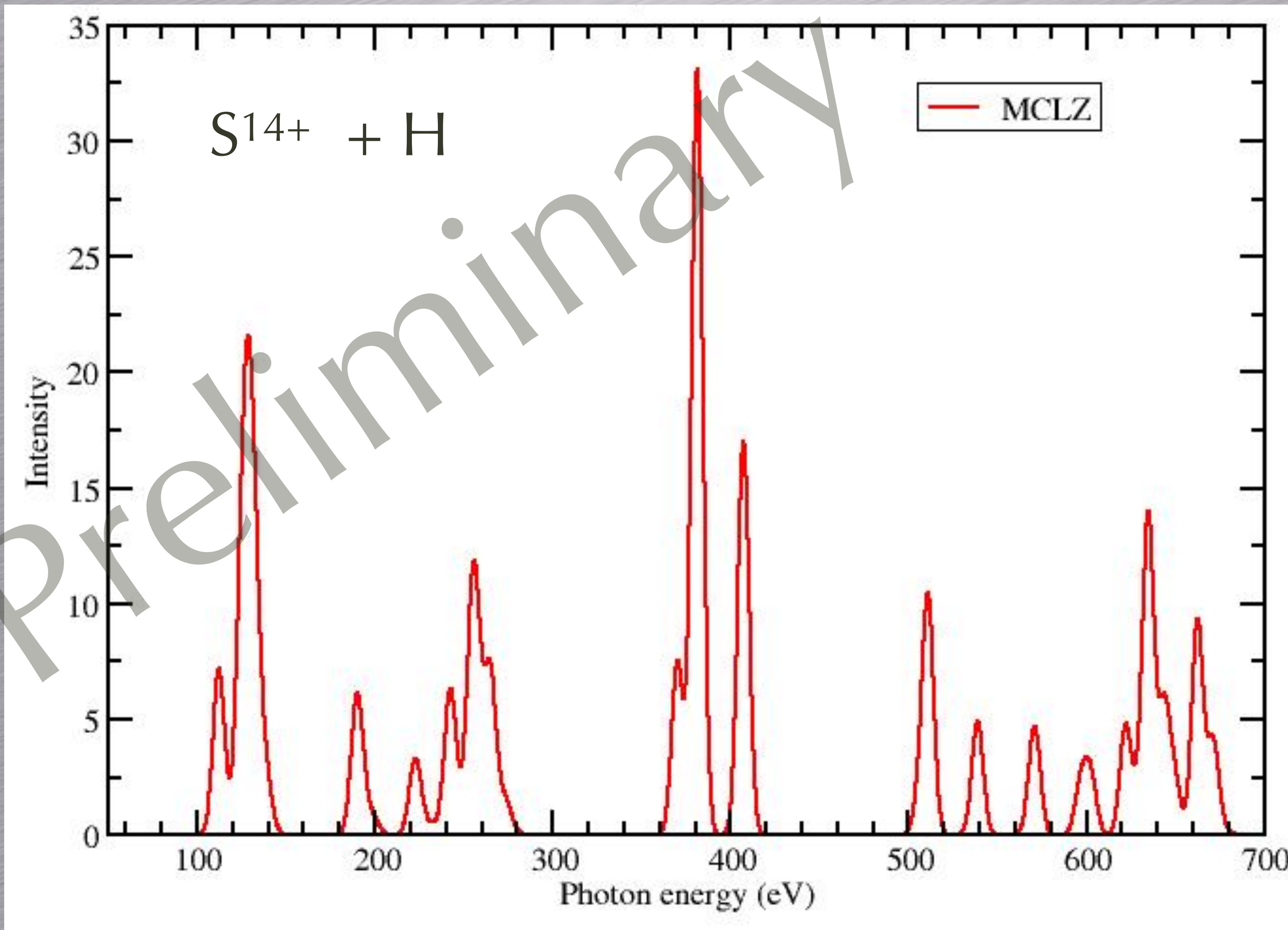


Mg^{11+} and Mg^{12+} discrepancies

- DCAI tends to populate lower n-values than SEC
- Suppresses high-n transition lines
- He-like ion measurement appears to have larger triplet population
- Should non-adiabatic coupling depend on spin?
- Topics to explore with joint Clemson-Auburn-GSFC-Livermore-UGA measurements focused on double-capture

Li-like S CX emission

MCLZ 1 keV/u



4.5 eV resolution

Summary

- Reviewed Kronos database for CX X-ray emission - single electron capture only
- Most cross section data obtained with MCLZ method
- Some QMOCC, AOCC, CTMC, and prior recommended cross sections
- Includes more than 300 collision systems
- Dominant uncertainty in the potential difference at the avoided-crossings (R_x)

The Future

- New Kronos release coming soon
- Moving to multi-electron systems w/ MCLZ
- New QMOCC and AOCC codes in development
- Benchmarking to measurements
- Optimize LZ parameters with machine learning
- Double capture and fine-structure