Recent Developments of the NIST Atomic Data Program

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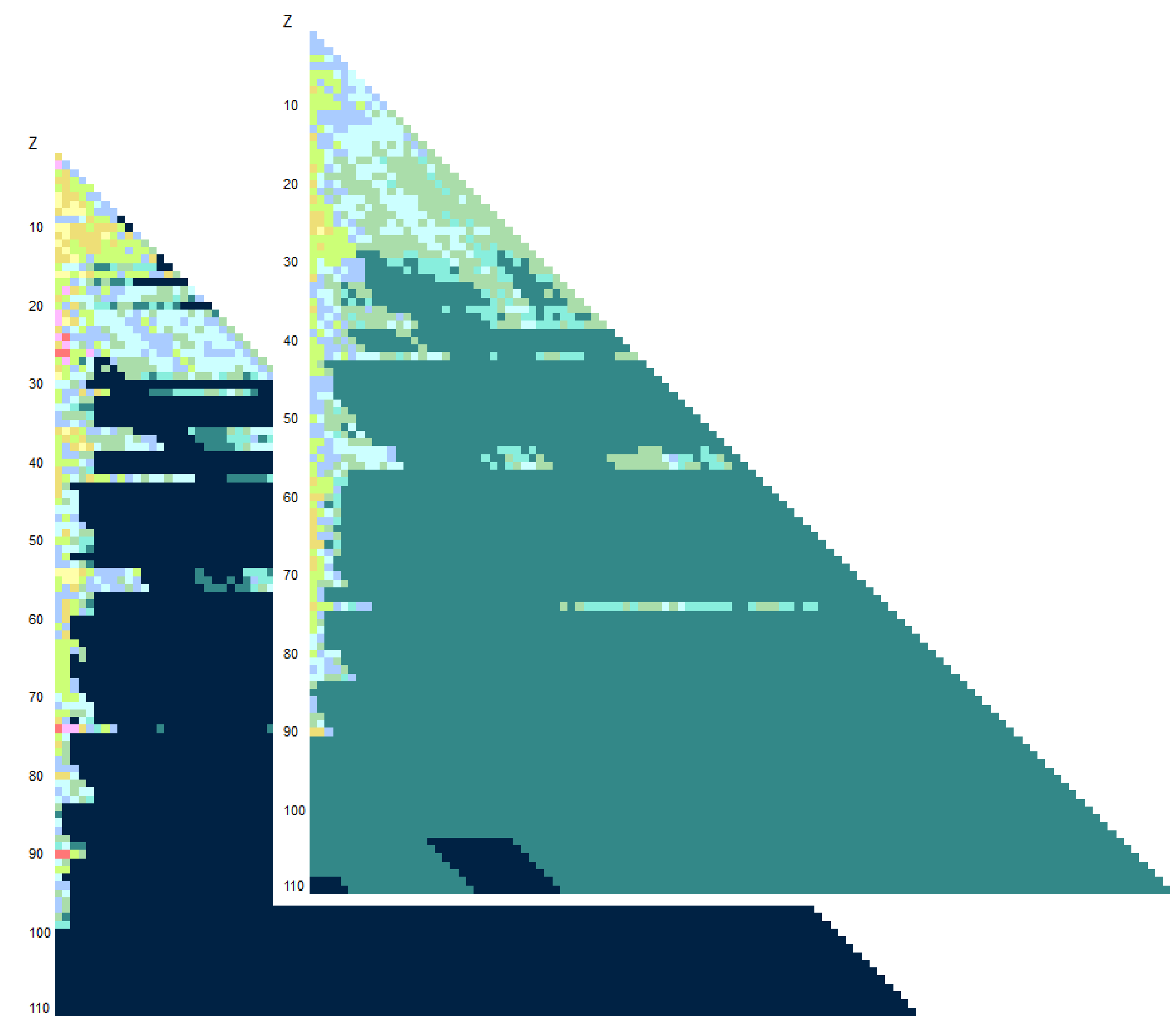

DCN Meeting, IAEA, Sep 4 2017

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Plan

- Staff
- Atomic Spectra Database
  - New version and contents
  - LIBS database
- Bibliographic Databases
- Compilations, modeling and measurements
- Interactions with other data centers
- Conclusions

The Atomic Spectroscopy Data Center: 2017

- Physicists
  - A. Kramida
  - G. Nave
  - Yu. Ralchenko
  - J.N. Tan
  - J. Reader
- Computer support
  - K. Olsen
  - R. Ibacache

- Contractors
  - E.B. Saloman
  - V.I. Azarov
- Guest researchers
  - C. Froese Fischer
  - T. Das
  - H. Kunari
  - Dipti
  - E. Takacs (EBIT)

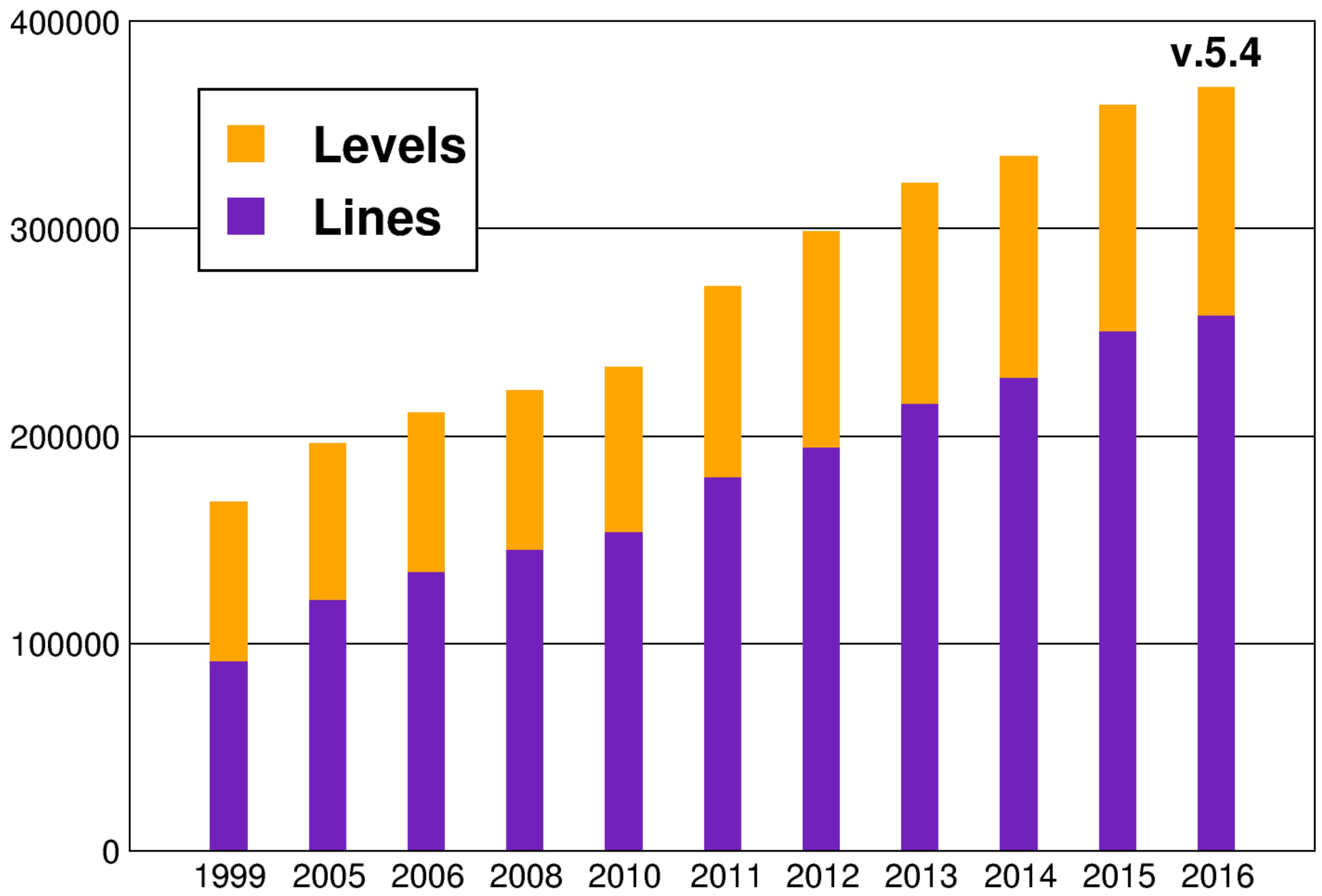
Papers published by the Atomic Spectroscopy Group in 2015-2017

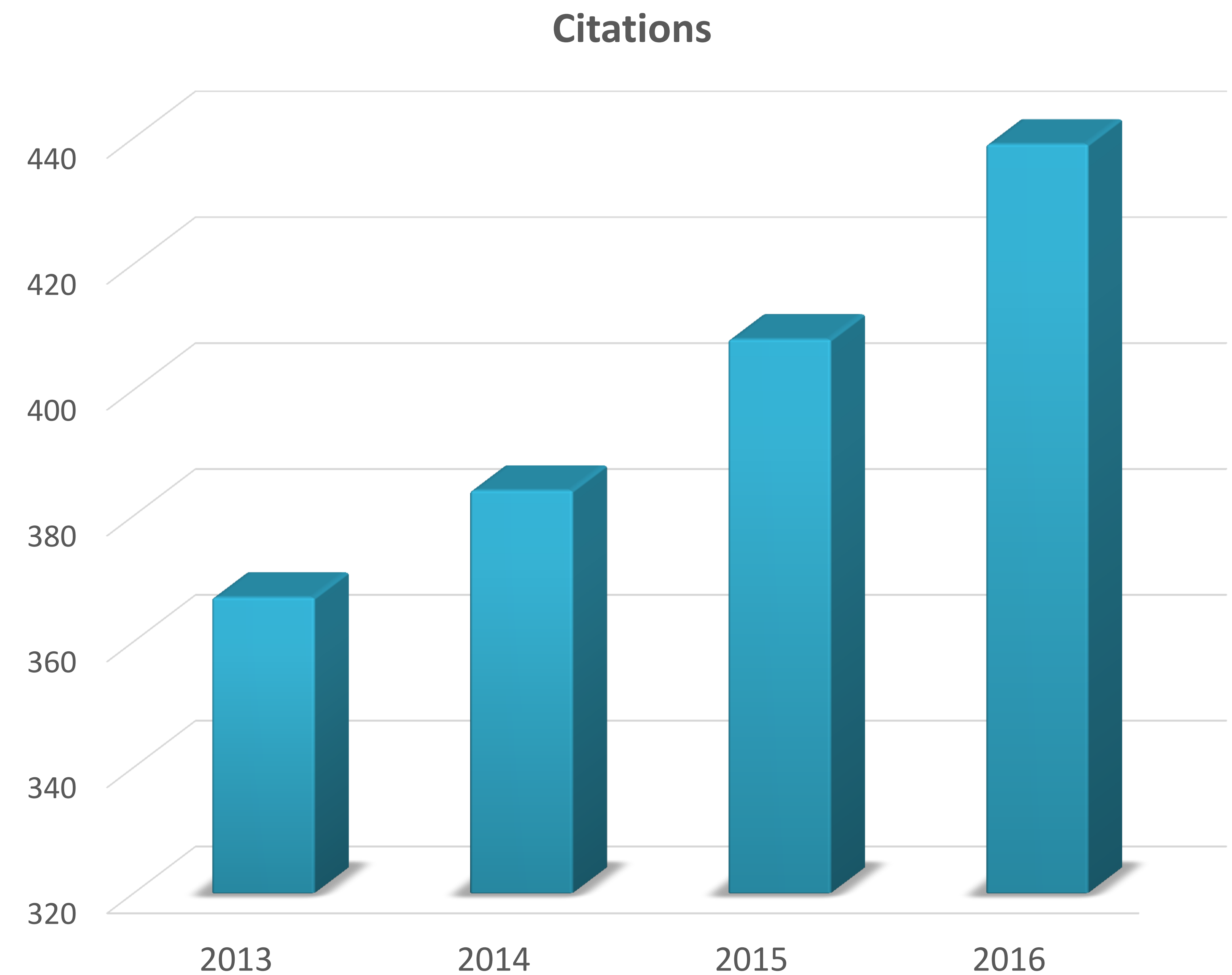
- W.L.Wiese et al, Spectral properties of heavy elements of fusion interest, APID-17 (2017).
- E. B. Saloman and A. Kramida, Critically Evaluated Energy Levels, Spectral Lines, Transition Probabilities, and Intensities of Singly Ionized Vanadium (V II), Astrophys. J., Suppl. Ser. **231**, 19 (2017)
- E. B. Saloman and A. Kramida, Critically Evaluated Energy Levels, Spectral Lines, Transition Probabilities, and Intensities of Neutral Vanadium (V I), Astrophys. J., Suppl. Ser. **231**, 18 (2017)
- R. Piron, F. Gilleron, Y. Aglitskiy, H.-K. Chung, C. J. Fontes, C. B. Hansen, O. Marchuk, H. A. Scott, E. Stambulchik, and Yu. Ralchenko, Review of the 9th NLTE Code Comparison Workshop, High En. Dens. Phys. **23**, 38–47 (2017)
- A. Kramida, Configuration Interactions of Class 11: An Error in Cowan's Atomic Structure Theory, Comput. Phys. Commun. **215**, 47–48 (2017)
- A. Kramida, G. Nave, and J. Reader, The Cu II Spectrum, Atoms **5**, 9 (2017)
- J. Reader and M. D. Lindsay, Spectrum and Energy Levels of Five-Times Ionized Zirconium (Zr VI), Phys. Scr. **91**, 025401 (2016); Erratum: **92**, 039501 (2017)
- M. Wyatt and G. Nave, Evaluation of Resolution and Periodic Errors of a Flatbed Scanner Used for Digitizing Spectroscopic Photographic Plates, Appl. Opt. **56**, 3744–3749 (2017)
- G. Shafir,…, Yu. Ralchenko, and Y.E. Krasik, Characterization of inductively coupled plasma generated by a quadruple antenna, PSST **26**, 025005 (2017).
- V. I. Azarov and R. R. Gayasov, Revised and Extended Analysis of the Eighth Spectrum of Platinum (Pt VIII), At. Data Nucl. Data Tables **115-116**, 369–384 (2017)
- V. I. Azarov and R. R. Gayasov, The Seventh Spectrum of Platinum (Pt VII): Analysis of the (5d4+5d36s)–5d36p Transition Array, At. Data Nucl. Data Tables **115-116**, 344–368 (2017)
- V. I. Azarov and R. R. Gayasov, The Sixth Spectrum of Platinum (Pt VI), At. Data Nucl. Data Tables **115-116**, 309–343 (2017)
- V. A. Dzuba, M. S. Safronova, U. I. Safronova, and A. Kramida, Ionization Potentials of Superheavy Elements No, Lr, and Rf and Their Ions, Phys. Rev. A **94**, 042503 (2016)
- M. L. Dubernet, …, Yu. Ralchenko, et al, The Virtual Atomic and Molecular Data Centre (VAMDC) Consortium, J. Phys. B **49**, 074003 (2016)
- Yu. Ralchenko, Validation and Verification of Collisional-Radiative Models, in *Modern Methods in Collisional-Radiative Modeling of Plasmas*, Ch. 8, 181–208 (Edited by Yu. Ralchenko, Springer, New York, 2016)
- J. Reader, Spectrum and Energy Levels of Four-Times Ionized Yttrium (Y V), Atoms **4**, 31 (2016)
- K. Townley-Smith, G. Nave, J. C. Pickering, and R. J. Blackwell-Whitehead, Hyperfine Structure Constants for Singly Ionized Manganese (Mn II) Using Fourier Transform Spectroscopy, Mon. Not. R. Astron. Soc. **461**, 73–78 (2016)
- D. G. Smillie, J. C. Pickering, G. Nave, and P. L. Smith, The Spectrum and Term Analysis of Co III Measured Using Fourier Transform and Grating Spectroscopy, Astrophys. J., Suppl. Ser. **223**, 12 (2016)
- V. I. Azarov and R. R. Gayasov, The Fourth Spectrum of Platinum (Pt IV): Determination of the 5d7, 5d66s and 5d66p Configurations, At. Data Nucl. Data Tables **108**, 118–153 (2016)
- V. I. Azarov and R. R. Gayasov, The Fourth Spectrum of Iridium (Ir IV), At. Data Nucl. Data Tables **108**, 81–117 (2016)

NIST Atomic Spectra Database

- **v. 5.4 (September 2016)**
  - Major updates
    - E/λ/A: **Co III, Sr II, Zr VI, Pt IV-V, Ir IV, Pb I, Ra I-II**
    - λ/A: **Y I-II, Mo O, Rh I, Nd II, Eu I, Pr II, Dy I, Tm I, Lu I, Ta I, Ir I**
    - A uncertainties & bibliography: **Cu I-II, Zn I-II, Ge I-II, Cd I-II, Sn I, Cs I, Hg I, Tl I, U I**
    - IP: **Zr VI, Nd III, Pm III, Sm III, Lu III, Ra II**

NIST ASD content and citations





v.5.4:
110,000 levels
258,000 lines

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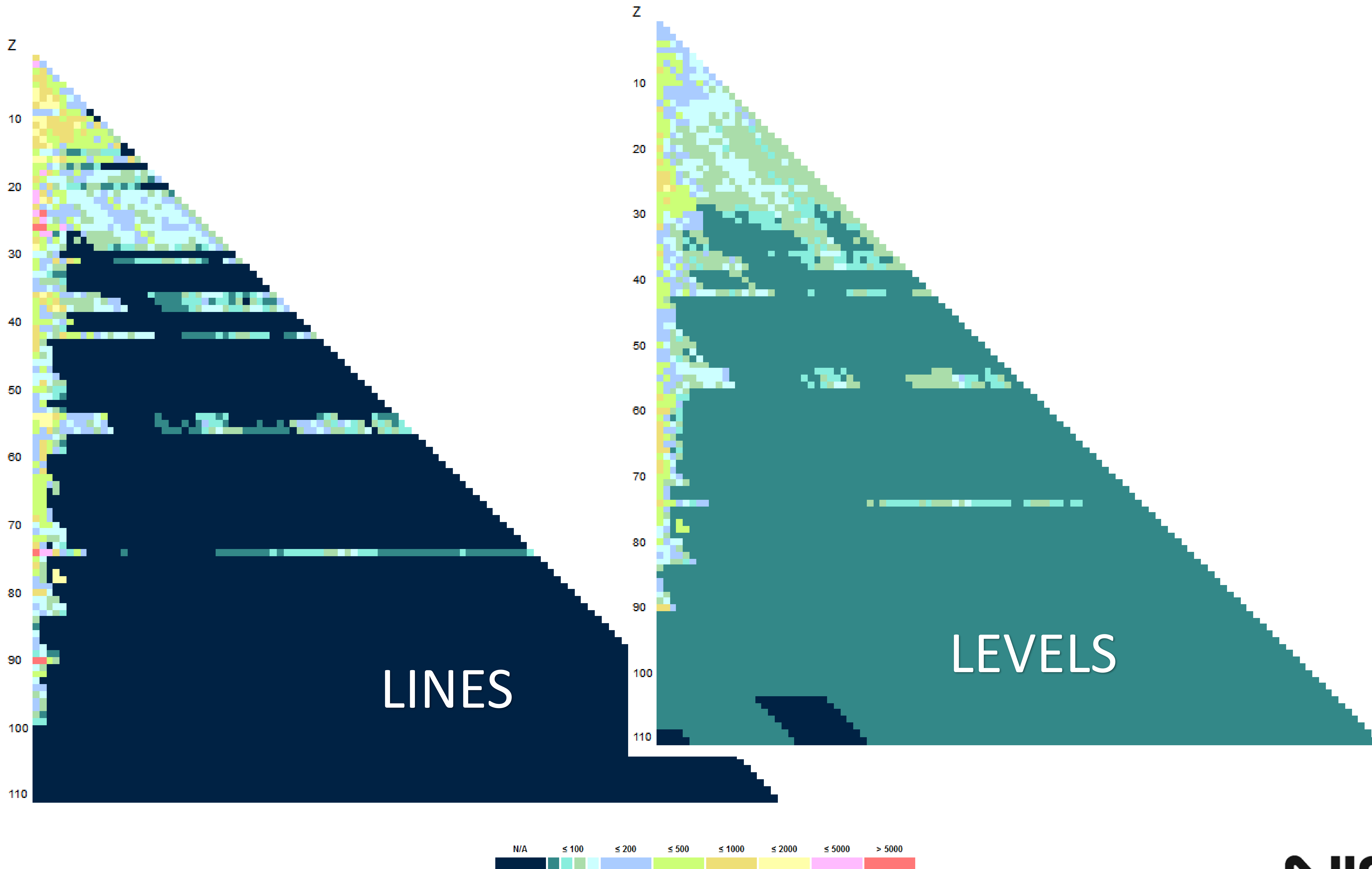
Detailed content of ASD 5.4



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Planned additions to ASD v.5.5 (Oct 2017)

Spectra	IP revised	Levels added	Lines added	TP added
Y V	1	81	525	600
Cu II		107	1990	548
V I		81	3228	761
V II	1	84	3371	1742
Lu II, Hf II-III, No I-II, Lr I-III, Rf I-IV	12			
Pt VI		212	1390	1390
Pt VII		176	759	759
Pt VIII		67	349	349
C I	1	131	624	238
Total	**15**	**939**	**12236**	**6387**

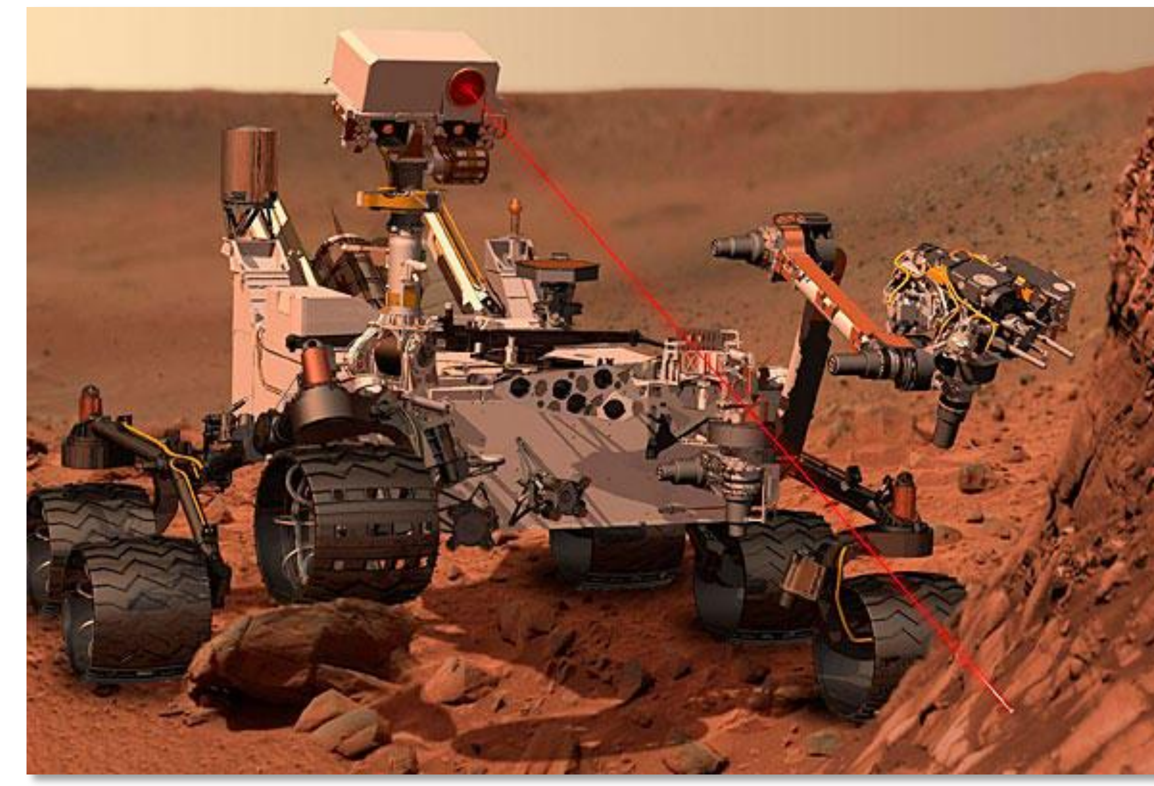
New NIST LIBS Database:
Laser Induced Breakdown Spectroscopy

https://physics.nist.gov/LIBS

NIST LIBS Database

Please specify Element

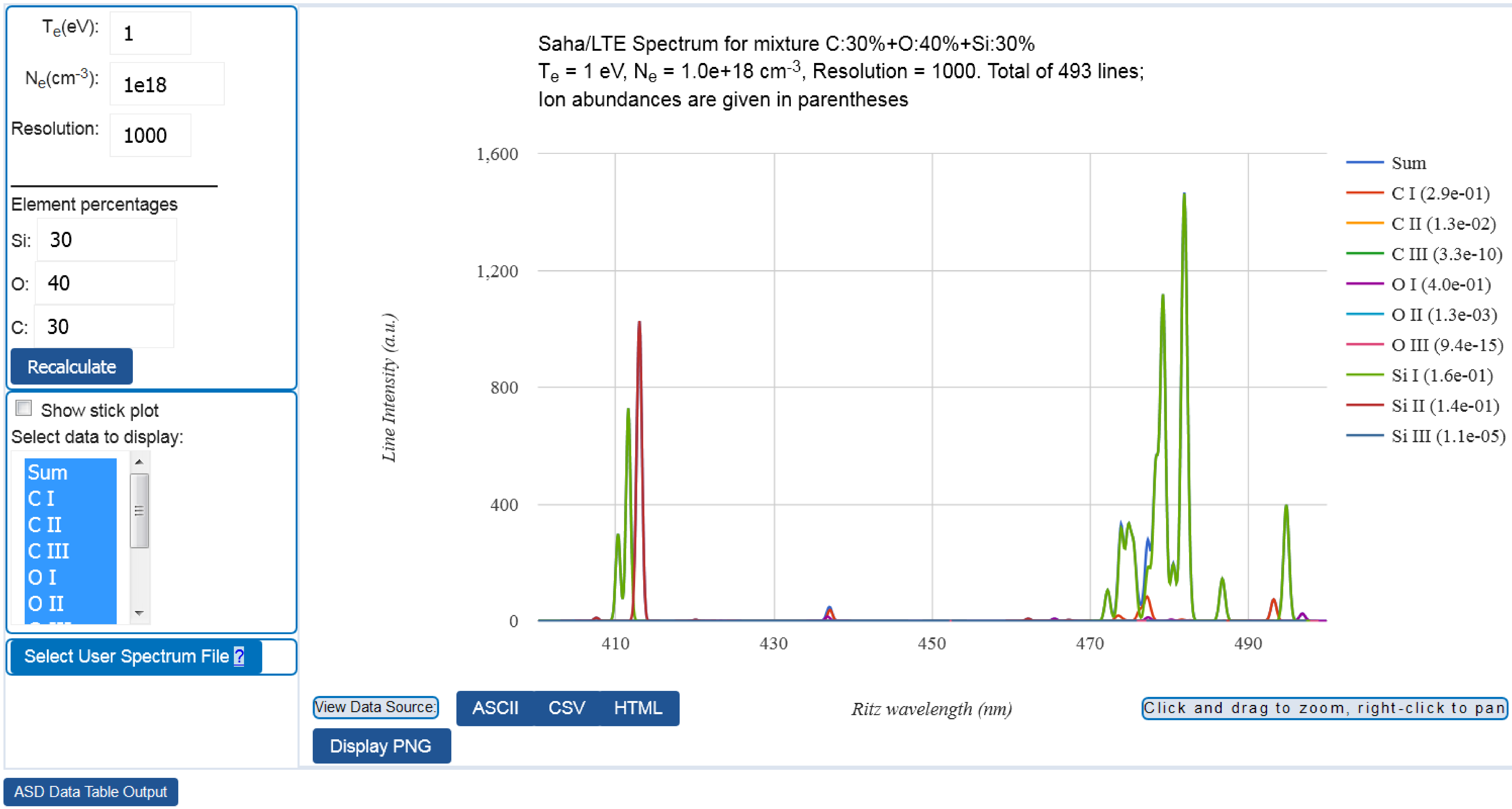
Element:	
Percentage:	100
Lower Wavelength:	200
Upper Wavelength:	600
Wavelengths in:	(•) Vacuum (< 200 nm) Air (200 - 2000 nm) Vacuum (> 2000 nm) ( ) Vacuum (all wavelengths)
Units:	nm
Resolution:	1000
T_e(eV):	1
N_e(cm^{-3}):	1e17



Credit: NASA

- Calculation of Saha/LTE spectra for the first three ions of any element or combination thereof in ASD
- Similar to the Saha/LTE interface of ASD
- Rich graphical services
- Arbitrary plasma parameters and spectrum resolution

LIBS DB output example



- Offers various selection and zooming options
- A user can upload a file for comparisons

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Bibliographic databases

http://www.nist.gov/pml/data/asbib/index.cfm

- Principal developer: A. Kramida
- Updated regularly (~2 weeks)

- **Atomic Energy Levels and Spectra**
  - **20,018** references, 1802-2017
- **Atomic Transition Probabilities**
  - **9,380** references, 1914-2017
- **Atomic Lines Broadening and Shifts**
  - **6,923** references, 1889-2017

- Annually submitted to IAEA

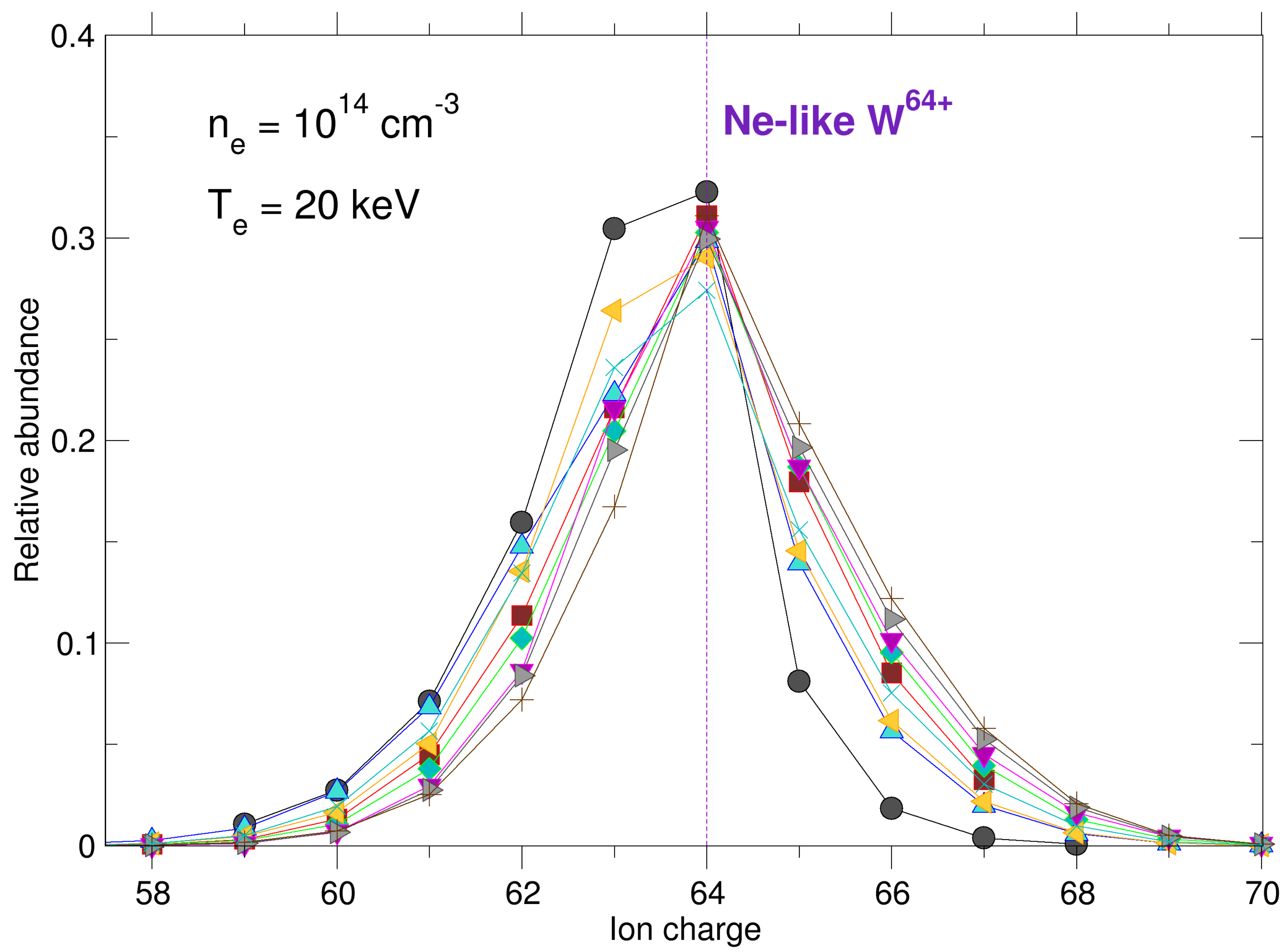
- Search options
  - Elements/ions
  - Isoelectronic sequence
  - Word/patterm
  - Publication years
  - Publication source
  - Method type
  - Keywords
  - General category
  - Specific subjects of interest

New data: 2016-2017

- **Compilations and data**
  - **V I-II** (Saloman & Kramida, 2017)
  - **Cu II** (Kramida et al, 2017)
  - **Zr VI** (Reader & Lindsay, 2017)
  - **Pt IV, VI-VIII** (Azarov & Gayazov, 2016-2017)
  - **Y V** (Reader, 2016)
  - **Mn II** (Tonwley-Smith et al, 2016)
  - **Co III** (Smilley et al, 2016)
  - **Ir IV** (Azarov & Gayazov, 2016)
- **EBIT Measurements**
  - Dielectronic resonances in highly-charged **W** and **Yb**
  - **Y XXVII-XXXVII**
  - **Yb XXXIV-XLV**
  - He- and Li-like **Ar**
  - Isotope shifts in **Xe XLIV**

THEORY: charge exchange spectra for W^{64+}+H collisions

Yu. Ralchenko & D.R. Schultz



W^{64+}: the most abundant ion in the core…
…however, there is no realistic data for its interactions with the neutral H beam particles

Classical Trajectory Monte Carlo

- **pCTMC** (Abrines & Percival 1966, Olson & Salop 1977)
  - Original and most frequently employed
  - Microcanonical distribution reproduces QM electronic *momentum* (**p**) probability distribution
- **rCTMC** (Hardie & Olson 1983, Cohen 1985)
  - reproduces QM electronic *radial* (**r**) probability distribution

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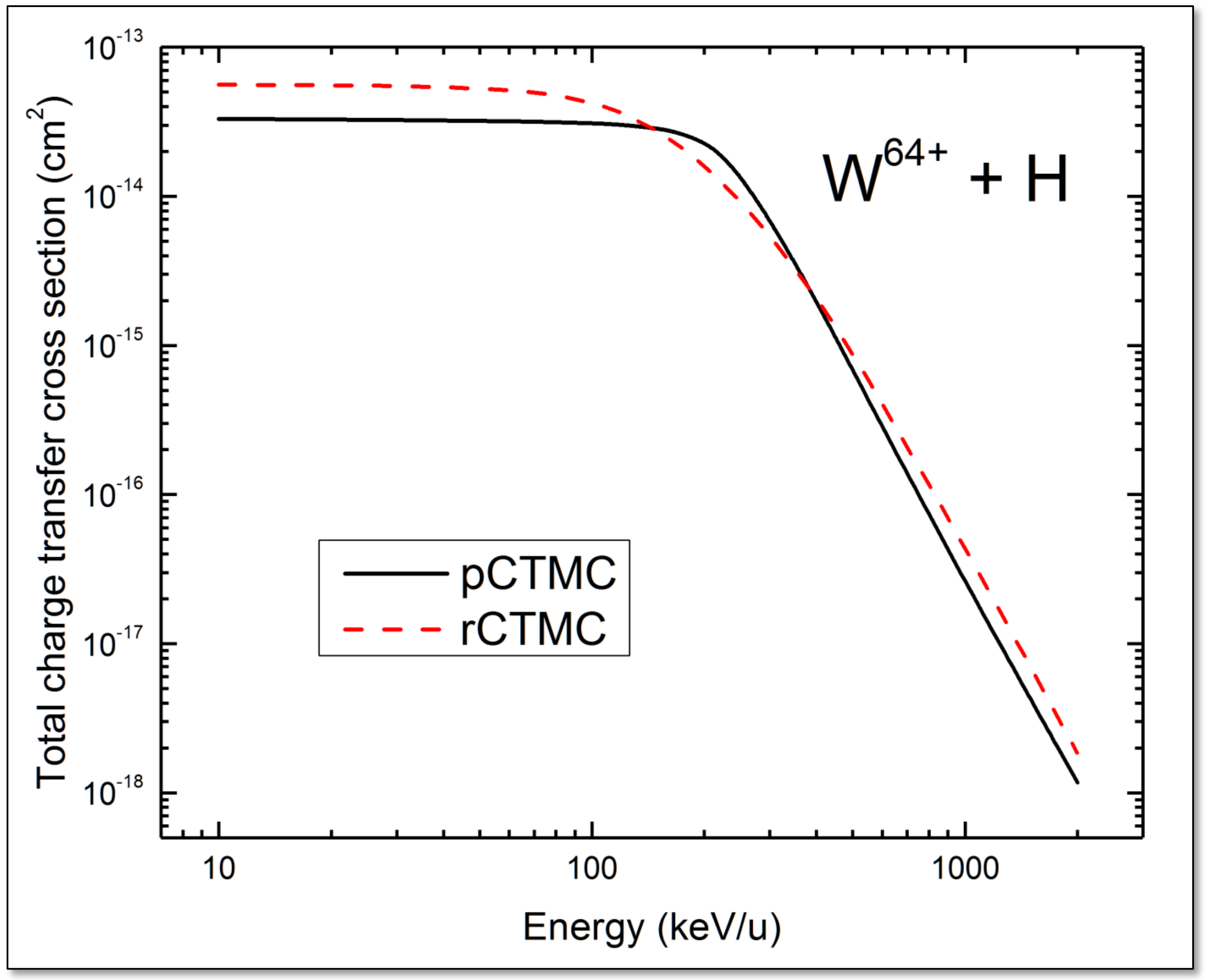
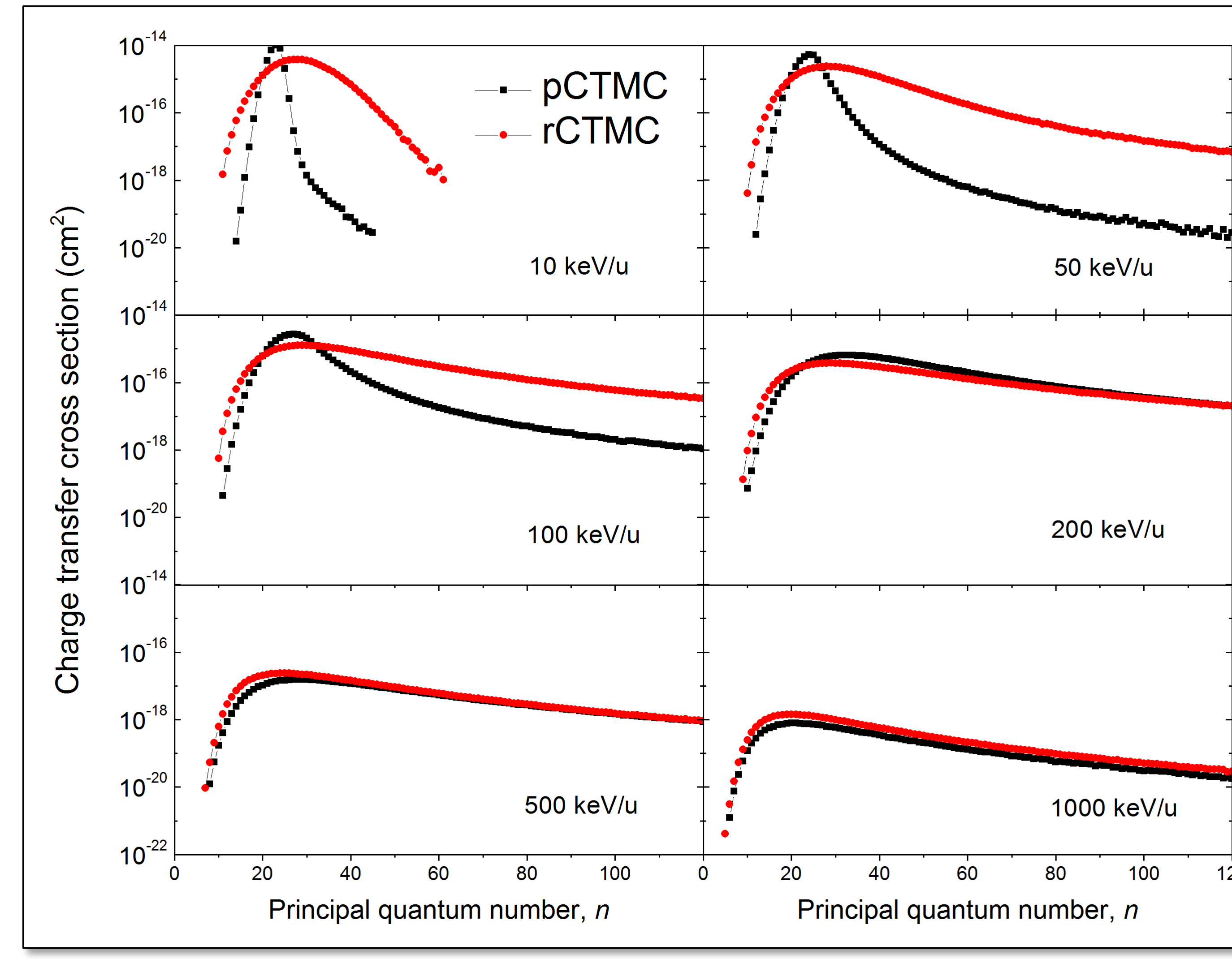
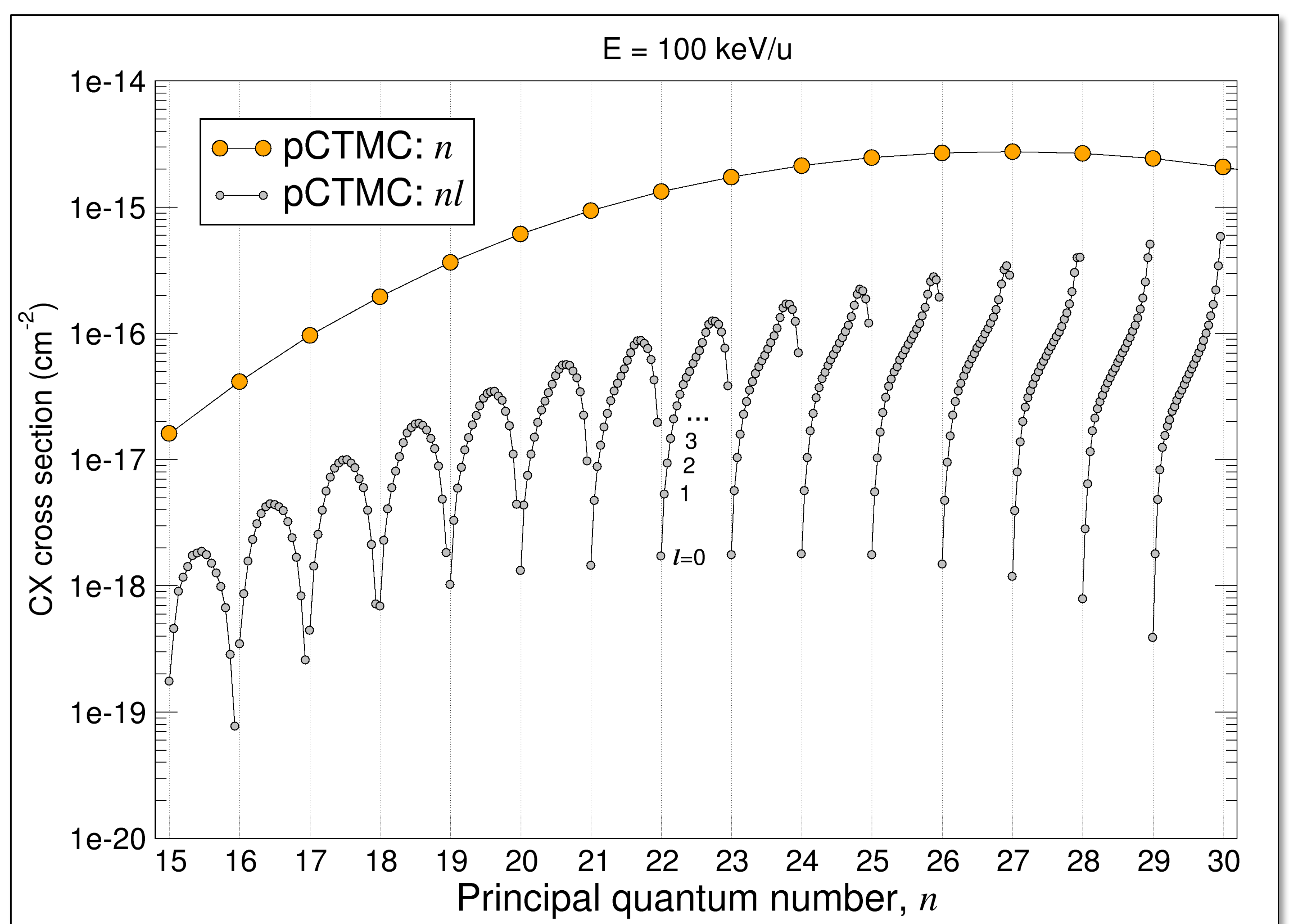
Total, *n*- and *nl*-selective cross sections







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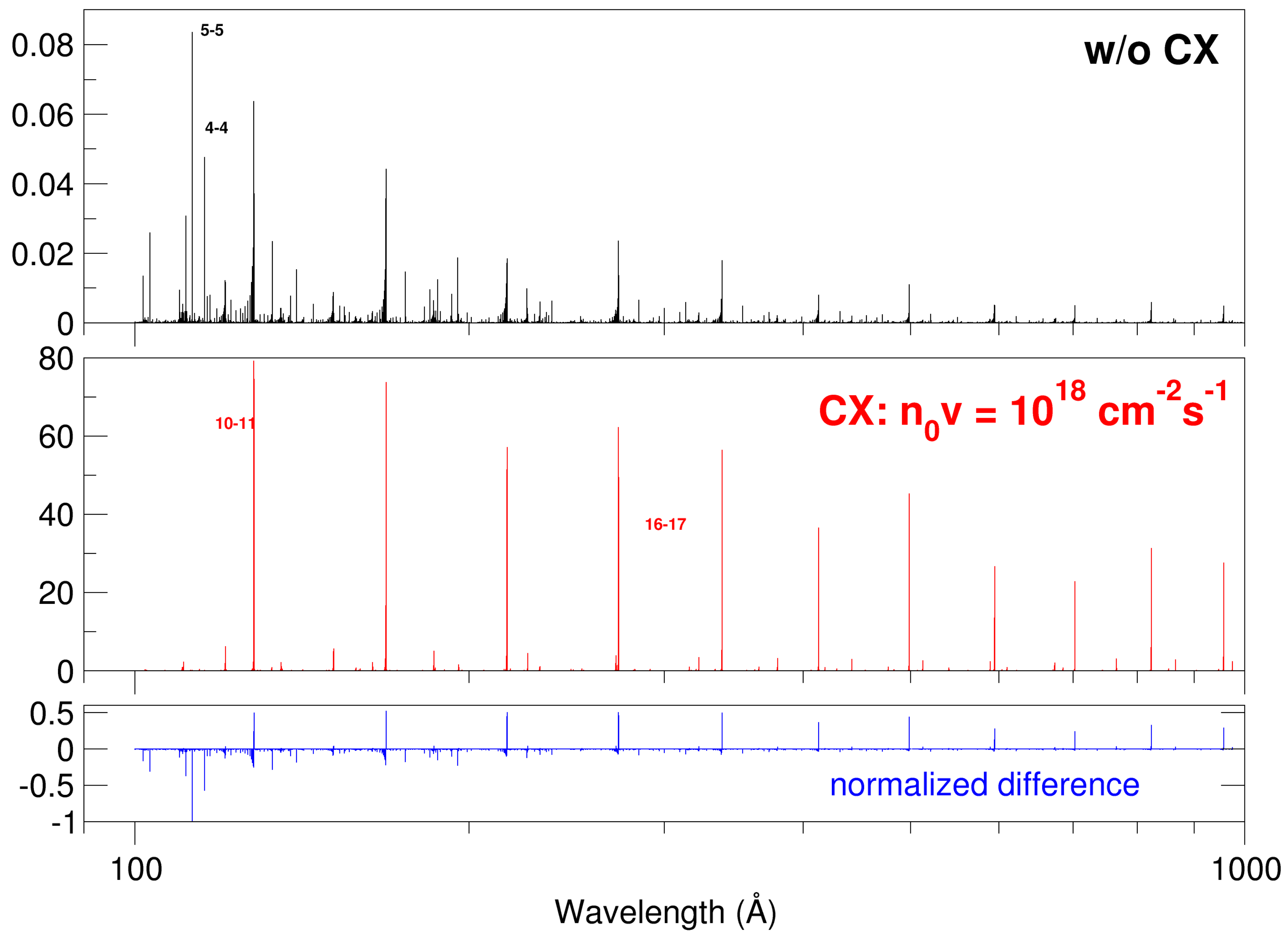
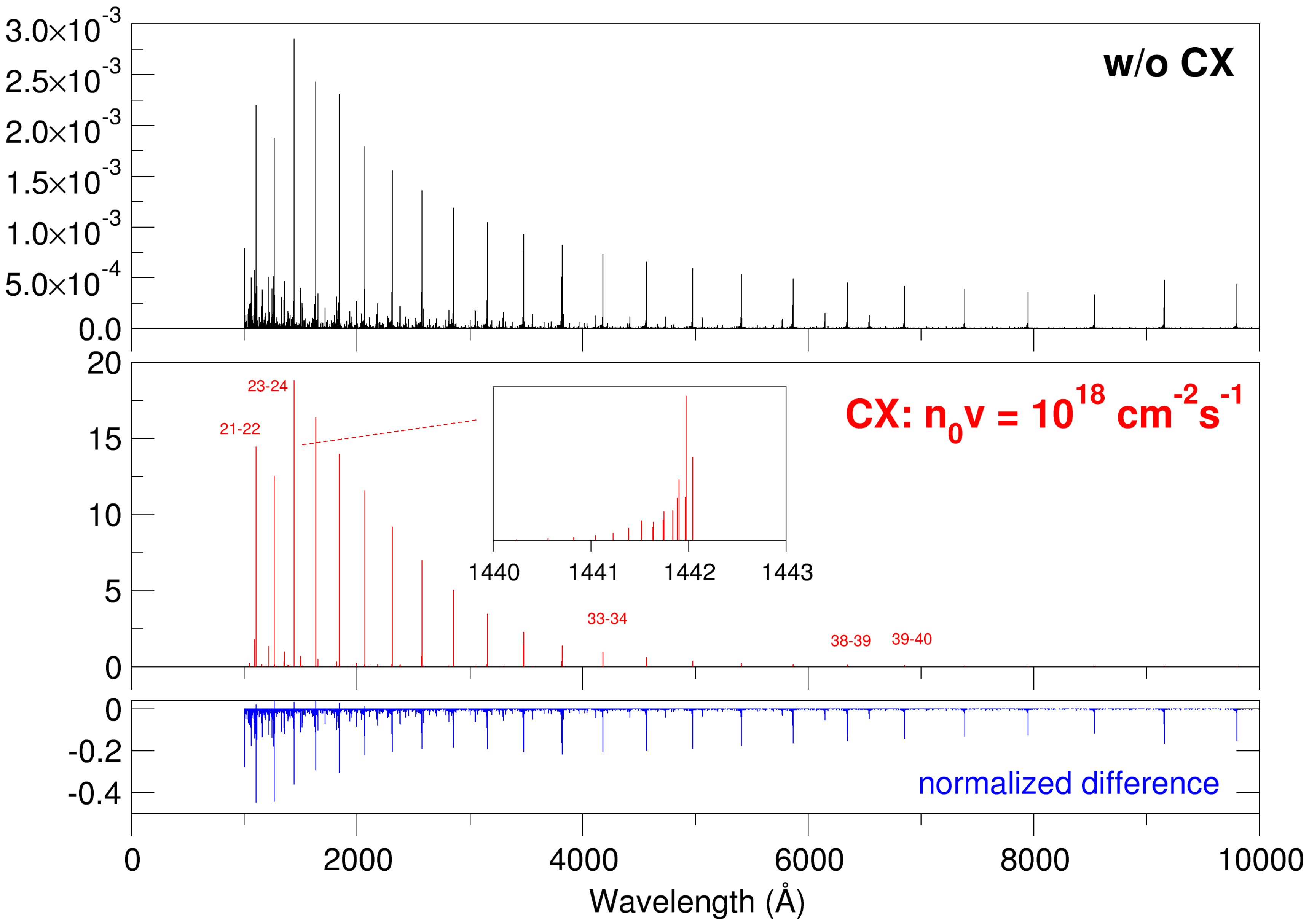
Examples of calculated spectra

CR model: Na-like and Ne-like (g.s. only); ~6000 FS levels; 20 keV & 10^{14} cm^{-3}
All important physical processes (including collisions with protons) are taken into account

pCTMC 100 keV/u: 100 - 1000 Å

pCTMC 100 keV/u: 1000 - 10000 Å



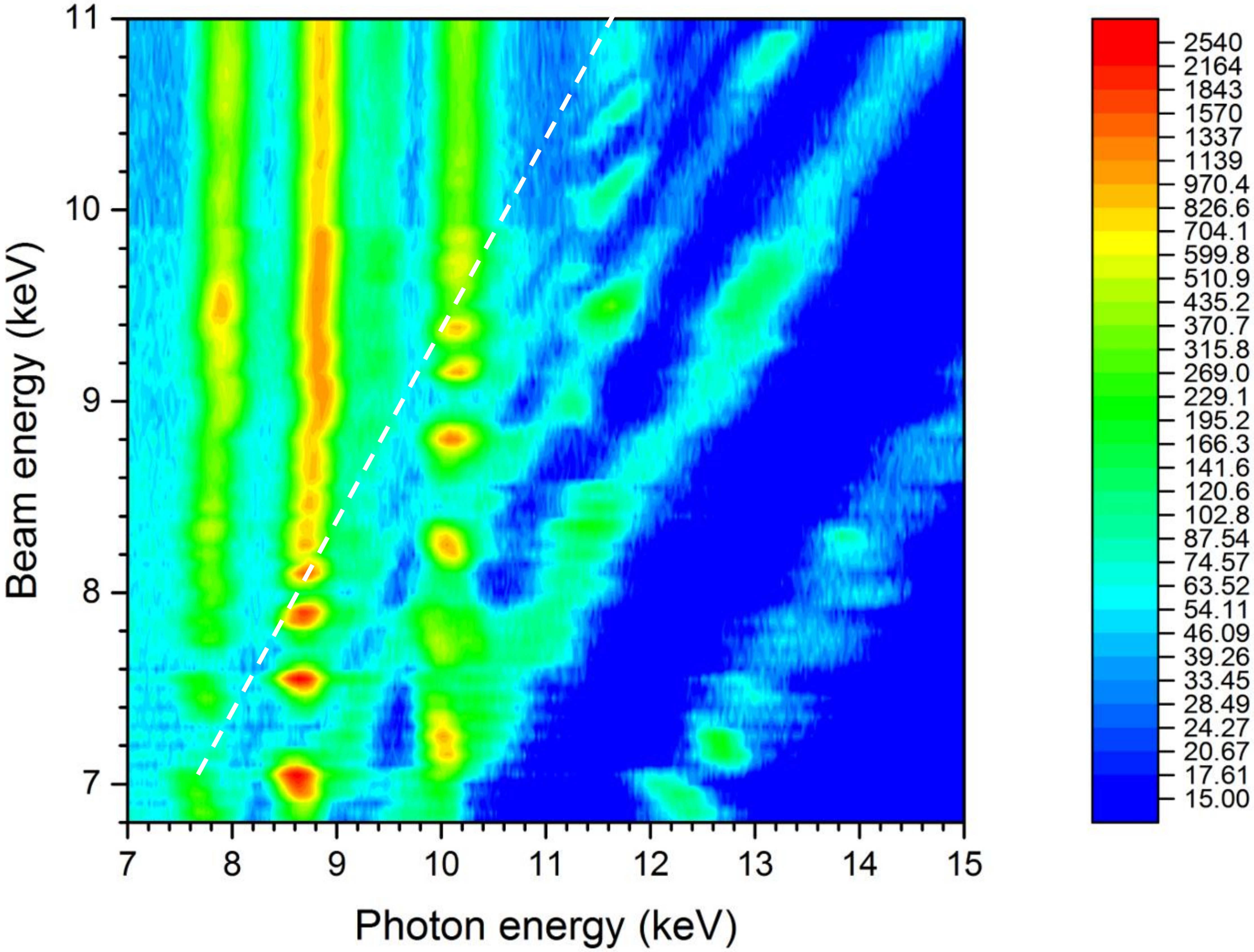


Strongest: Δn=1

NIST EBIT:
Inner-shell DR resonances in highly-charged W ions

A.A. Borovik, Jr., Dipti, et al, to be published

NIST EBIT: W for E_b = 7-11 keV

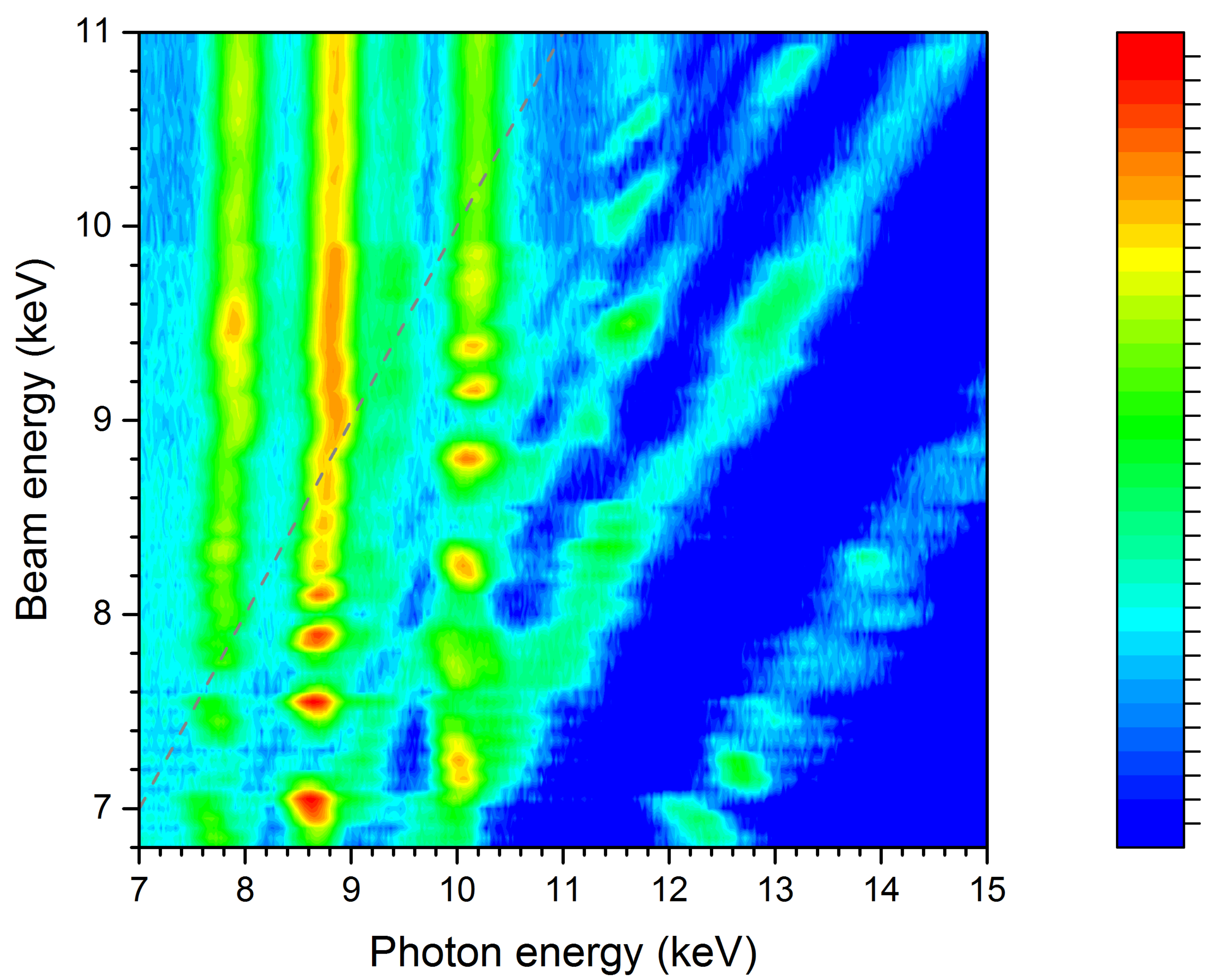


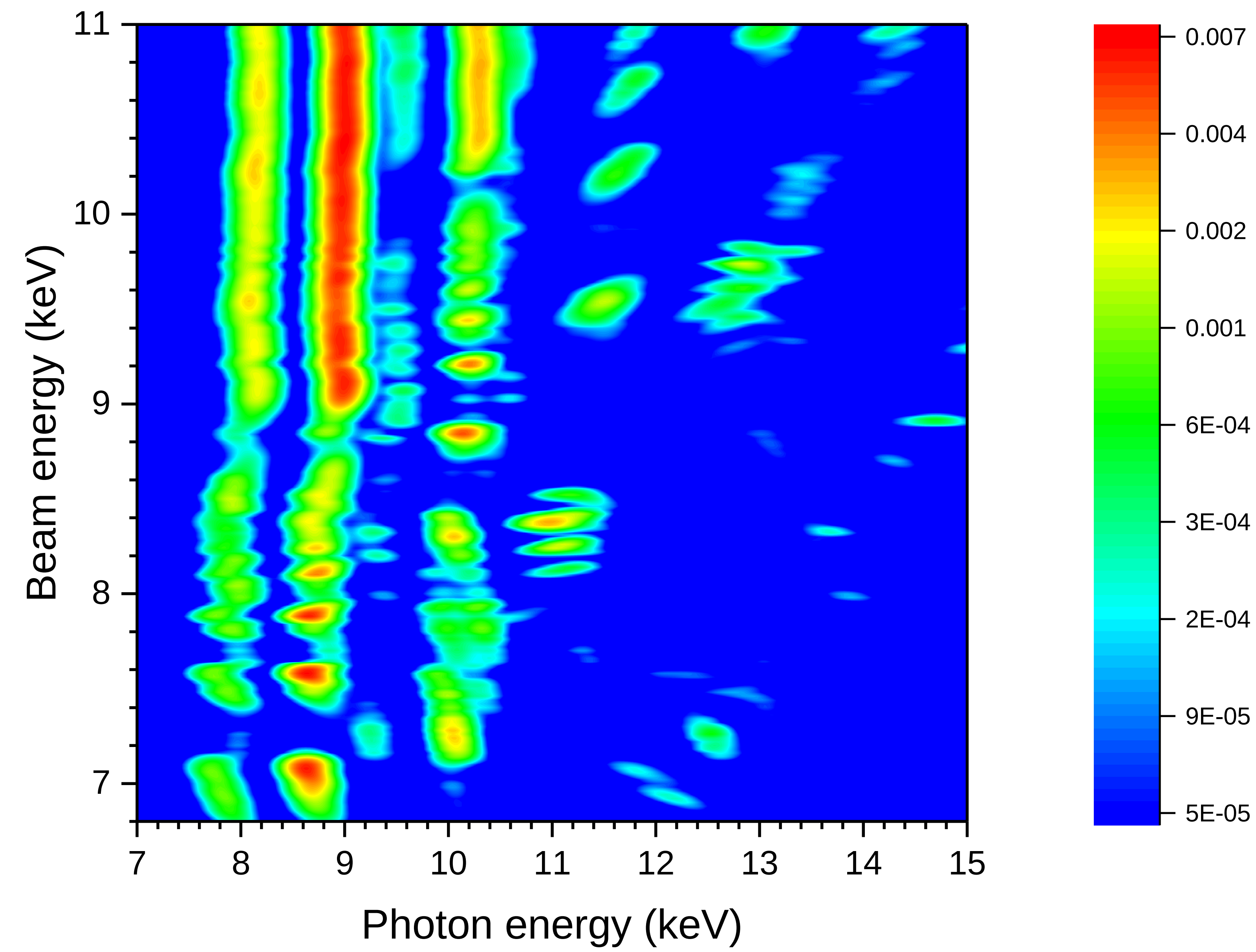
What to include in the CR model (NOMAD):

- W^{50+}-W^{64+}
- Data: relativistic Flexible Atomic Code (M.F. Gu)
- Low exp resolution (~150 eV): relativistic configurations are good
- >50,000 RCs
    - $n_{max} \leq 9$
    - $n_{max} \leq 15$
    - millions of transitions
- Gaussian EEDF of the beam

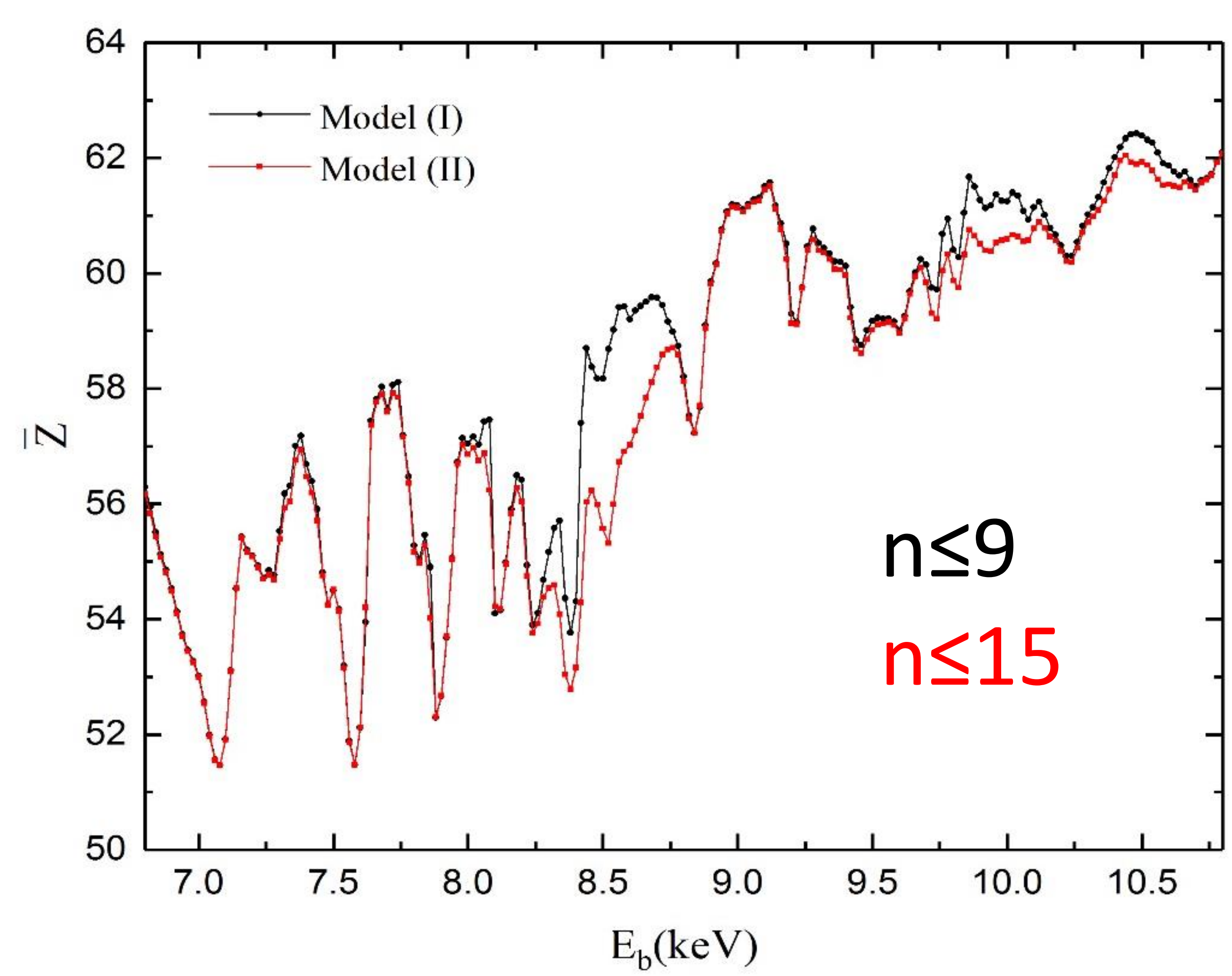
Experiment: W, beam 7-11 keV

Theory: NOMAD





Each feature due to contribution from several ions: energy is almost the same BUT: intensity depends on the balance



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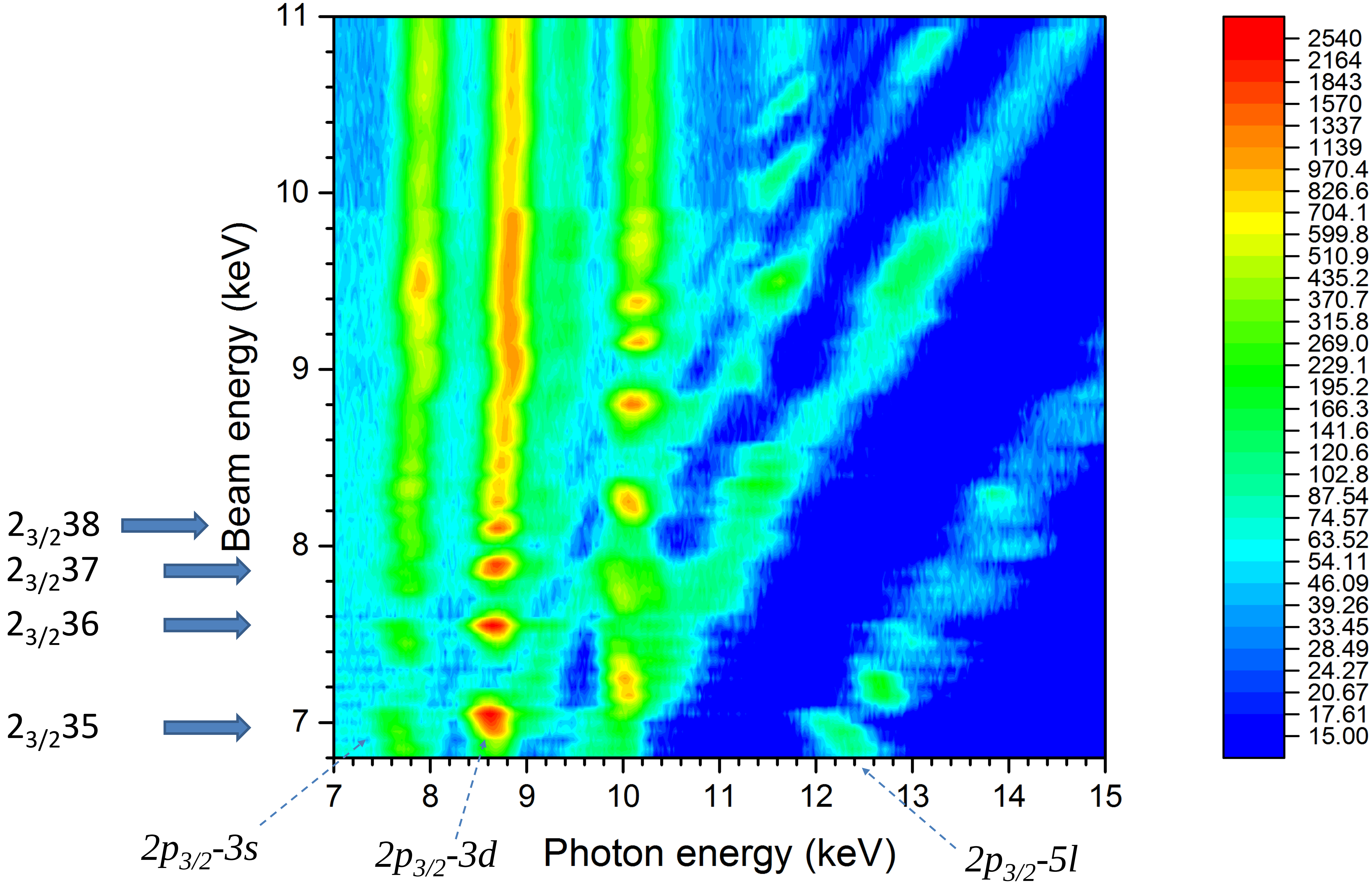
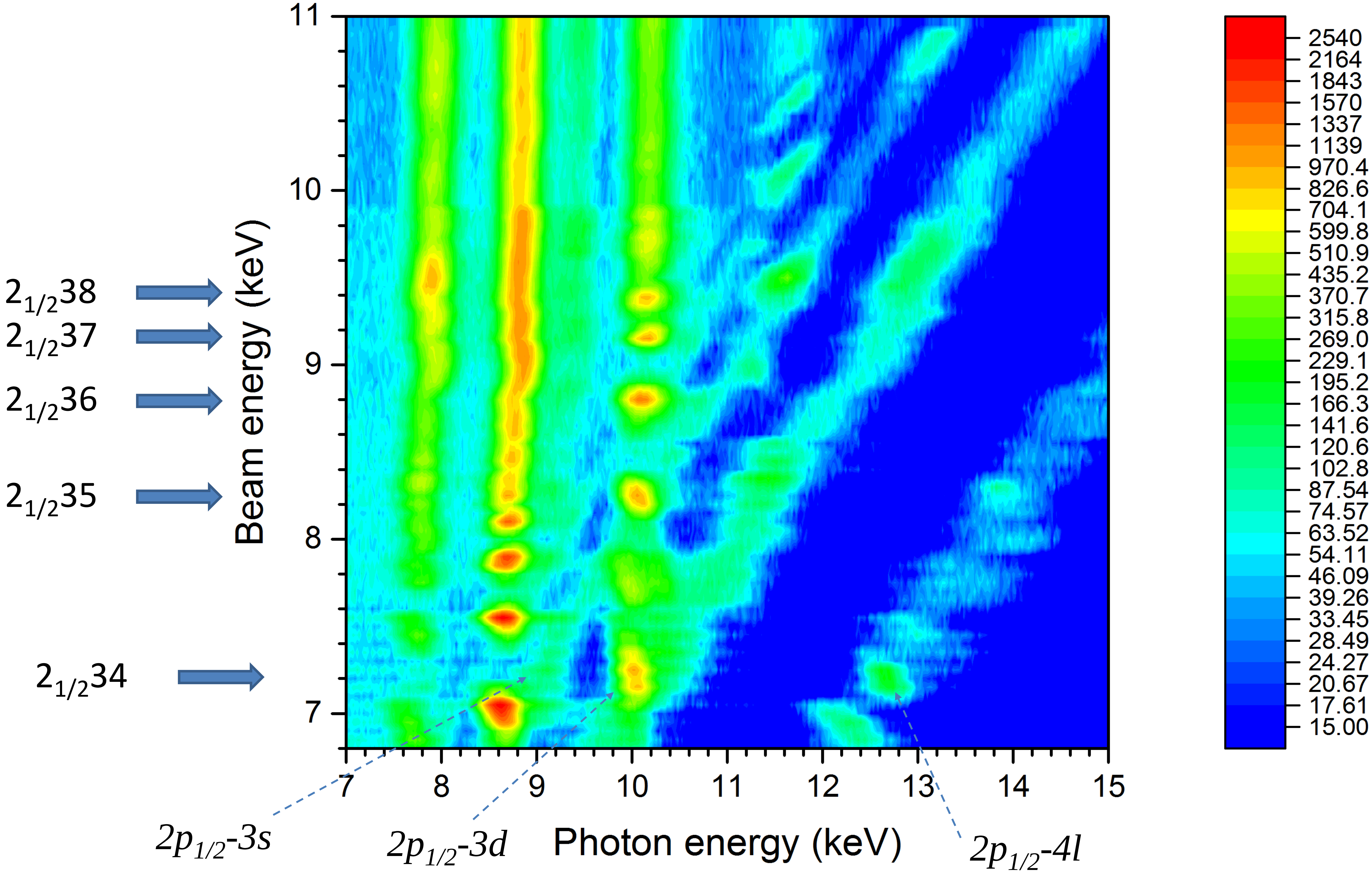
$$1s^2 2s^2 \mathbf{2p^6} 3s^2 3p^m \mathbf{3d^k} + e \rightarrow 1s^2 2s^2 \mathbf{2p^5} 3s^2 3p^m \mathbf{3d^{k+1} nl}$$



$L_{3/2}Mn$

Every spectral feature is identified

$$1s^2 2s^2 \mathbf{2p^6} 3s^2 3p^m \mathbf{3d^k} + e \rightarrow 1s^2 2s^2 \mathbf{2p^5} 3s^2 3p^m \mathbf{3d^{k+1} nl}$$



$L_{1/2}Mn$

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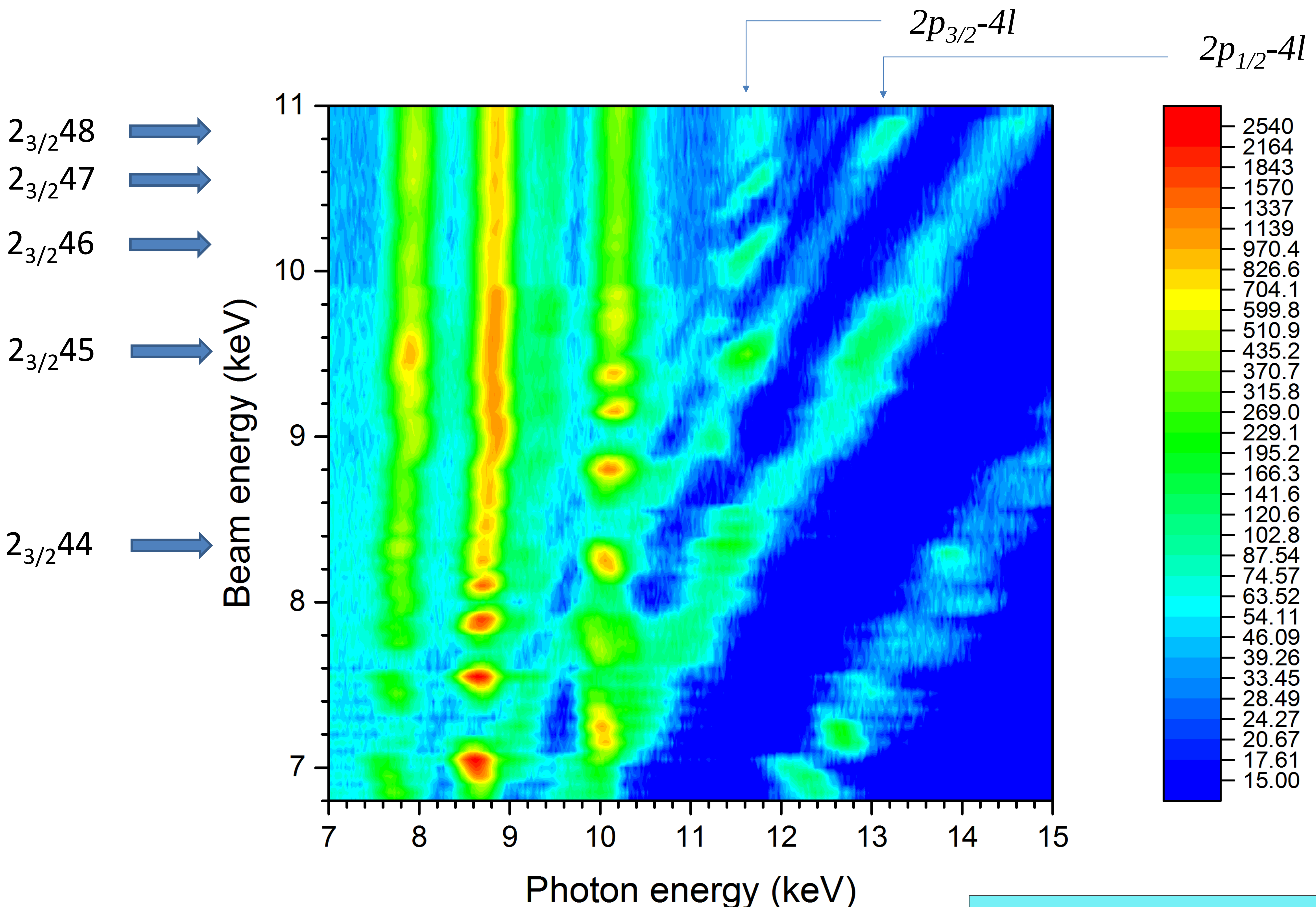
$$1s^2 2s^2 \mathbf{2p^6} 3s^2 3p^m \mathbf{3d^k} + e \rightarrow 1s^2 2s^2 \mathbf{2p^5} 3s^2 3p^m \mathbf{3d^k 4lnl'}$$



LNn

Future plans:
Better resolution

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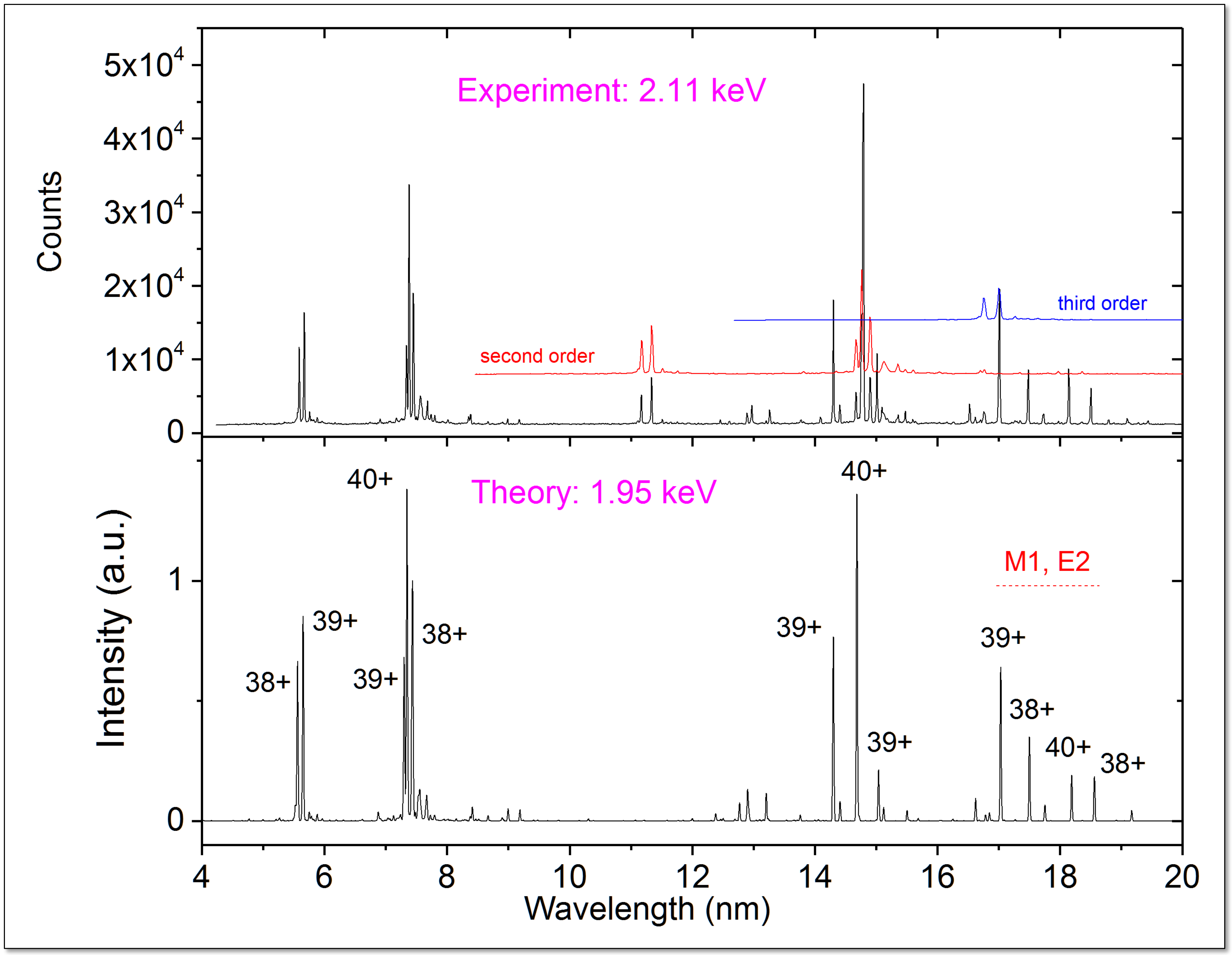
EBIT EUV spectra of Yb



Model for Yb:

- Ion stages: 33+ to 44+
- About 10,000 **FS levels**
- About 50,000,000 transitions

4l-4l' transitions in Zn-, Ga-, and Ge-like ions

Identified dozens of new 4-4 spectral lines in highly-charged ions of Yb

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Online Collisional-Radiative Modeling: FLYCHK

- FLYCHK
  - CR code developed at LLNL (H.-K. Chung, R.W. Lee)
  - Time-dependent, non-Maxwellian, opacity effect, radiation field,…
  - http://nlte.nist.gov/FLY
  - >**900** users from all over the world

Interaction with other Data Centers

- **IAEA AMDU**
  - **Evaluation of Be I collisional data** (*Yu.Ralchenko*)
  - **Bibliographic data** (*A.Kramida*)
  - **ICTP-IAEA School and Workshop, Feb 2017** (*Yu.Ralchenko*)
- **VAMDC**
  - **External partner with SUP@VAMDC**
  - **Meeting at Paris** (2017)
- **Conferences**
  - ICAMDATA
  - ASOS
  - ICPEAC
  - APiP
  - NLTE Workshops
  - …

Conclusions

- NIST Atomic Data Center continues collection, evaluation, and dissemination of accurate atomic spectroscopic data relevant to fusion and other fields of research
- Funding issues do affect connections with the fusion community