Current Status of the NIST Atomic Data Program

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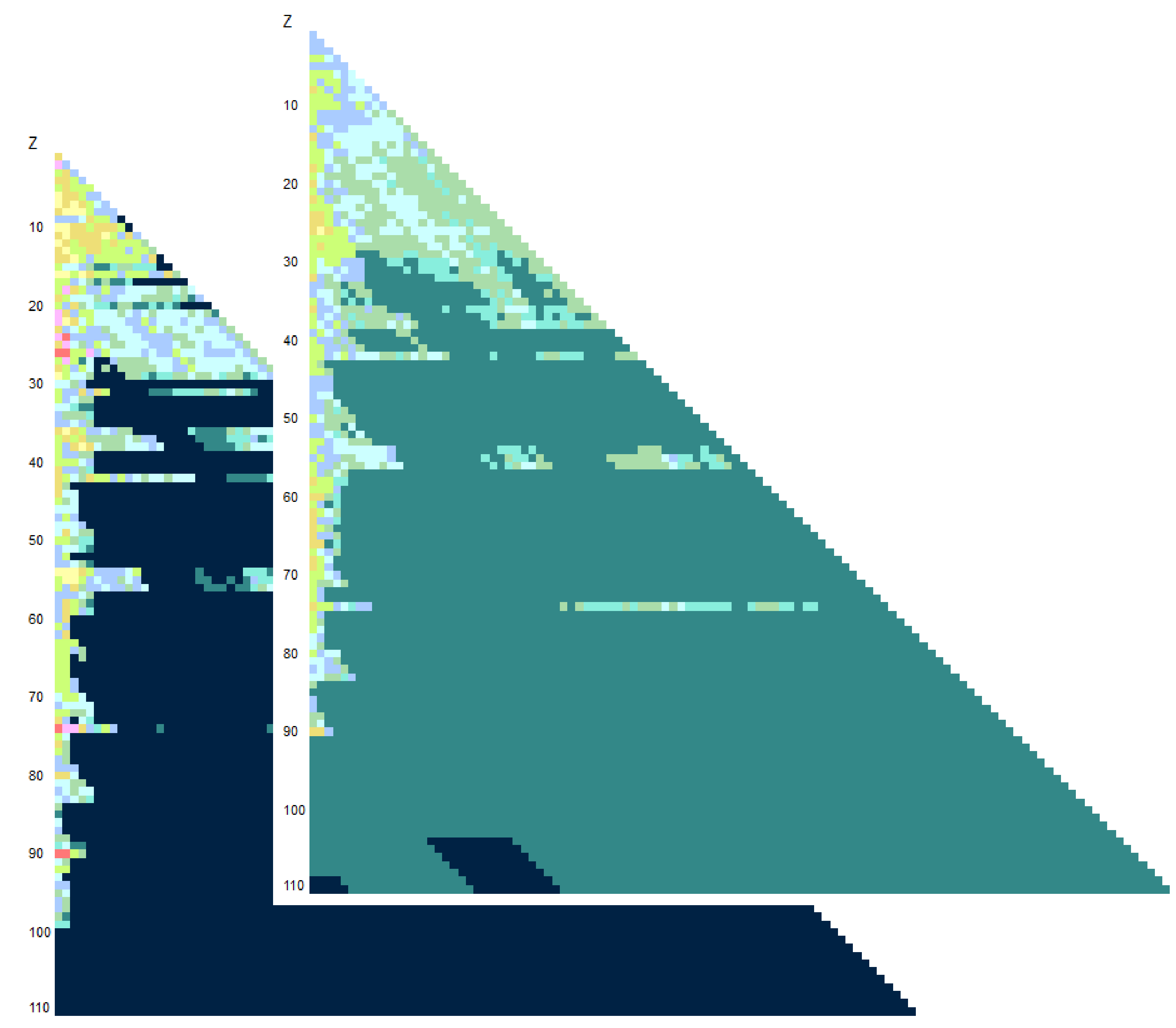

DCN Meeting, IAEA, Vienna, 2015

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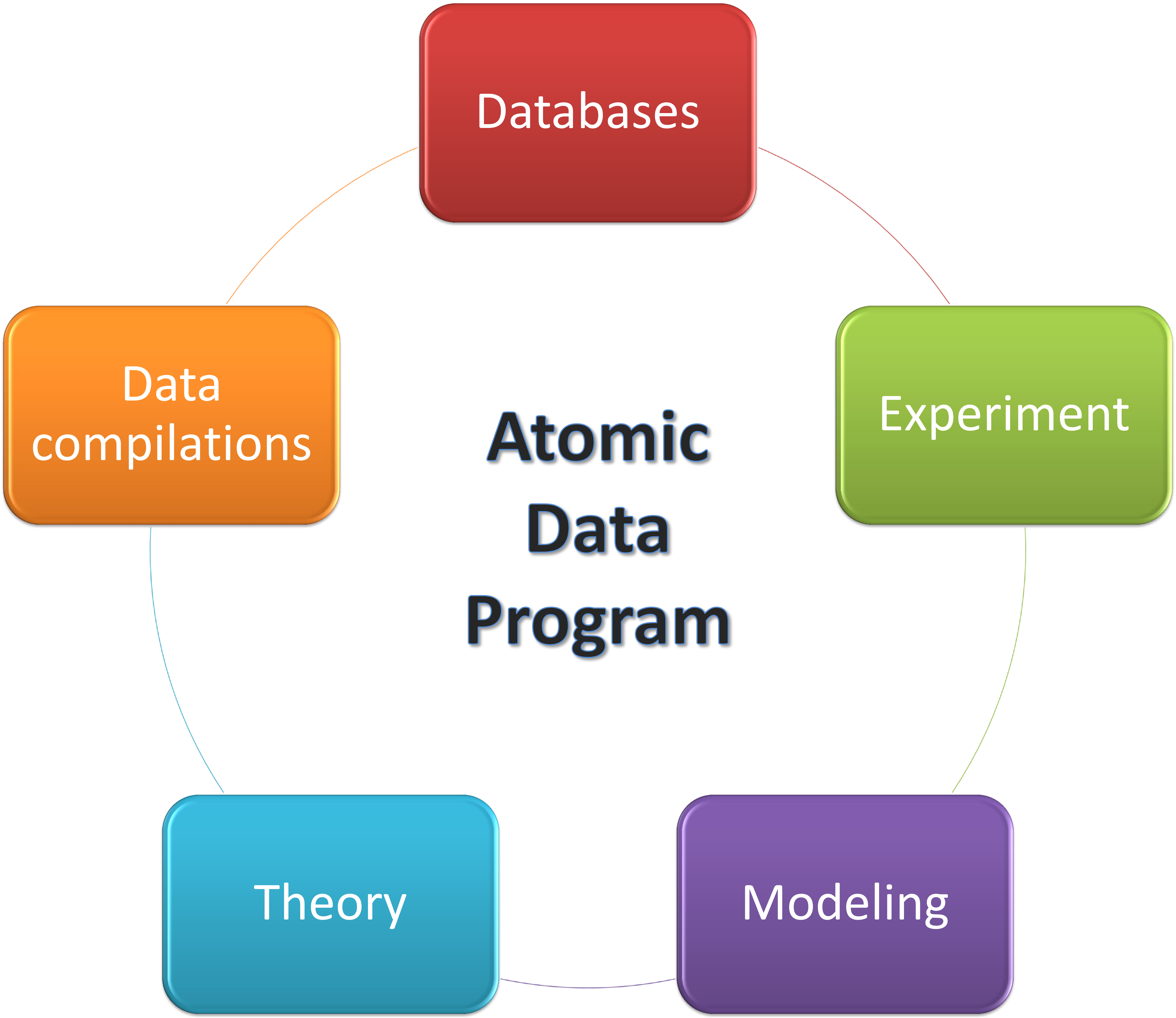

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Plan

- Staff
- Atomic Spectra Database
  - New versions and contents
- Bibliographic Databases
- Compilations, modeling and measurements
  - Examples: Mo V, highly-charged Er
  - O^{6+}+A charge exchange
- Interactions with other data centers
  - ICTP-IAEA School
- Conclusions

The Atomic Spectroscopy Data Center: 2015

- Physicists
  - A. Kramida
  - G. Nave
  - Yu. Ralchenko
  - J. Reader
- Postdoctoral Fellows
  - M. Wood
  - J. Dreiling
- Computer support
  - K. Olsen
  - R. Ibacache

- Contractors
  - E.B. Saloman
  - V.I. Azarov
- Guest researchers
  - C. Froese Fischer
    - …
  - T. Das
  - H. Kunari
  - Many other visitors…
- Losses
  - J.D. Gillaspy
  - Y.A. Podpaly

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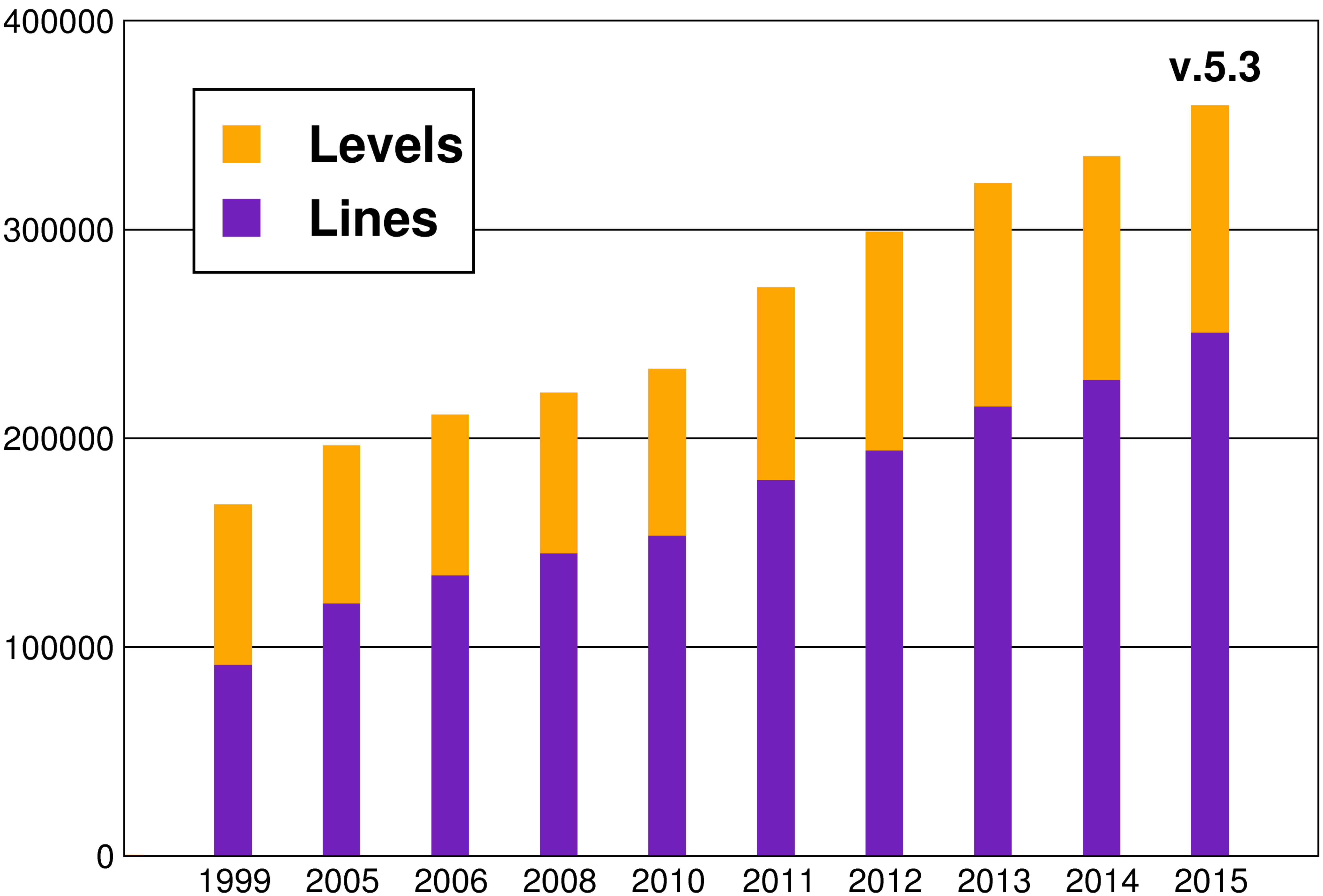
NIST Atomic Spectra Database

- v. 5.2 (September 2014)
  - Major updates
    - Cr I-II, Cu I, Fe V, Al I-VII
    - New data content plots
- v. 5.3 (October 2015)
  - Major updates:
    - Th I-III: from **950** to **20120** lines, from **6** to **1481** levels
    - W VIII: 103 levels, 193 lines
    - Sn II, Mo V, F V-VIII, Ne VI-IX
  - New diagnostic module for low-density (astrophysical) plasmas
    - Ions of C, N, O, Ne, Mg, Si, S, Ar, Ca, Fe, Ni
  - Ionization energies updated for a number of ions
  - Multi-component Saha/LTE spectra generation

Developers:
A. Kramida
K. Olsen
Yu. Ralchenko

NIST ASD content



v.5.3:

109,000 levels

250,000 lines

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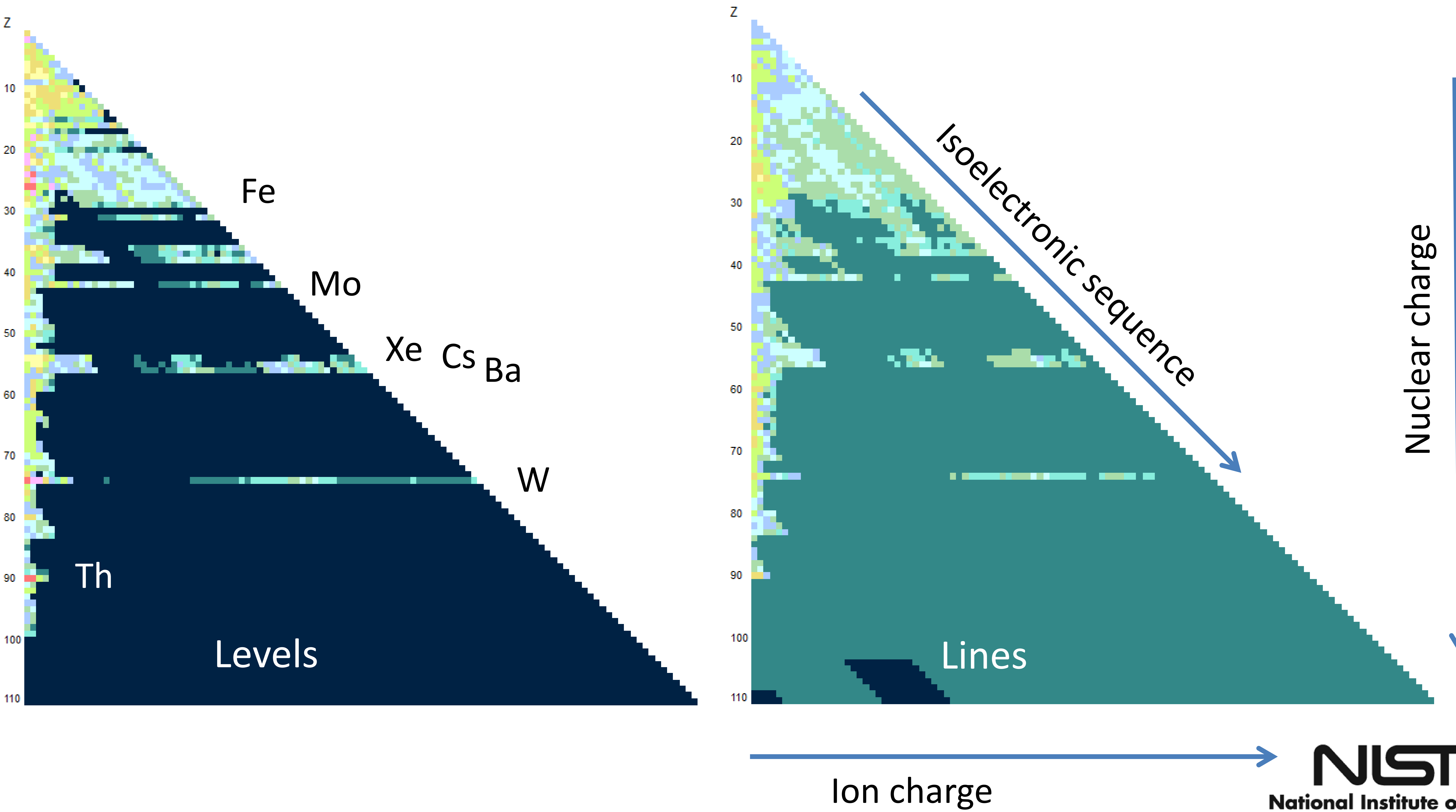
Detailed content of ASD 5.3



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New ASD Diagnostic Module (Astro)

Calculation: U. Feldman, CHIANTI (2013)

Additional Criteria

Lines:
- ○ All
- ○ Only with transition probabilities
- ○ Only with energy level classifications
- ○ ~~Only with observed wavelengths~~
- ◉ Only with diagnostics

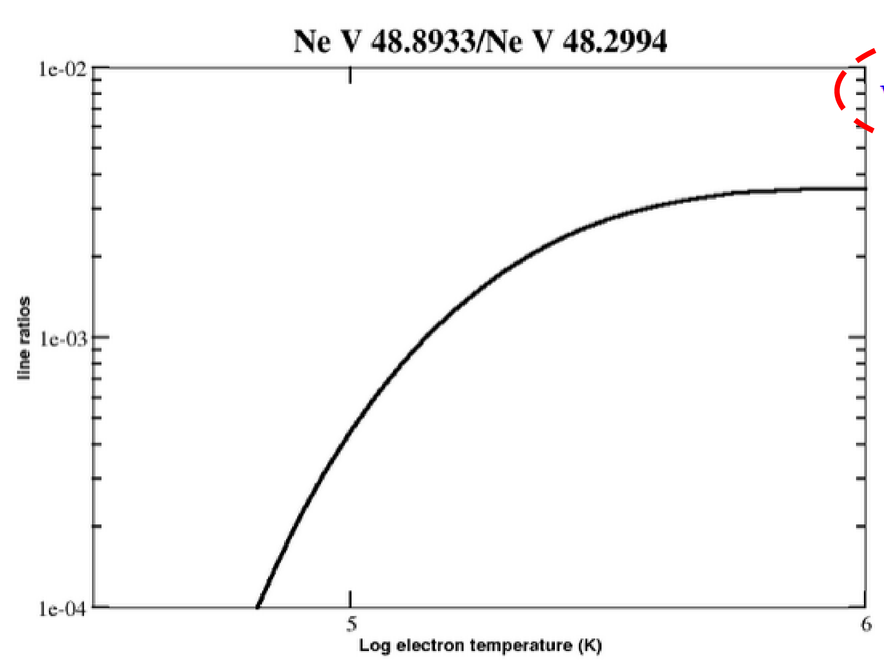
☑ Include diagnostics data

Ne V

Observed Wavelength Vac (nm)	Ritz Wavelength Vac (nm)	Rel. Int. (?)	A_{ki} (s^{-1})	Acc.	Lower Level Conf., Term, J	Upper Level Conf., Term, J	Type	TP Ref.	Line Ref.	Diagnostics Line Ratio
35.8474	35.8474	1000bl	7.3e+09	E	$2s^22p^2$ ^3P 1	$2s2p^3$ $^3S°$ 1		T425LS	L11744	density
36.5591	36.5593	2000	1.35e+10	E	$2s^22p^2$ ^1D 2	$2s2p^3$ $^1P°$ 1		T425	L11744	density
48.2993	48.2994	1000*	3.0e+09	E	$2s^22p^2$ ^3P 2	$2s2p^3$ $^3P°$ 2		T425LS	L11744	temperature
	48.8933	m			$2s2p^3$ $^3P°$ 2	$2p^4$ ^3P 2			L11744	temperature

NIST Atomic Spectra Database Temperature Diagnostics Data

Spectrum	Ritz Wavelength (nm)	Lower Level	Upper Level	Electron Density (cm^{-3})
Ne V	48.8933	$2s2p^3$ $^3P°_2$	$2p^4$ $^3P_2$	1e+10
Ne V	48.2994	$2s^22p^2$ $^3P_2$	$2s2p^3$ $^3P°_2$	

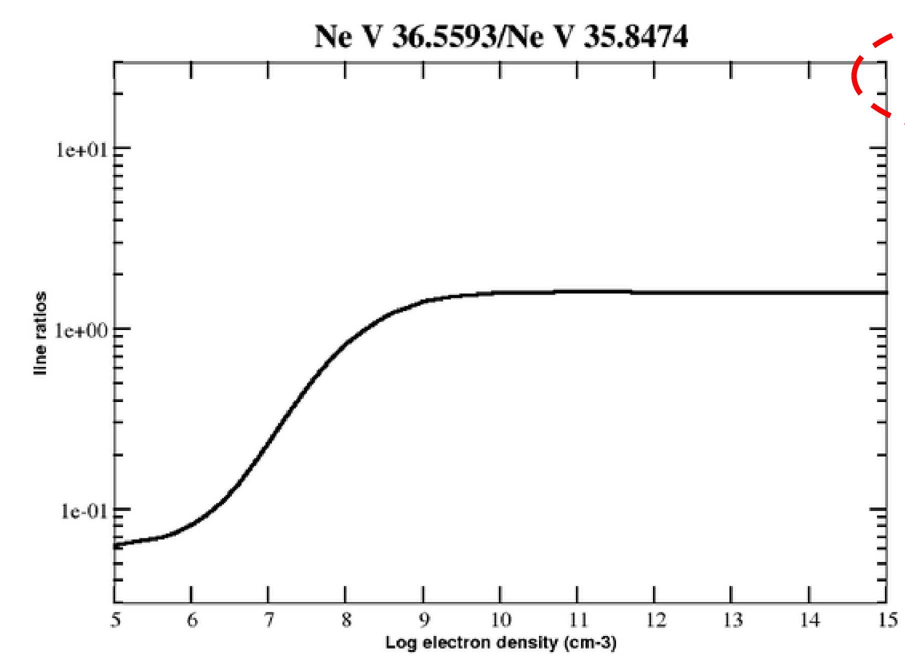


View Graph Data

The line intensity ratios were calculated by U. Feldman (NRL) using the CHIANTI database (2013).

NIST Atomic Spectra Database Diagnostics Data

Spectrum	Ritz Wavelength (nm)	Lower Level	Upper Level	Density Sensitivity Range (cm^{-3})
Ne V	36.5593	$2s^22p^2$ $^1D_2$	$2s2p^3$ $^1P°_1$	1e+06-3e+08
Ne V	35.8474	$2s^22p^2$ $^3P_1$	$2s2p^3$ $^3S°_1$	



View Graph Data

The line intensity ratios were calculated by U. Feldman (NRL) using the CHIANTI database (2013).

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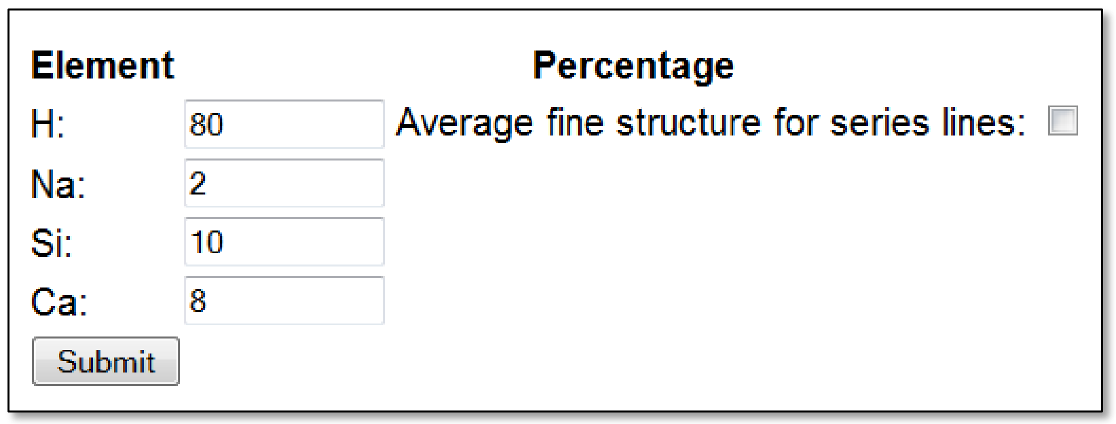
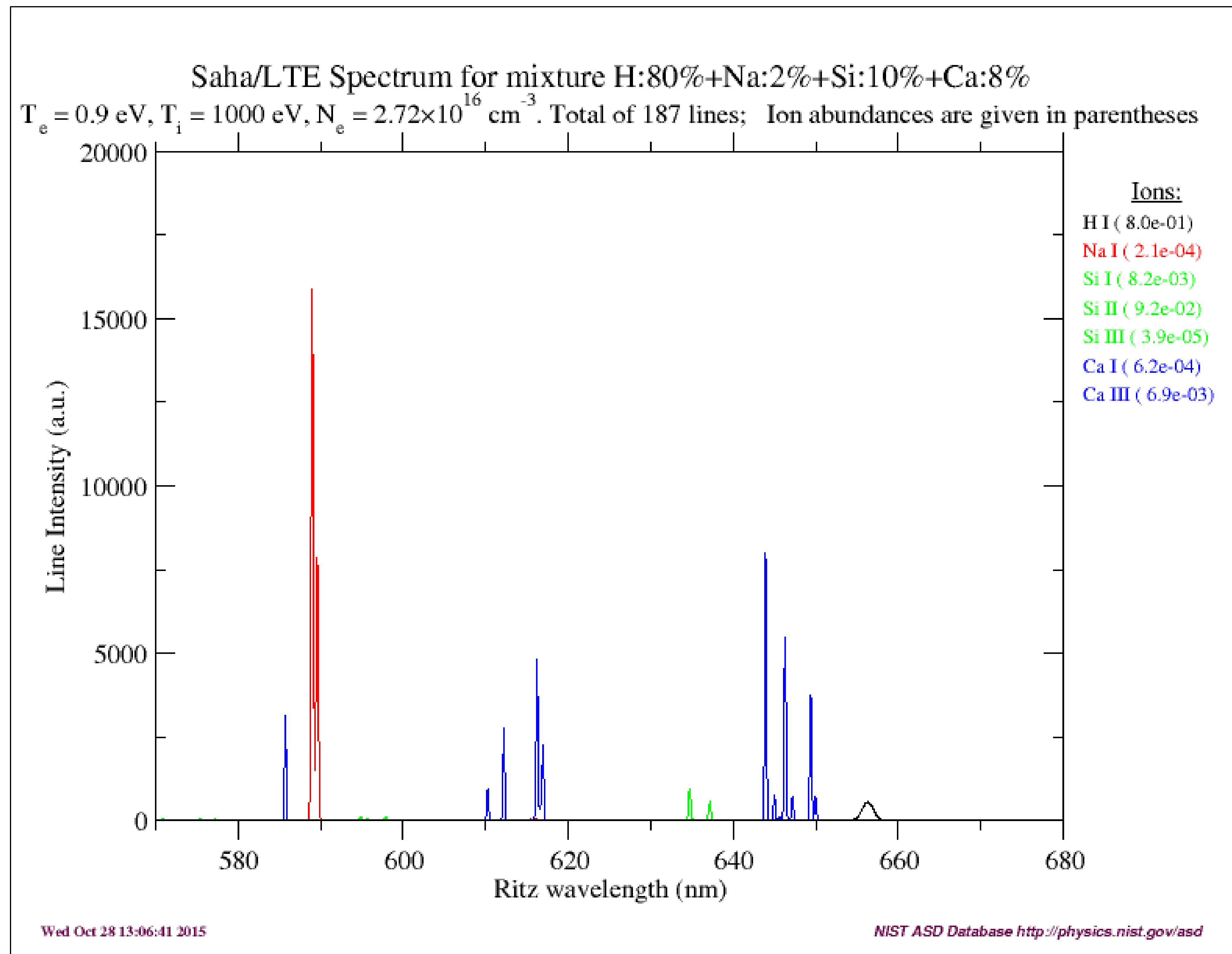
New ASD module: Multi-component Saha/LTE spectra (LIBS applications)



Output:

- List of all lines
- Bibliography
- Data
  - Relative line intensities
  - Doppler-broadened spectrum
  - Total spectrum
- Graphics
  - PDF
  - EPS
  - PNG



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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**
  - **19,221** references, 1802-2015
- **Atomic Transition Probabilities**
  - **9,069** references, 1914-2015
- **Atomic Lines Broadening and Shifts**
  - **6,862** references, 1889-2015

- 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

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Theory

- **Atomic structure** (**C. Froese Fischer**, A. Kramida, Yu. Ralchenko)
  - MCDHF (GRASP2K code)
  - N-like ions (F-Kr)
  - Ne-like ions (Mg-Kr)
  - C-like ions (Ar-Zn)
  - General theoretical analysis (electron-nucleus interactions, some specific transitions, ionization potentials)
  - Auger states in W^+

- **Modeling** (Yu. Ralchenko)
  - Collisional-radiative modeling (NOMAD code)
  - Support of EBIT experiments
  - Laser-produced plasmas (NRL)
  - LCLS spectra
  - Single and multiple charge exchange for O^{6+}+A
    - Monte-Carlo simulations of multiple CX
  - Be CR model
  - NLTE-8 Workshop (2013)

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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
  - **>770** users from all over the world

FLYCHK

New data: 2014-2015

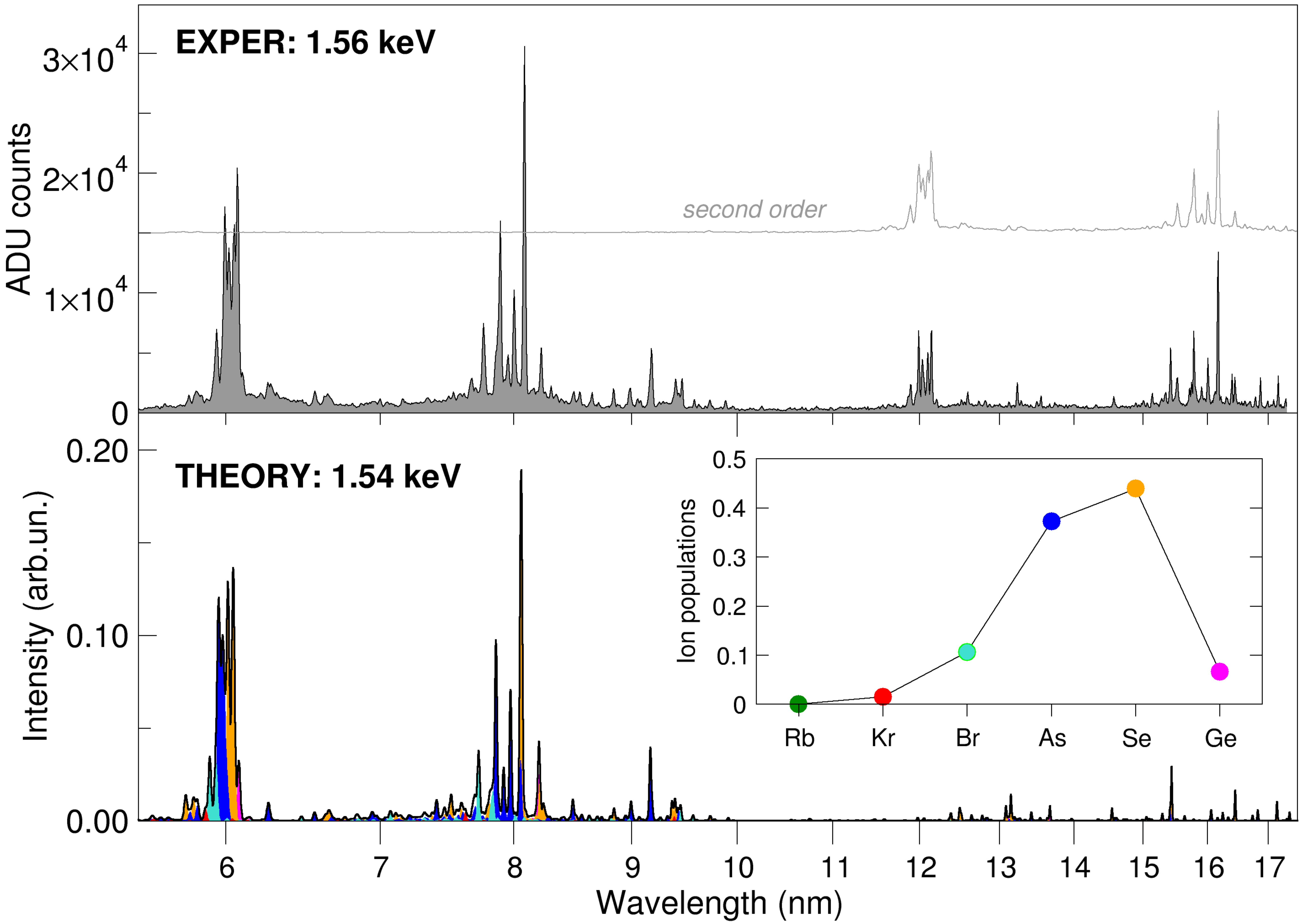
- **Published Compilations**
  - **Th I-III** (Redman et al, 2014)
  - **Fe I** (Ruffoni et al, 2014)
  - **Cr II** (Sansonetti and Nave, 2014)
  - **Fe V** (Kramida, 2014)
  - **Sn II** (Kunari et al, 2014)
  - **Mo V** (Reader and Tauheed, 2015)
- **To be published (completed)**
  - V I
  - Ir IV, Pt IV, Pt V
- **EBIT Measurements**
  - Kr XXI-XXXIV
  - Ba (numerous ions)
  - Dy XXX-XXXIX
  - W XXXV-XLI
  - Sm XXVII-XXXV
  - Er XXXIII-XLI

Mo V

- **Reader and Tauheed**, *J Phys B* **48**, 144001 (2015)
- Spectrum measured between 200 and 4700 Å
- **900** lines and **260** levels classified, of these 600 and 130 are new
- Many values were revised
- Theoretical analysis of all spectra
- Hatree-Fock simulations with least-square fits
- Ritz wavelengths determined for **380** lines, uncertainties from 0.0003 to 0.002 Å
- Oscillator strengths calculated for all classified lines
- Ionization energy determined to be **54.417±0.019** eV

Experiment vs simulations: **Er**

Podpaly et al, *J Phys B* **48**, 025002 (2015)



NIST EBIT
MeVVA injection

CR code NOMAD
~6000 levels
~3,000,000 transitions
Non-Maxw EEDF

4-4 E1 and M1
Transitions (60 new)

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Experiment at JPL: O^{6+}+H_2,He

- ECR source for production of $^{18}O^{6+}$
- Collisions with **H_2** and **He** (gas cell)
- Ion energies:
  - 3.5 keV·q (**1.17 keV/u**)
  - 7 keV·q (**2.33 keV/u**)
- Velocities: **464 km/s** and **671 km/s**
- Current: **5-20 nA**
- Gas pressure: **(6.5-12)×10^{-3} Pa**
- No indication of metastables

J.R. Machacek, D.P. Mahapatra, D.R. Schultz, Yu. Ralchenko. A. Chutjian, J. Simcic, R.J. Mawhorter, Phys. Rev. A **90**, 052708 (2014)

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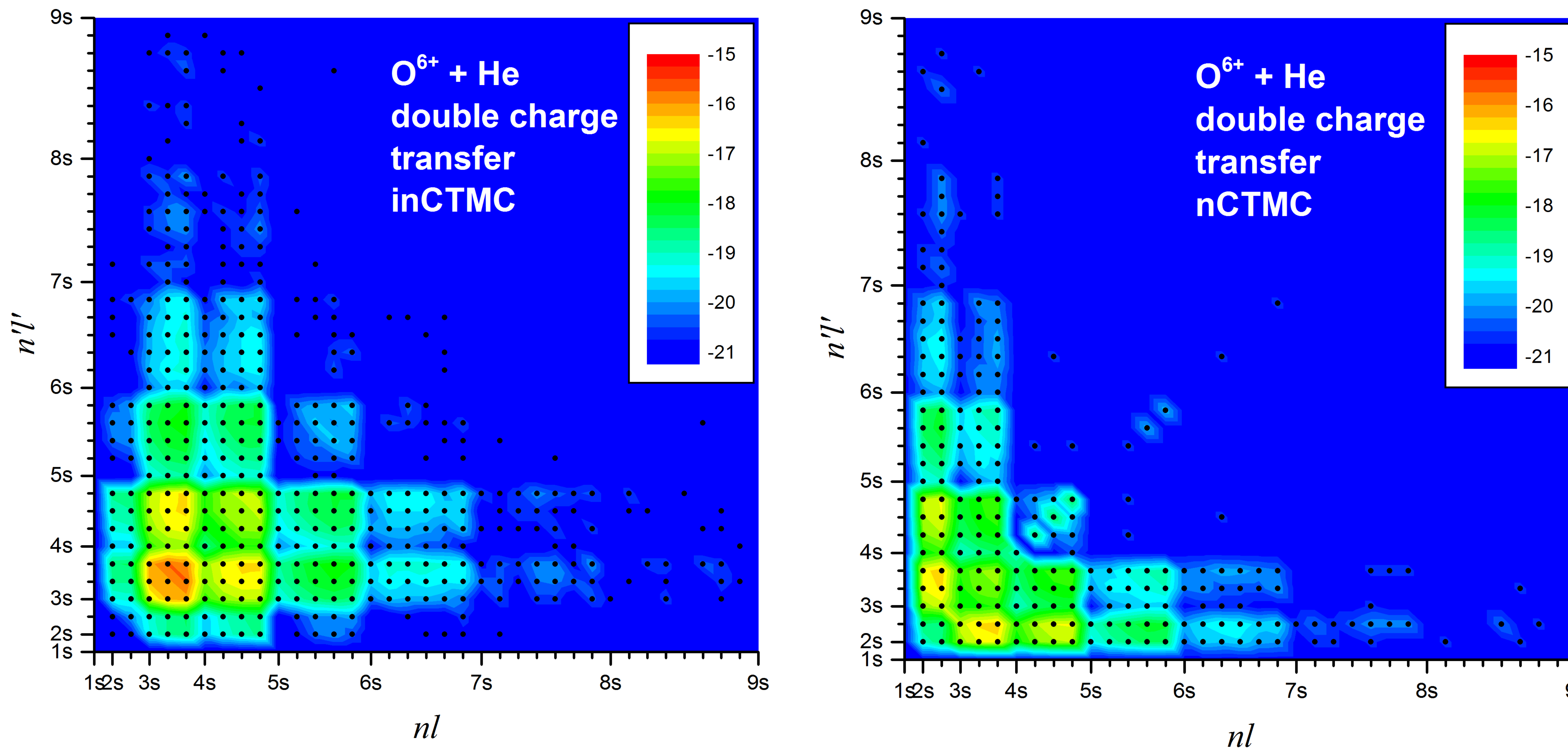
Calculated CTMC DCX cross sections O^{6+}+ He (2.33 keV/u):

Distribution over the final states

log(σ) vs (*nl*,*n′l′*)



Most of important states are autoionizing!!!

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$$\frac{d\widehat{N}(t)}{dt} = \hat{A} \cdot \widehat{N}(t)$$

Rate equation solution

$$\widehat{N}(0) = \widehat{N}_{CTMC}$$

Integration until stabilization

Matrix size: ~ 4500 x 4500 levels

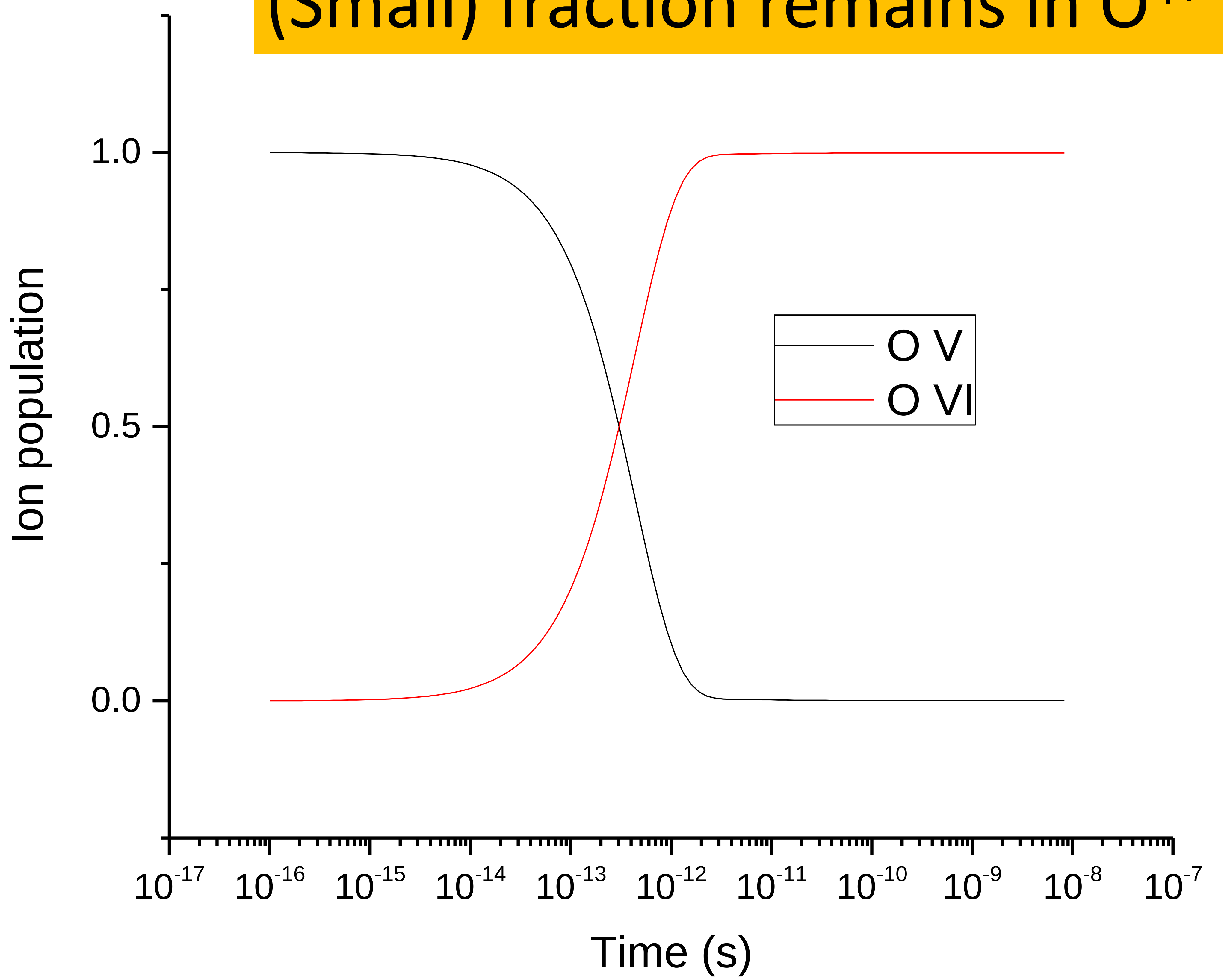
SCX and DCX: CTMC

Atomic data (FAC):

- Energy levels
- Radiative rate
- **Autoionization** rates
- **No collisional processes**

TD CR code NOMAD
Ralchenko & Maron (2001)

(Small) fraction remains in O^{4+}



Experiment (JPL) vs theory (CTMC+CR)

Cross Section (in 10^{-15} cm^2)		He		H_2	
		1.17 keV/u	2.33 keV/u	1.17 keV/u	2.33 keV/u
$\sigma_{6,5}$	present experiment	**1.16** ± 0.08	**1.34** ± 0.09	**4.24** ± 0.29	**4.24** ± 0.29
	present theory	**1.32**	**1.39**	**4.64**	**4.37**
$\sigma_{6,4}$	present experiment	**0.116** ± 0.008	**0.107** ± 0.008	**0.118** ± 0.008	**0.096** ± 0.007
	present theory	**0.173**	**0.175**	**0.066**	**0.073**

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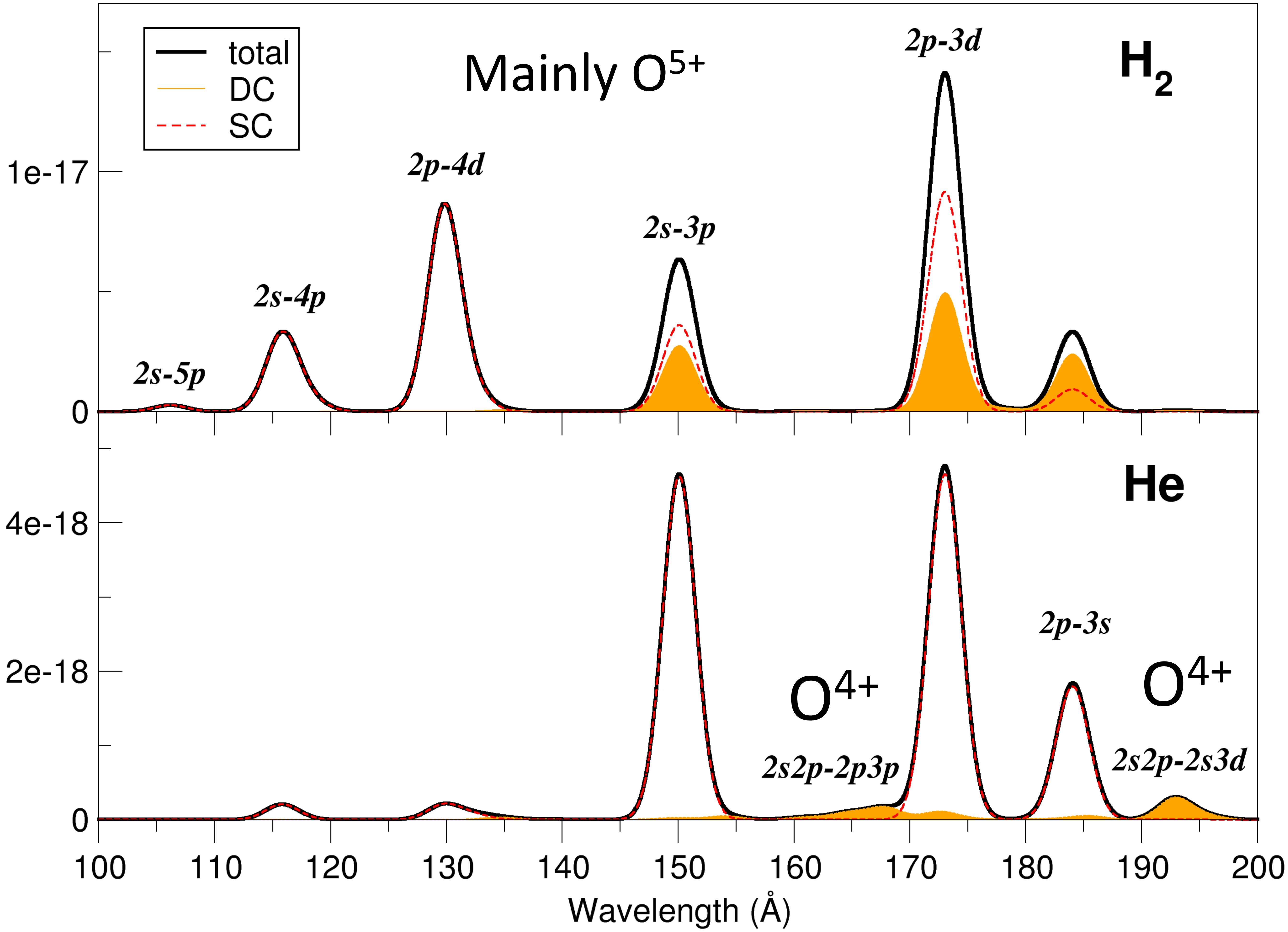
Contribution of Single and Double CX: $O^{6+}+H_2$,He at 1.17 keV/u



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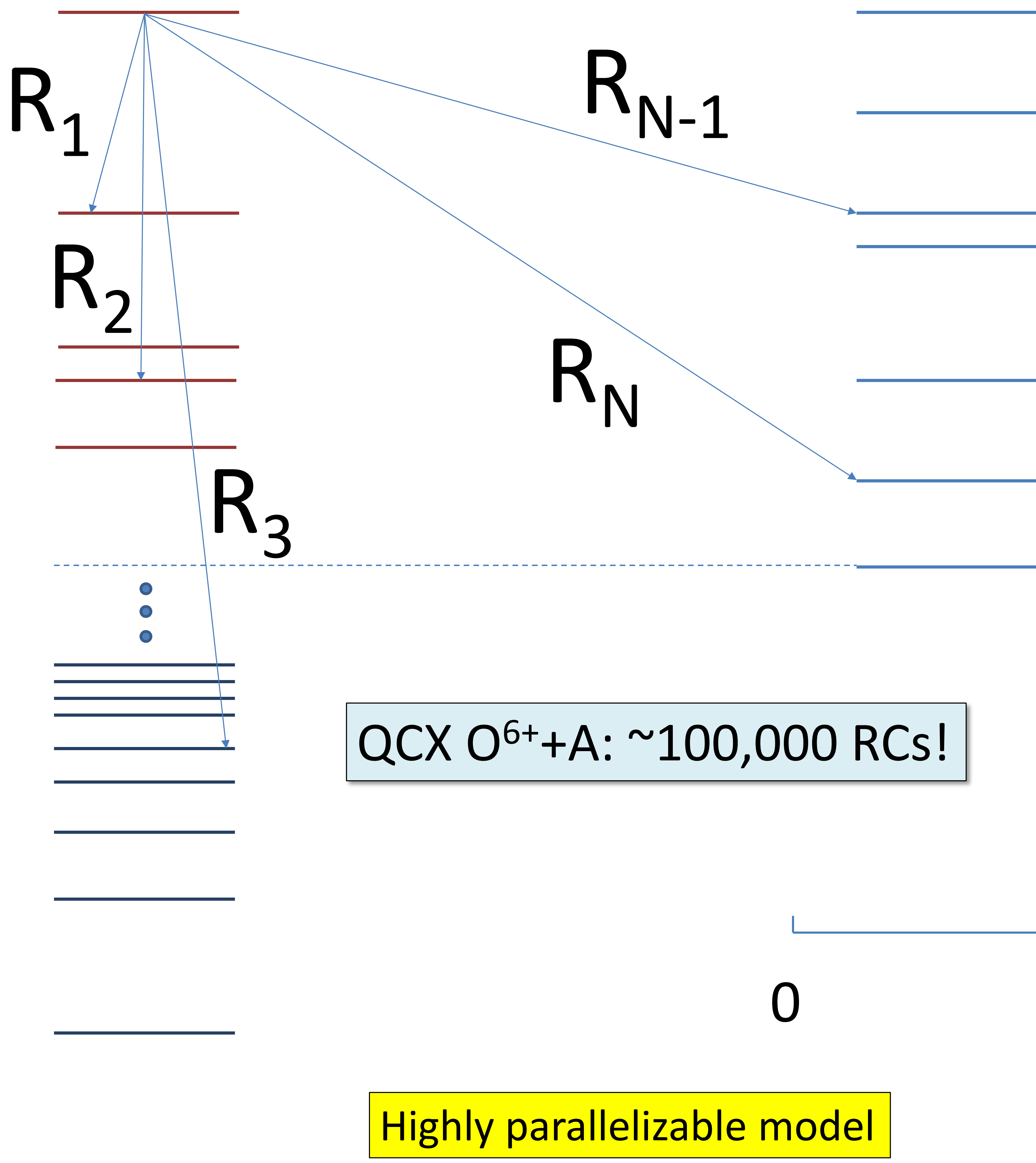
Monte Carlo approach to MCX stabilization

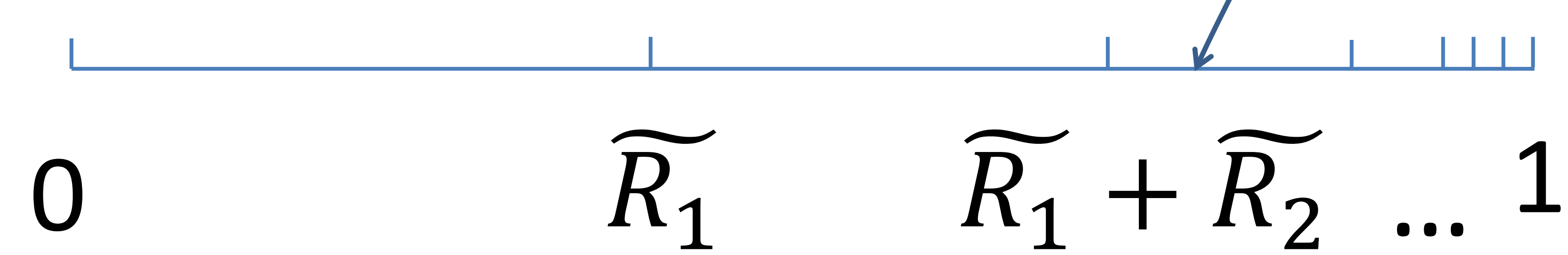
1. Normalize
2. Sort
3. Random pick
4. Proceed until stabilized
5. Repeat **999,999** times
6. Weight with CTMC CS's



QCX O^{6+}+A: ~100,000 RCs!

$$\widetilde{R}_i = \frac{R_i}{\sum_k R_k}$$

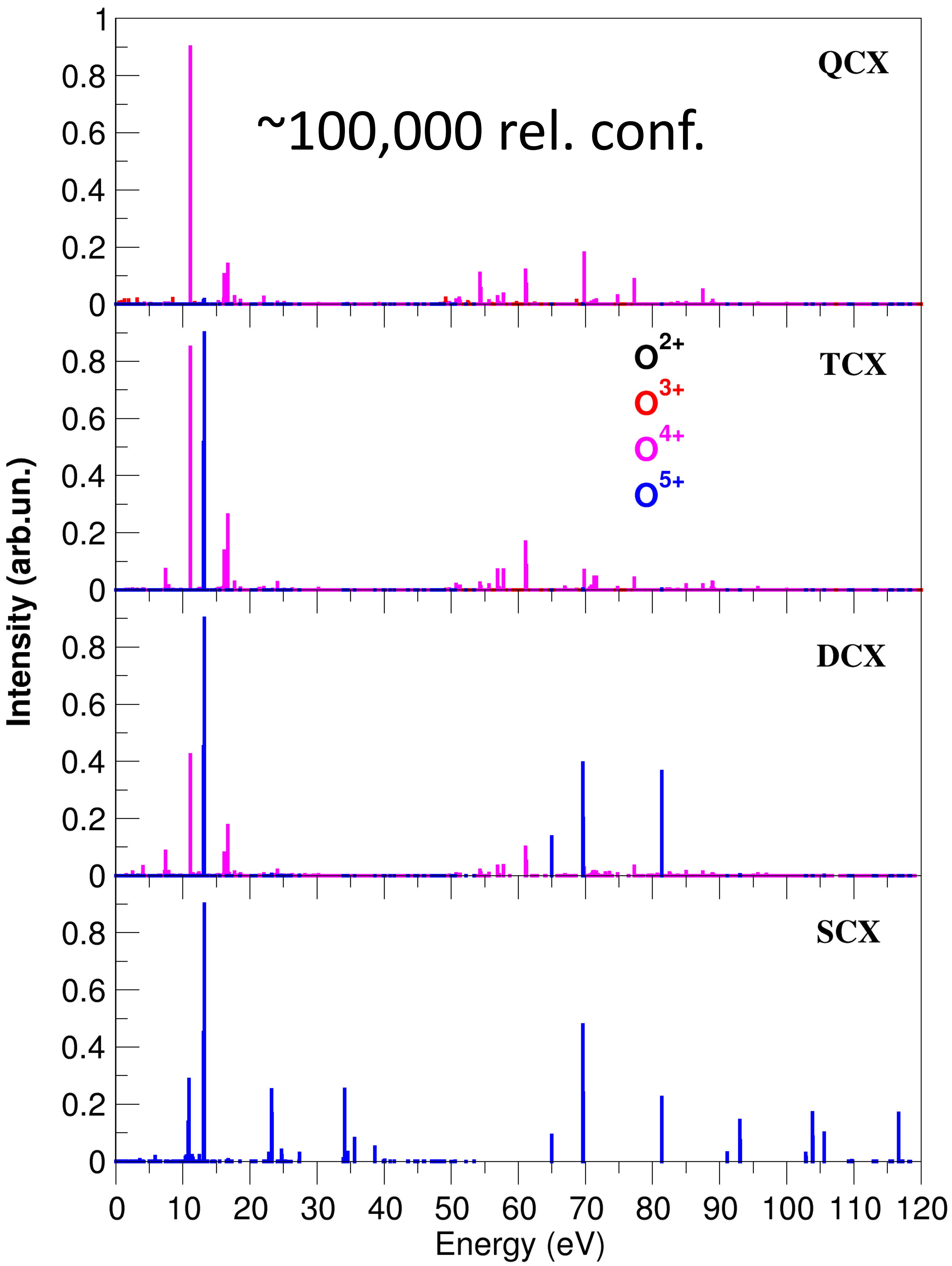
$$\widetilde{R}_1 \leq \widetilde{R}_2 \leq \widetilde{R}_3 \ldots$$



Highly parallelizable model

Ralchenko & Schultz, to be published

Multiple CX Monte Carlo Spectra



But: final ion distributions (effective cross sections) are less accurate for multielectron CX

O^{6+} + molecule: ratio EXP/TH

E(keV/u)	SCX	DCX	TCX
1.17	1.0	1.2	7.2
2.33	1.0	1.5	5.8

Machacek et al, Ap.J. (2015)

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Interaction with other Data Centers

- IAEA AMDU
  - CRP on tungsten
  - Code Centre Network
  - Joint IAEA-ITAMP TM on uncertainty assessment
  - IAEA TM on AMPMI Data for Fusion (Korea)
  - ICTP-IAEA School and Workshop
  - CM on Be/C/Ne data
- VAMDC
  - External partner with SUP@VAMDC
  - Meeting at NIST (2014)
  - Finalizing VAMDC access to ASD

Joint ICTP-IAEA School and Workshop on Modern Methods in Plasma Spectroscopy

- Directors: H.-K. Chung, B.J. Braams, Yu. Ralchenko
- March 16-27 2015
- 37 students from developing and developed countries
- 10 lecturers, 18 lectures, 4 computer classes (GRASP2K, FLYCHK, ATOMIC, CRETIN)
- 46 workshop participants

The Abdus Salam
International Centre for Theoretical Physics
www.ictp.it

Joint ICTP-IAEA Advanced School and Workshop on Modern Methods in Plasma Spectroscopy

16 - 27 March 2015
ICTP, Miramare – Trieste, Italy

DIRECTORS
H.-K. Chung and B. J. Braams
(IAEA, Austria)
Yu. Ralchenko
(NIST, USA)

LOCAL ORGANIZER
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(ICTP, Trieste)

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(Technion, Israel)
H.-K. Chung
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C.J. Fontes
(LANL, USA)
P. Jönsson and J. Ekman
(Malmö Univ, Sweden)
H.-J. Kunze
(Ruhr-Univ, Germany)
O. Marchuk
(FZ Jülich, Germany)
Yu. Ralchenko
(NIST, USA)
H. A. Scott
(LLNL, USA)

DEADLINE
2 November 2014

- Lectures
  - Atomic structure
  - Radiative processes
  - Atomic collisions
  - Line shapes and broadening
  - Opacities and radiation transport
  - Experimental techniques
  - Diagnostic methods
    - Industrial plasmas
    - Magnetic fusion
    - Astrophysics
    - Dense plasmas

www-amdis.iaea.org/Workshops/ICTP2015

Conclusions

- NIST Atomic Spectroscopy Data Center continues collection, evaluation, and dissemination of accurate atomic spectroscopic data relevant to fusion
- We actively interact with data users and data providers to define priorities in data compilations
- New data and data manipulation tools are regularly added to the existing databases