Fudan University China

SPECTROSCOPY STUDIES OF MODERATELY CHARGED TUNGSTEN, SULFUR, AND CHLORINE IONS AT THE SH-HTSCEBIT

Jun Xiao

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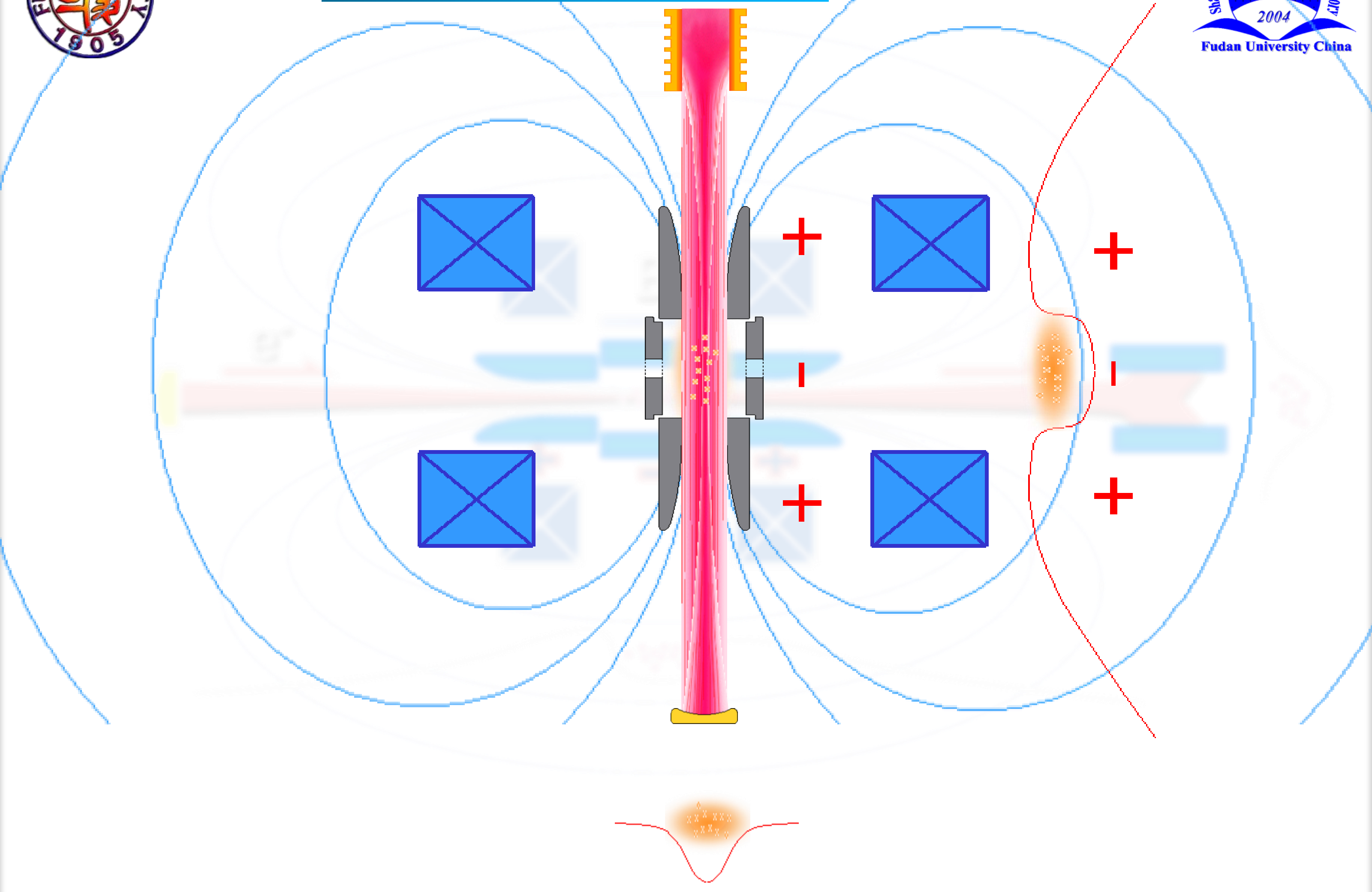
Paris， 2023-07-12

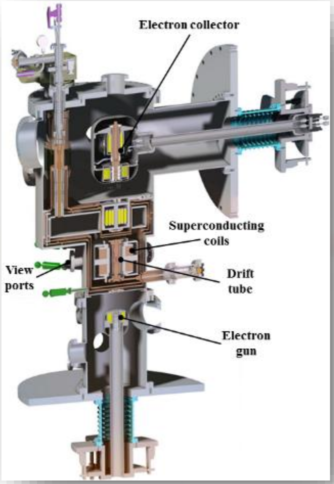
Outline

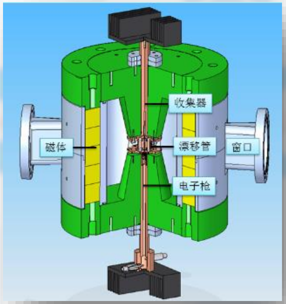
- Background
- Tungsten Spectroscopy
- Chlorine& Sulfur Spectroscopy
- Summary

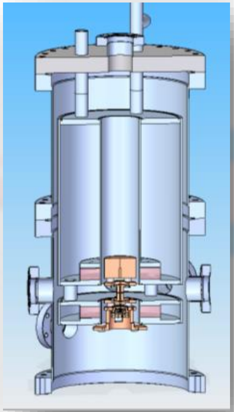
Electron Beam Ion Trap, EBIT



The Shanghai EBITs







ShanghaiEBIT~150keV

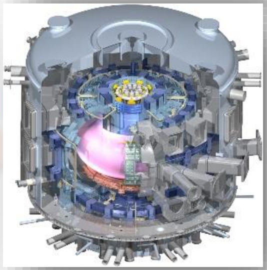
SH-PermEBIT~60eV

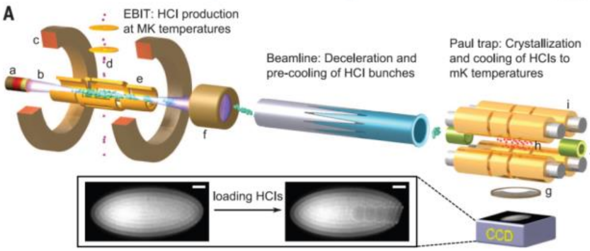
SH-HtscEBIT~30eV

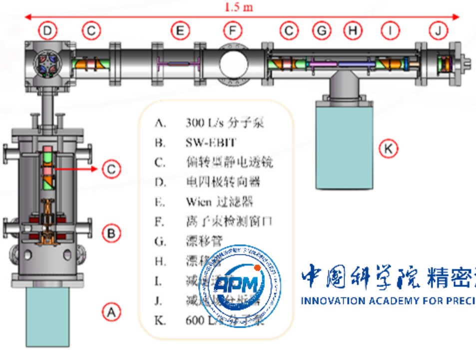
Livermore, NIST, Heidelberg, Tokyo, …EBITs

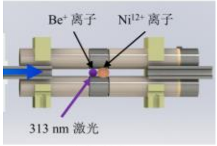
What can EBIT do?

- Dielectronic Recombination
- Provide atomic data for astrophysical, ICF, MCF plasma
- For Plasma Diagnostics, e.g. Ne, Te, B…
- Fundamental studies e.g. QED Test…
- HCI clock
- …









线形离子阱

中国科学院 精密测量科学与技术创新研究院
INNOVATION ACADEMY FOR PRECISION MEASUREMENT SCIENCE AND TECHNOLOGY, CAS

Outline

EBIT HCI

Spectroscopy

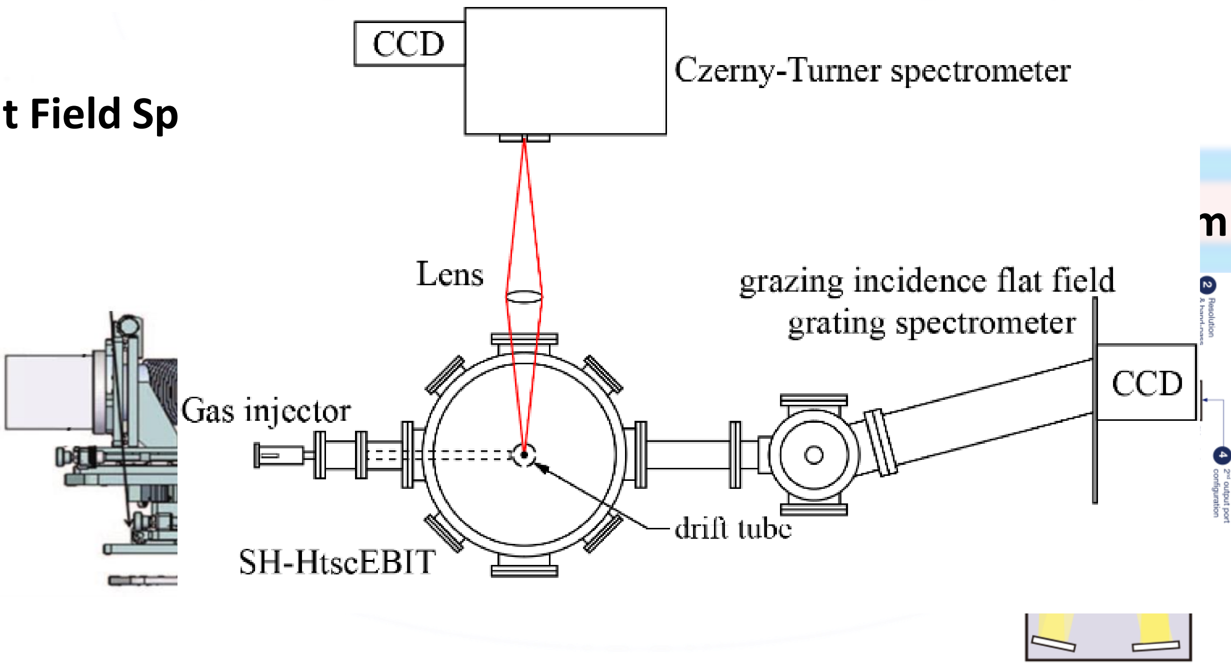
W

S Cl

SH-HtscEBIT and Experimental Setup

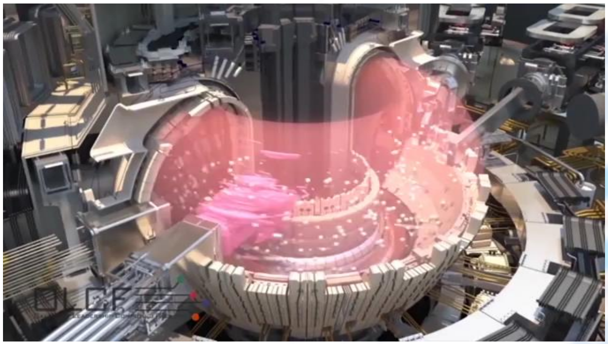
Flat Field Sp

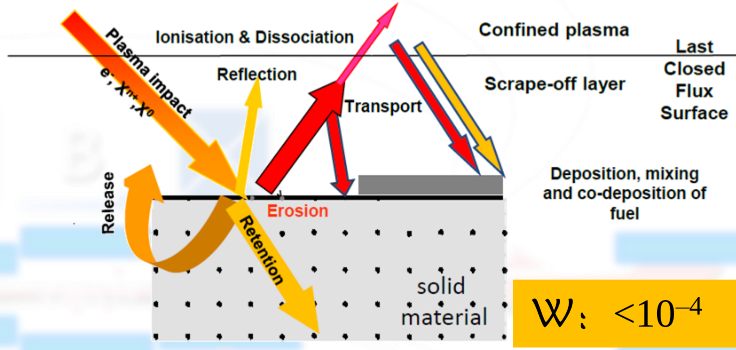
mrock



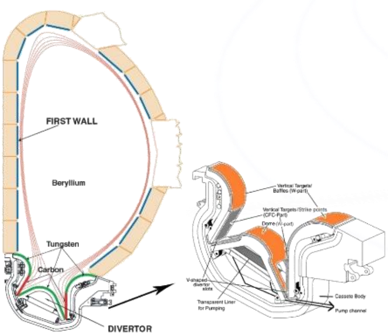
SH-HtscEBIT and Experimental Setup

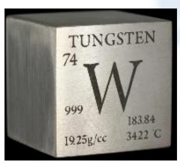
Part I:Tungsten data are needed!

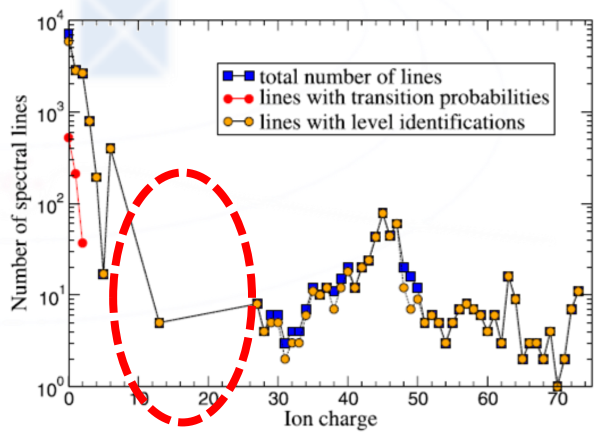




W： $<10^{-4}$



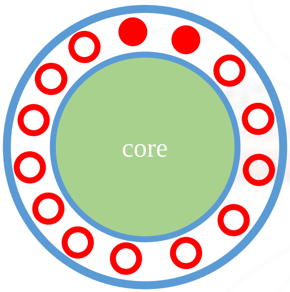




Moderately Charged Tungsten Ions

open 4*f* electrons

W^{27+}–W^{25+}

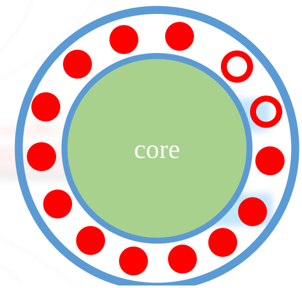


	Ground state
W^{27+}	$4d^{10}4f^{1}$
W^{26+}	$4d^{10}4f^{2}$
W^{25+}	$4d^{10}4f^{3}$
W^{24+}	$4d^{10}4f^{4}$

W^{16+}–W^{24+}

W^{7+}–W^{15+}

	Ground state
W^{7+}	$4f^{13}\,5s^2\,5p^6$
W^{8+}	$4f^{14}\,5s^2\,5p^4$
W^{9+}	$4f^{14}\,5s^2\,5p^3$
W^{10+}	$4f^{14}\,5s^2\,5p^2$
W^{11+}	$4f^{13}\,5s^2\,5p^2$
W^{12+}	$4f^{14}\,5s^2$
W^{13+}	$4f^{13}\,5s^2$
W^{14+}	$4f^{12}\,5s^2$
W^{15+}	$4f^{11}\,5s^2$
	$4f^{11}\,5s^1$



PHYSICAL REVIEW A **102**, 042818 (2020)

Identification of visible lines from multiply charged W^{8+} and W^{9+} ions

Priti,[1,*] Momoe Mita,[1] Daiji Kato,[2,3] Izumi Murakami,[2,4] Hiroyuki A. Sakaue,[2] and Nobuyuki Nakamura[1]
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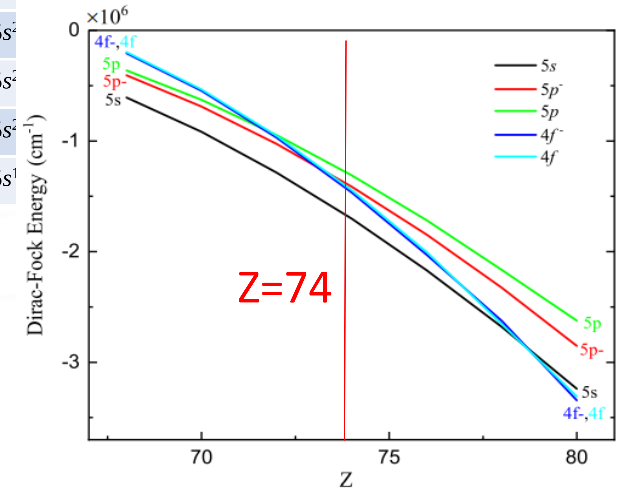


Theoretical Methods

$$H_{DC} = \sum_{i=1}^{N} h_d(i) + \sum_{i<j}^{N} \frac{1}{r_{ij}}$$

$$\Psi(\Gamma PJ) = \sum_{i=1}^{M} c_i \Phi(\Upsilon_i PJ)$$

FAC
- Relativistic Configuration Interaction(RCI)
- Relativistic Many-Body Perturbation Theory(RMBPT)

GRASP Multi configuration Dirac-Hartree-Fock(MCDHF)

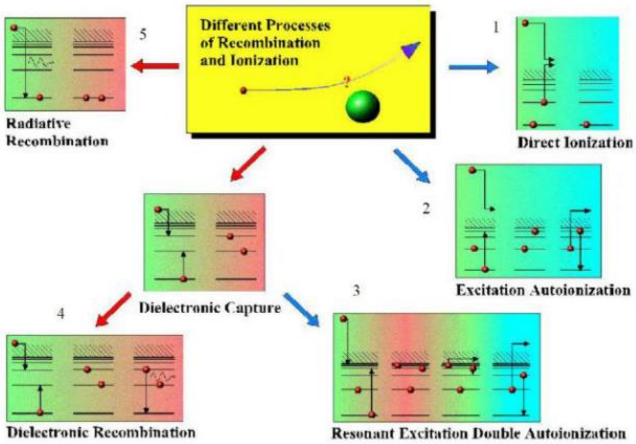
$$I_{i,j}(\lambda) \propto N_i A_{i,j} \phi(\lambda)$$

Collisional Radiative Model(CRM)

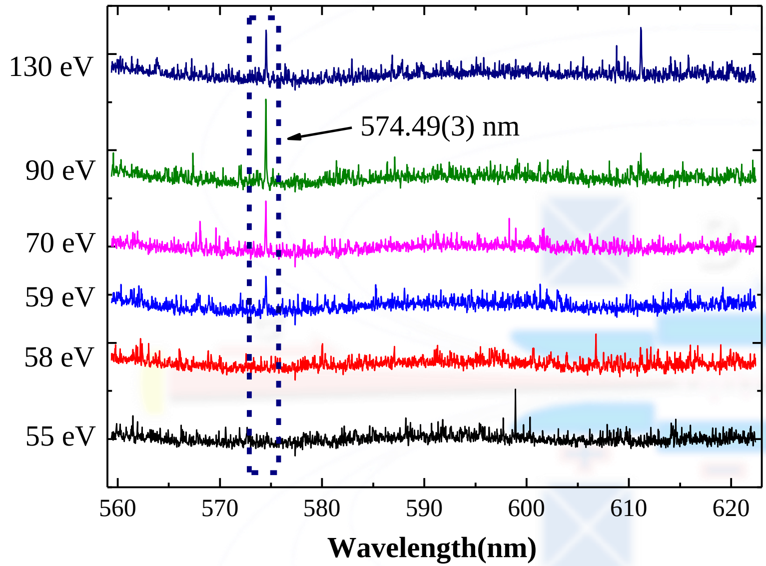
$$\frac{dN_i}{dt} = \sum_{j>i}\left(A^r_{j\to i}N_j\right) + \sum_{j<i}\left(C^e_{j\to i}N_j n_e\right) + \sum_{j>i}\left(C^d_{j\to i}N_j n_e\right) - \sum_{j<i}\left(A^r_{i\to j}N_i\right) - \sum_{j>i}\left(C^e_{i\to j}N_i n_e\right) - \sum_{j<i}\left(C^d_{i\to j}N_i n_e\right)$$

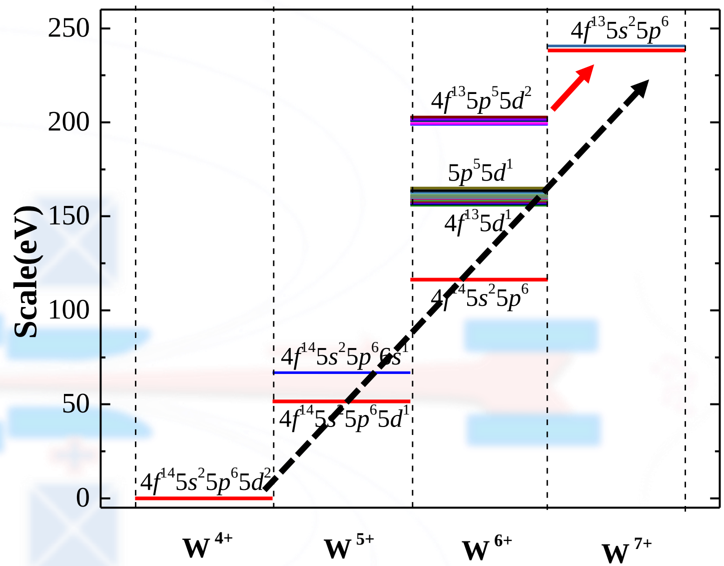
collisional (de)excitation
radiative decay

$$\frac{dN_i}{dt} = 0 \qquad \sum_i N_i = 1$$

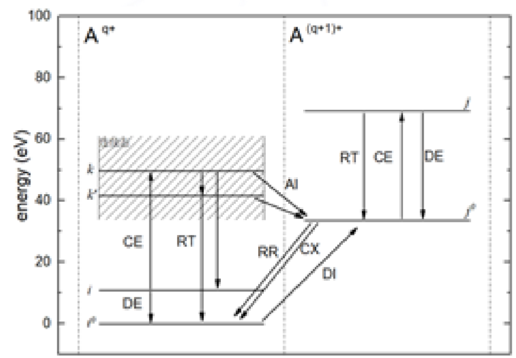


Indirect Ionization from W^{4+}–W^{7+}





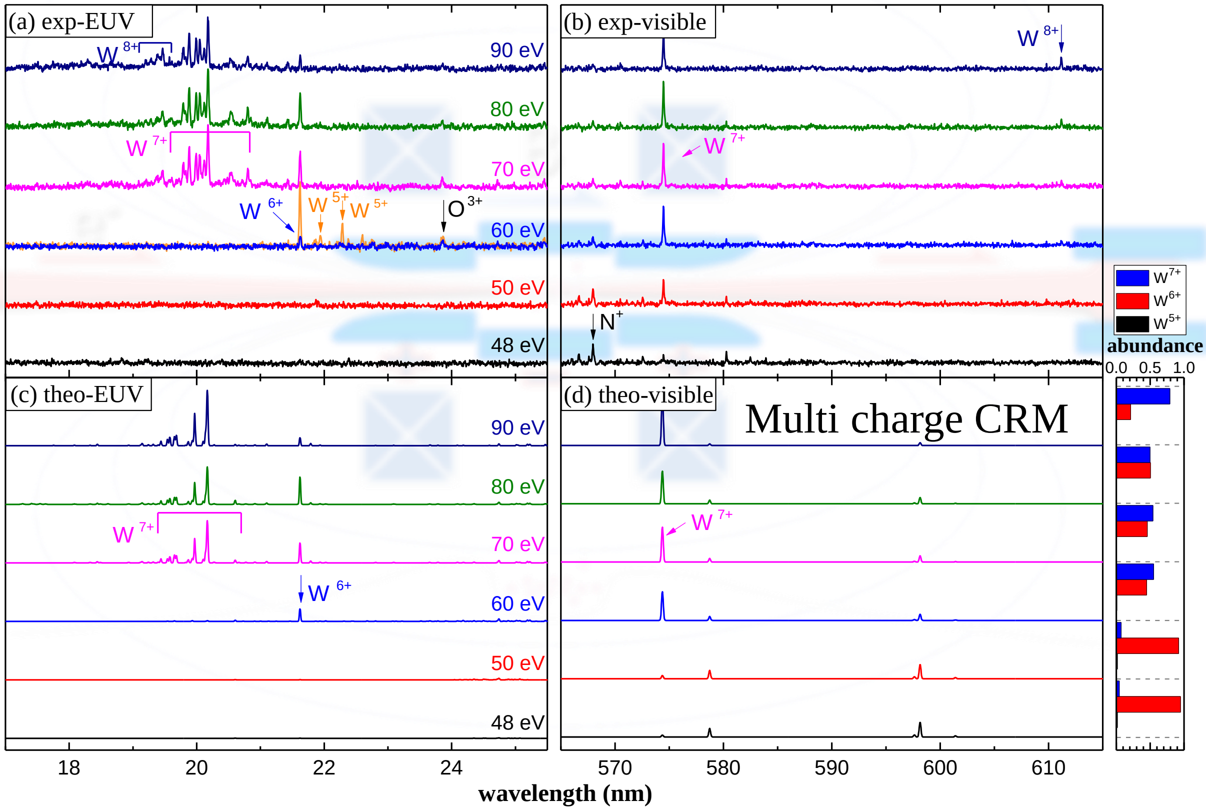
$$
\begin{aligned}
\frac{dN_i}{dt} &= \sum_{k>i}(A_{ki}^{RT}N_k) + \sum_h(A_{hi}^{AI}N_h) - \sum_{k<i}(A_{ik}^{RT}N_i) - \sum_j(A_{ij}^{AI}N_i) \\
&+ \left[\sum_{k<i}(C_{ki}^{CE}N_k) + \sum_{k>i}(C_{ki}^{DE}N_k) + \sum_h(C_{hi}^{DI}N_h) + \sum_j(C_{ji}^{RR}N_j)\right]n_e \\
&- \left[\sum_{k>i}(C_{ik}^{CE}N_i) + \sum_{k<i}(C_{ik}^{DE}N_i) + \sum_j(C_{ij}^{DI}N_i) + \sum_h(C_{ih}^{RR}N_i)\right]n_e \\
&+ \sum_j(C_{ji}^{CX}N_j)n_{cx} - \sum_h(C_{ih}^{CX}N_i)n_{cx} = 0
\end{aligned}
$$



Collaborated with C.Y. Cheng, J.G. Li, K. Wang

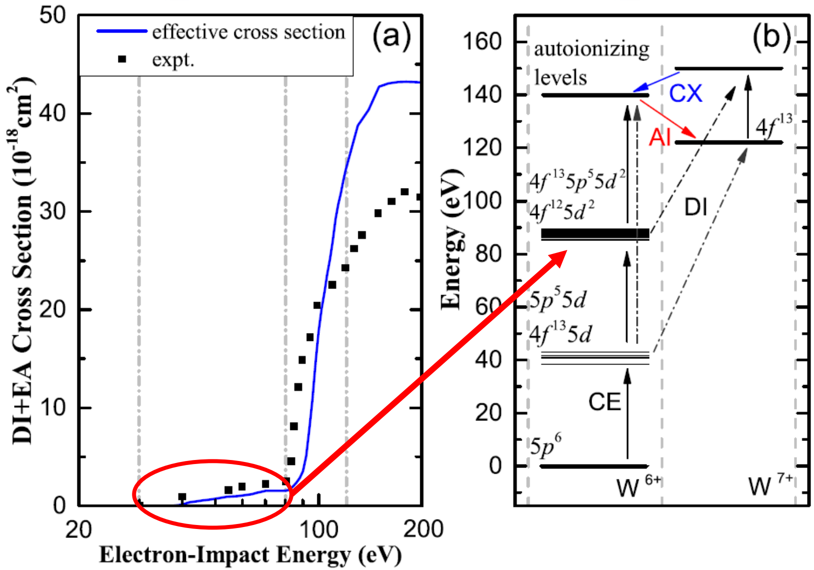
Q. Lu et. al, PRA, 99, 042510 (2019)

Indirect Ionization from W^{4+}–W^{7+}



C.L. Yan et. al, PRA, 105, 032830 (2022)

Indirect Ionization from W^{4+}–W^{7+}



W^{6+}： 50–80 eV(solid line)， ground to $4f^{13}5p^55d^2$ & $4f^{12}5d^2$， to EA

80–122 eV(dashed line)， ground to $5p^55d$ & $4f^{13}5d$， to EA

W^{5+}： 35–65 eV， ground to $5p^55d^2$和$4f^{13}5d^2$， to EA

C.L. Yan et. al, PRA, 105, 032830 (2022)

Large scale RCI calculation for W^{8+}

W^{8+}: 3 "ground states"

gs1:
$4f^{14}5s^{2}5p^{4}$

Single excitation :
$4f^{14}5s^{2}5p^{3}5f$
$4f^{14}5s5p^{4}5d$ …

Double excitation:
$4f^{14}5s^{2}5p^{2}5d^{2}$
$4f^{14}5p^{6}$ …

gs2:
$4f^{13}5s^{2}5p^{5}$

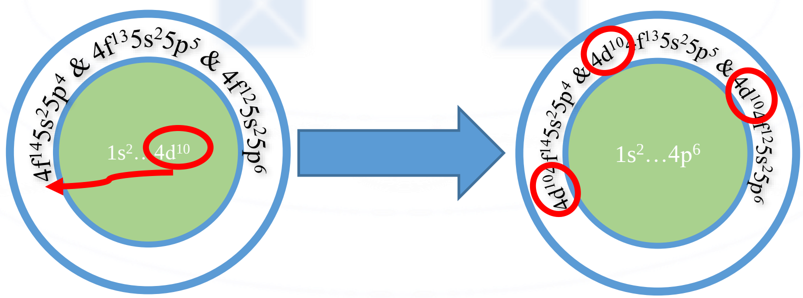
Single excitation
$4f^{13}5s^{2}5p^{4}5f$
$4f^{13}5s5p^{5}5d$ …

Double excitation:
$4f^{13}5s^{2}5p^{3}5d^{2}$
$4f^{13}5p^{6}5f$ …

gs3:
$4f^{12}5s^{2}5p^{6}$

Single excitation
$4f^{12}5s^{2}5p^{5}5f$
$4f^{12}5s5p^{6}5d$ …

Double excitation:
$4f^{12}5s^{2}5p^{4}5d^{2}$
$4f^{12}5p^{6}5d^{2}$ …



537,988levels

the 4 *d* and 4 *f* electron correlation

Modified FAC1.1.5 to large scale calculation

PHYSICAL REVIEW A **103**, 022808 (2021)

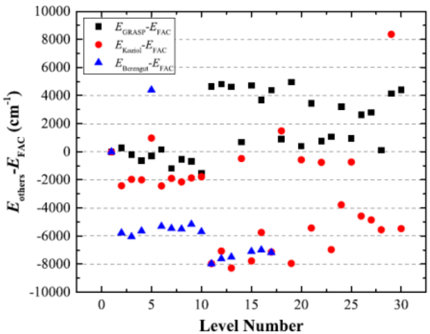
Visible spectra of W^{8+} in an electron-beam ion trap

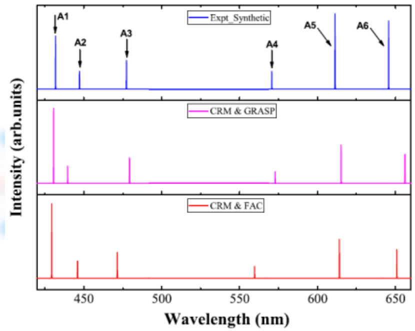
Q. Lu (陆祺峰),[1] C. L. Yan (严成龙),[1] J. Meng (孟举),[2] G. Q. Xu (许帼芹),[1] Y. Yang (杨洋),[1] C. Y. Chen (陈重阳),[1] J. Xiao (肖君),[1,*] J. G. Li (李冀光),[2,†] J. G. Wang (王建国),[2] and Y. Zou (邹亚明)[1]

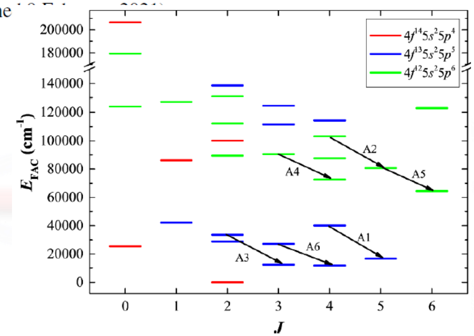
[1]*Shanghai EBIT Laboratory, Key Laboratory of Nuclear Physics and Ion-Beam Application (MOE), Institute of Modern Physics, Fudan University, Shanghai 200433, China*

[2]*Institute of Applied Physics and Computational Mathematics, Beijing 100088, China*

(Received 25 September 2020; accepted 26 January 2021; publishe...







Key	跃迁	λ^a_{FAC}	λ^b_{FAC}	λ_{GRA}	D^a_{FAC}	D^b_{FAC}	D_{GRA}	I_{CRM}	A_{FAC}	A_{GRA}
A1	9→4	425.2	429.4	430.6	−1.6	−0.6	−0.3	1.00	1.8[2]	1.7[2]
A2	19→13	440.4	446.0	439.6	−1.5	−0.3	1.7	0.23	1.6[2]	1.6[2]
A3	8→3	468.0	471.5	479.4	−2.0	−1.2	0.4	0.35	9.9[1]	9.1[1]
A4	17→12	558.6	559.6	572.8	−2.1	−1.9	0.4	0.16	8.6[1]	8.5[1]
A5	13→11	616.8	614.0	615.2	0.9	0.4	0.6	0.52	1.1[2]	1.1[2]
A6	6→2	644.3	651.0	656.1	−0.2	0.8	1.6	0.39	7.1[1]	6.6[1]

RCI 0.88%
MCDHF 0.83%

Phys. Rev. A. 2021, 103: 022808

More Spectroscopy works for W^{10+},W^{11+},W^{12+}

Journal of Quantitative Spectroscopy & Radiative Transfer 262 (2021) 107533

Contents lists available at ScienceDirect

Journal of Quantitative Spectroscopy & Radiative Transfer

journal homepage: www.elsevier.com/locate/jqsrt

ELSEVIER

Measurement and identification of visible lines from W^{10+}

IOP Publishing Journal of Physics B: Atomic, Molecular and Optical Physics

J. Phys. B: At. Mol. Opt. Phys. 55 (2022) 045001 (8pp) https://doi.org/10.1088/1361-6455/ac5432

Re-investigation and line identifications for W^{11+} in the visible range

Journal of Quantitative Spectroscopy & Radiative Transfer 279 (2022) 108064

Contents lists available at ScienceDirect

Journal of Quantitative Spectroscopy & Radiative Transfer

journal homepage: www.elsevier.com/locate/jqsrt

ELSEVIER

Experimental and theoretical investigations of visible spectra of W^{12+}

Check for updates

Q. Lu[a], N. Fu[a], C.L. Yan[a], F.H. Qu[a], Y. Yang[a], K. Wang[b,*], C.Y. Chen[a], Y. Zou[a], J. Xiao[a,*]

[a] Shanghai EBIT Laboratory, Key Laboratory of Nuclear Physics and Ion-Beam Application (MOE), Institute of Modern Physics, Fudan University, Shanghai 200433, China

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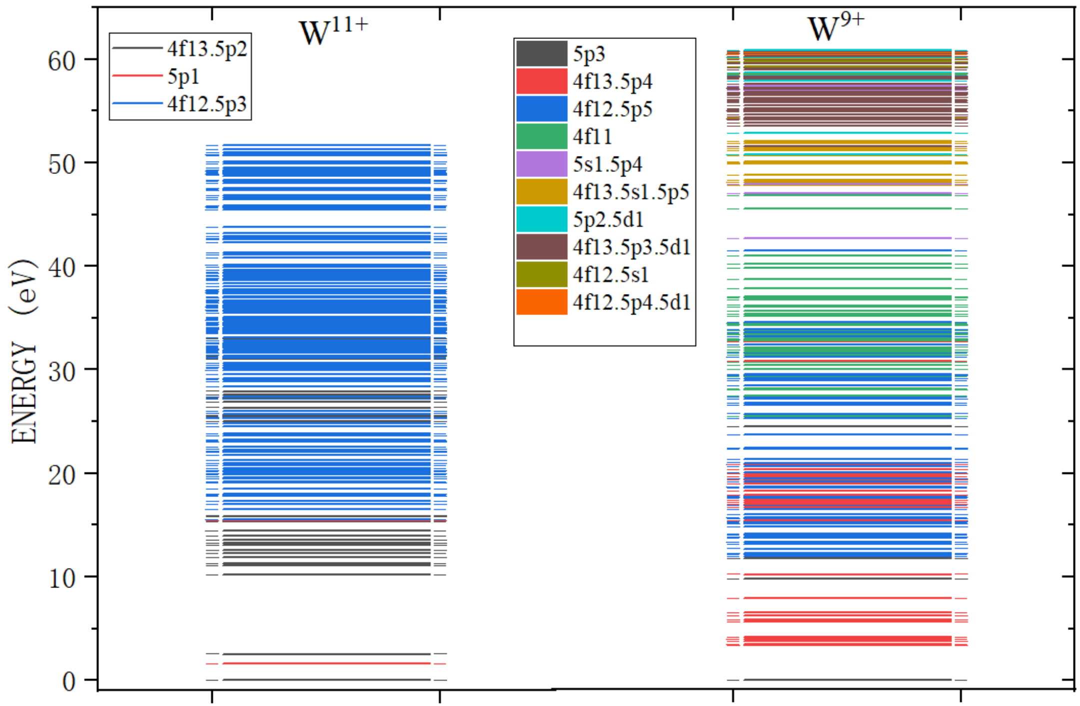
Side Product

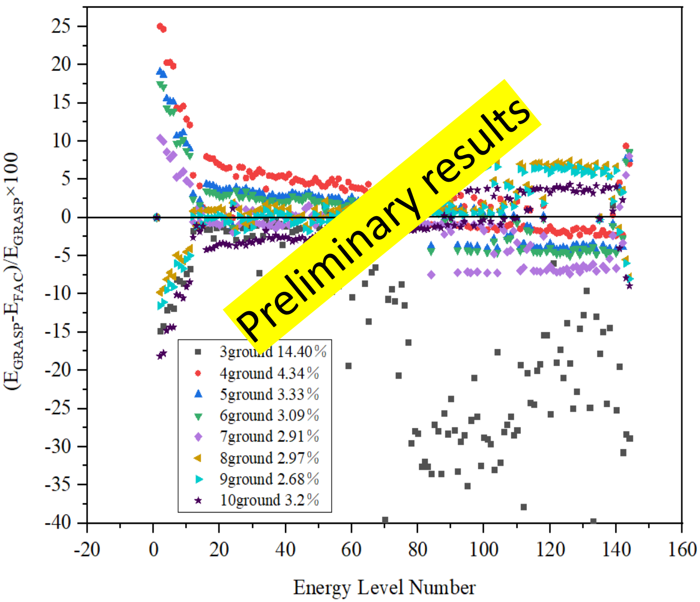
Large scale RCI calculation of energy levels in W^{9+}

Ground states selection

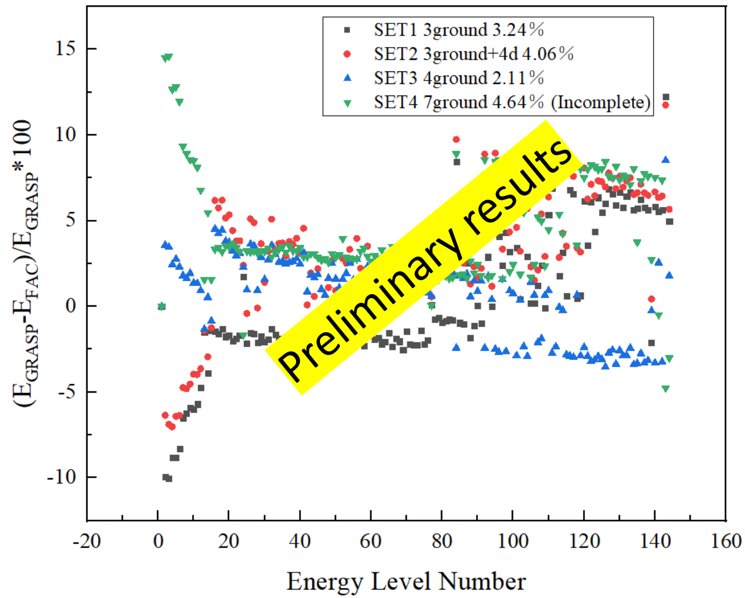


Comparison with GRASP :

Small-scale 68,164 energy levels



Large-scale 410,086 energy levels



- Large-scale calculation makes the deviation of 3-ground reduce from 14.40% to 3.24% and the deviation of 4-ground reduce from 4.34% to 2.11%

Priti et al. Phys Rev A 102:042818（2020）

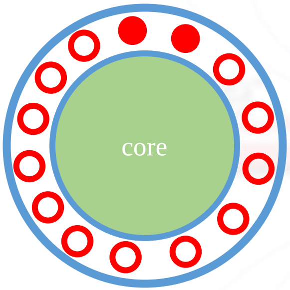
What's next?

open 4*f* electrons

W^{27+}–W^{25+}

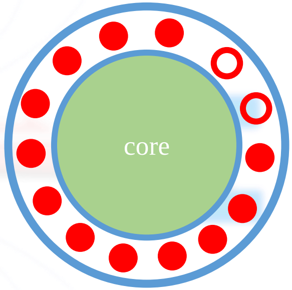
W^{16+}–W^{24+}

W^{7+}–W^{15+}



	Ground state
W^{27+}	$4d^{10}4f^{1}$
W^{26+}	$4d^{10}4f^{2}$
W^{25+}	$4d^{10}4f^{3}$
W^{24+}	$4d^{10}4f^{4}$

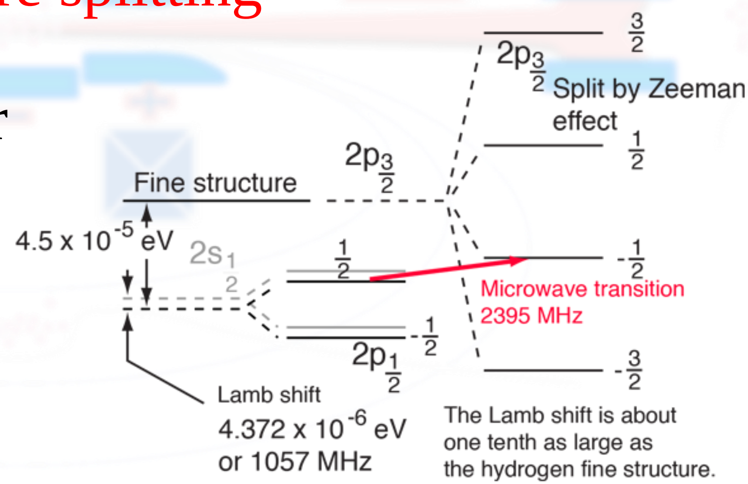
	Ground state
W^{7+}	$4f^{13}\,5s^2\,5p^6$
W^{8+}	$4f^{14}\,5s^2\,5p^4$
W^{9+}	$4f^{14}\,5s^2\,5p^3$
W^{10+}	$4f^{14}\,5s^2\,5p^2$
W^{11+}	$4f^{13}\,5s^2\,5p^2$
W^{12+}	$4f^{14}\,5s^2$
W^{13+}	$4f^{13}\,5s^2$
W^{14+}	$4f^{12}\,5s^2$
W^{15+}	$4f^{11}\,5s^2$
W^{14+}	$4f^{11}\,5s^1$



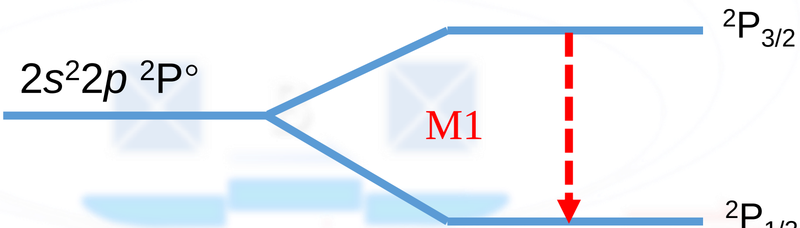
How to calculate more accurately for ions with Complex Electronic Structure?

Part II: HCI - Test QED

- Lamb shift
- Fine/ Hyperfine structure splitting
- Bound electron g-factor
- …



Fine structure of B-like ions



NIST Atomic Spectra Database Levels Data

S XII 53 Levels Found

Z = 16, B isoelectronic sequence

S^{11+}

Data on Landé factors and level compositions are not available for this ion in ASD

Primary data source	Query NIST Bibliographic Database for **S XII** (new window)
Martin et al. 1990	Literature on S XII Energy Levels

Configuration	Term	J	Level (eV)	Uncertainty (eV)	Reference
$2s^22p$	$^2P^\circ$	1/2	0.00000		L7237
		3/2	1.62857		
$2s2p^2$	^4P	1/2	24.0383+x		
		3/2	24.6326+x		
		5/2	25.4695+x		

M1 transition for Boron-like ions:

- Astrophysical plasma diagnostics;
- **Test quantum electrodynamic (QED);**
- Candidate transitions for HCI optical clock;

Collaborated with W.Q. Weng from IMP, Lanzhou

B-like Ions: Test QED

VOLUME 91, NUMBER 18 PHYSICAL REVIEW LETTERS week ending 31 OCTOBER 2003

High Precision Wavelength Measurements of QED-Sensitive Forbidden Transitions in Highly Charged Argon Ions

I. Draganić,[1,*] J. R. Crespo López-Urrutia,[1] R. DuBois,[2] S. Fritzsche,[3] V. M. Shabaev,[4] R. Soria Orts,[1] I. I. Tupitsyn,[1,4] Y. Zou,[5] and J. Ullrich[1]

[1]*Max-Planck Institut für Kernphysik, Saupfercheckweg 1, D-69117 Heidelberg, Germany*
[2]*University of Missouri-Rolla, Physics Building, Rolla, Missouri 65409-0640, USA*

PRL 98, 173004 (2007) PHYSICAL REVIEW LETTERS week ending 27 APRIL 2007

QED Calculation of the $2p_{3/2} - 2p_{1/2}$ Transition Energy in Boronlike Argon

A. N. Artemyev,[1,2] V. M. Shabaev,[1,2] I. I. Tupitsyn,[1,2] G. Plunien,[2] and V. A. Yerokhin[3]

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[2]*Institut für Theoretische Physik, TU Dresden, Mommsenstraße 13, D-01062 Dresden, Germany*
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(Received 20 February 2007; published 27 April 2007)

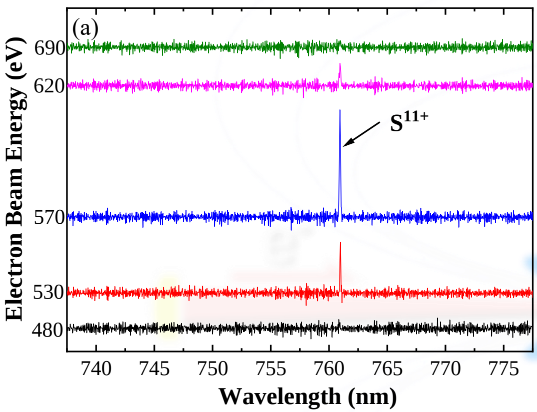
Table: Experimental values and accuracy for $^2P_{3/2} \rightarrow {}^2P_{1/2}$ transition energy

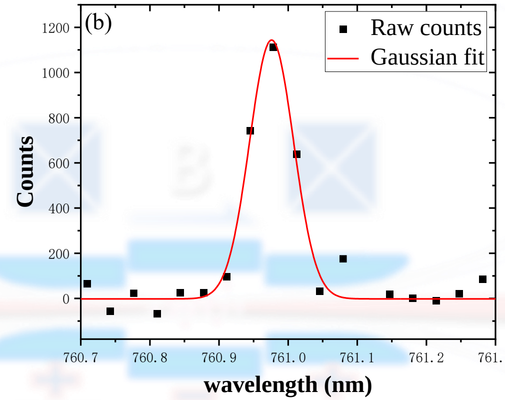
Ions	Expt. Energy(eV)	Accuracy
S^{11+}	1.6285(1)	7.61×10^{-5}
Cl^{12+}	2.1583(25)	1.16×10^{-3}
Ar^{13+}	**2.8090279(6)**	**2.14×10^{-7}**
K^{14+}	3.5963(31)	8.62×10^{-4}
Ca^{15+}	4.5397(37)	8.15×10^{-4}
Sc^{16+}	5.6583(4)	7.07×10^{-5}
Ti^{17+}	6.9732(4)	5.74×10^{-5}
V^{18+}	8.5061(50)	5.88×10^{-4}
Cr^{19+}	10.2815(17)	1.65×10^{-4}
Mn^{20+}	12.3100(12)	9.75×10^{-5}
Fe^{21+}	14.6640(35)	2.39×10^{-4}
Ni^{23+}	20.3286(68)	3.35×10^{-4}
Cu^{24+}	23.7154(93)	3.92×10^{-4}

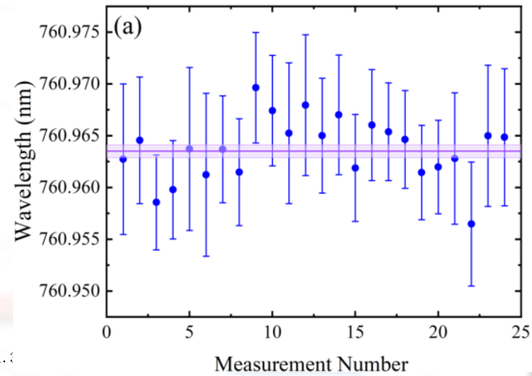
A. N. Artemyev et al., Phys. Rev. A 88, 032518 (2013)

Forbidden transition of B-like S^{11+} and Cl^{12+}

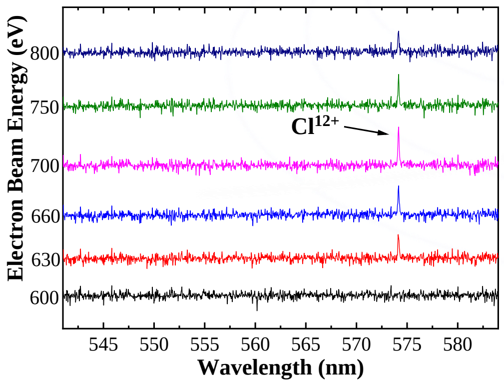
The experimental results

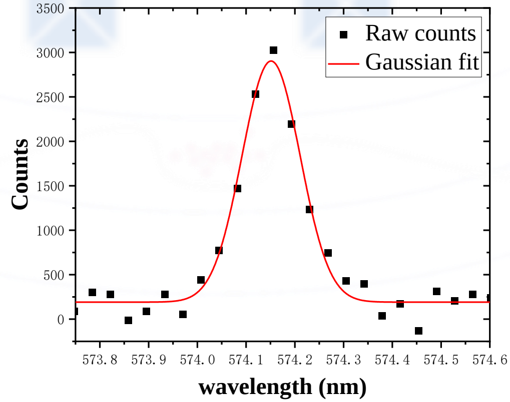


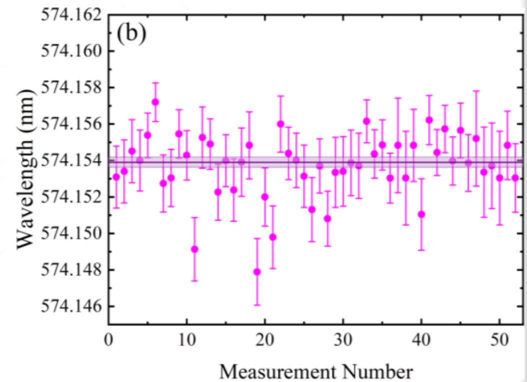




760.9635(29) nm







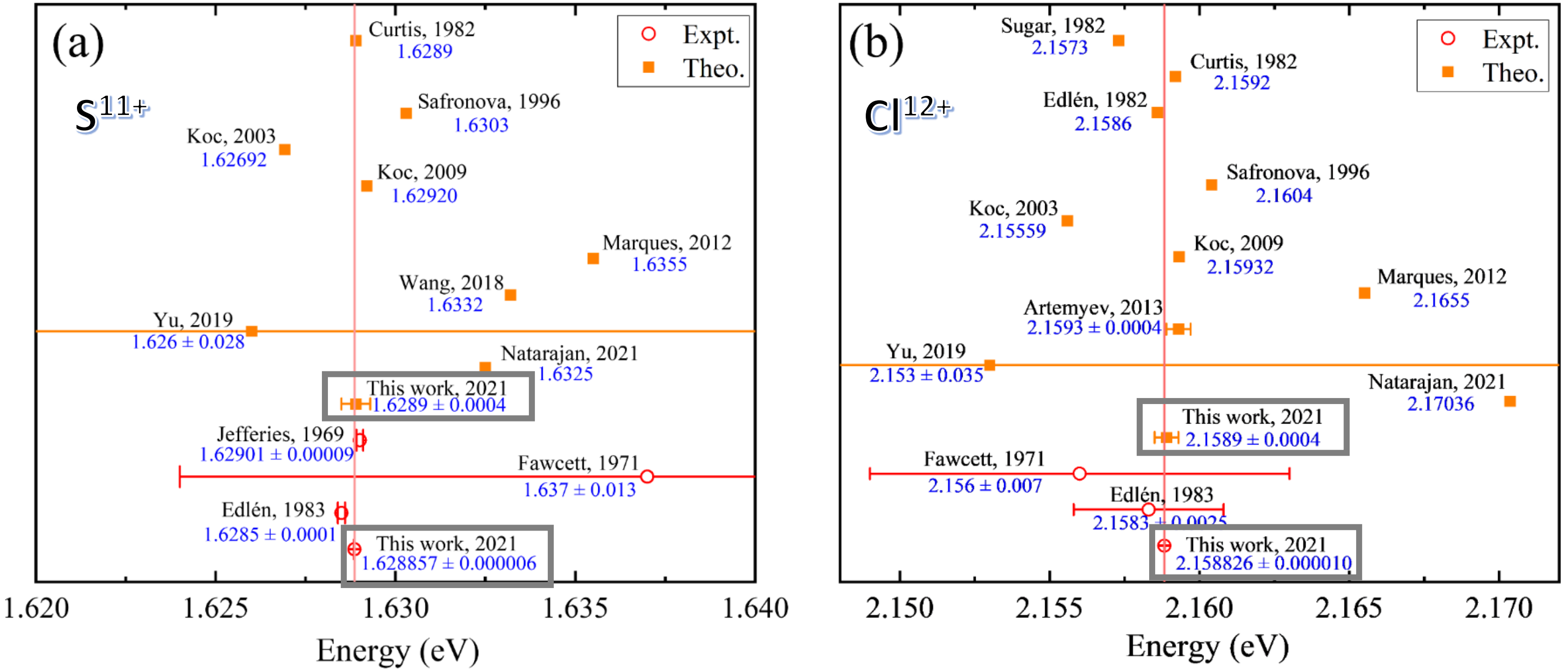
574.1539(26) nm

Forbidden transition of B-like S^{11+} and Cl^{12+}

Theoretical calculation results

	S^{11+} (eV)		Cl^{12+} (eV)	
	Core-Hartree	Kohn-Sham	Core-Hartree	Kohn-Sham
Dirac	1.76301	1.79581	2.32760	2.36827
Correlation,1	-0.08043	-0.11281	-0.10034	-0.14069
Correlation,2	-0.11063	-0.08568	-0.14108	-0.10825
Correlation,3	+0.0538(2)	0.0285(2)	+0.0687(2)	0.0356(2)
QED,1	0.00340	0.00343	0.00441	0.00448
QED,2	-0.0003(3)	-0.0003(3)	-0.0003(3)	-0.0004(3)
Recoil	-0.00009	-0.00009	-0.00008	-0.00008
Total	1.6289(4)	1.6289(4)	2.1589(4)	2.1589(4)
Final	1.6289(4)		2.1589(4)	
Expt.(This work)	1.628857(6)		2.158826(10)	
Expt.(prev.)	1.6285(1)		2.1583(25)	

Forbidden transition of B-like S^{11+} and Cl^{12+}

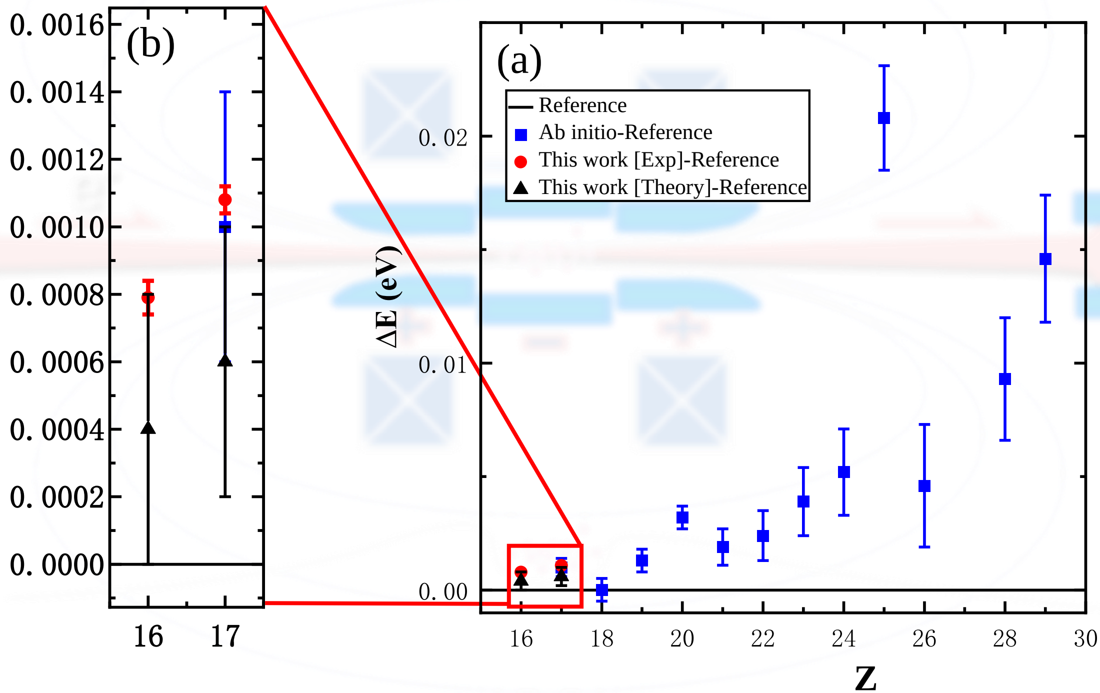


Increased by~20 times

Increased by~200 times

Forbidden transition of B-like S^{11+} and Cl^{12+}

Comparison of experimental and theoretical results of isoelectronic sequence boronlike ions



B. Edlén, Phys. Scr. 28, 483 (1983); I. Draganić et al, Phys. Rev. Lett. 91, 183001 (2003); A. N. Artemyev et al., Phys. Rev. A 88, 032518 (2013).

What's next?

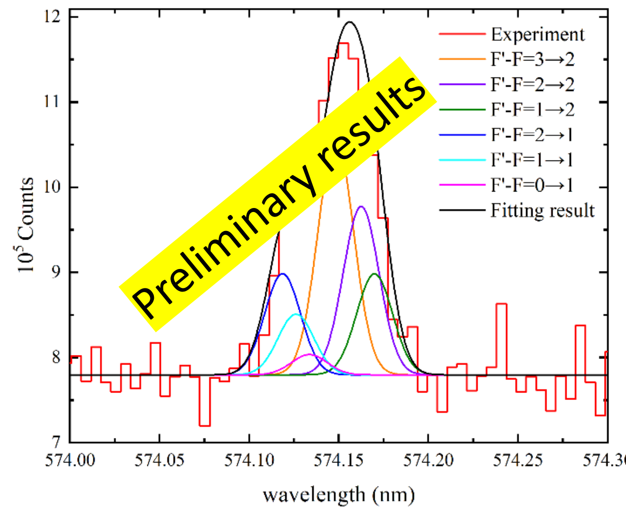
Hyperfine of B-like Ions

Extended Data Table 1 | Measured frequency ratios and absolute frequencies

Measurement	Value	Relative uncertainty
$R(^{40}Ar^{13+})$	1.057 769 387 587 480 94(11)	1.0×10^{-16}
$\nu(^{40}Ar^{13+})$	679 216 462 397 957.43(11) Hz	1.5×10^{-16}
$R(^{36}Ar^{13+})$	1.057 766 462 735 187 48(13)	1.2×10^{-16}
$\nu(^{36}Ar^{13+})$	679 214 584 287 424.91(12) Hz	1.7×10^{-16}
$\nu(^{40}Ar^{13+})$ - $\nu(^{36}Ar^{13+})$	1 878 110 532.51(11) Hz	5.7×10^{-11}

Optical frequency ratios $R(^{X}Ar^{13+}) = \nu(^{X}Ar^{13+})/\nu(^{171}Yb^{+}\ E3)$, derived transition frequencies $\nu(^{X}Ar^{13+})$, resulting isotope shift $\nu(^{40}Ar^{13+})-\nu(^{36}Ar^{13+})$ and total relative uncertainties of each of the measurements are given.

Nature **611**, 43-47 (2022)



the Fine Structure Splitting of : $2p^5$

Electron Correlation
Breit Interaction
QED: Self Energy(SE)+Vacuum Polarization(VP)

PHYSICAL REVIEW A **98**, 020502(R) (2018)

Rapid Communications

Proposal of highly accurate tests of Breit and QED effects in the ground state 2p⁵ of the F-like isoelectronic sequence

M. C. Li,[1] R. Si,[2] T. Brage,[1,3,*] R. Hutton,[1,†] and Y. M. Zou[1]
[1]*Shanghai EBIT Laboratory, Institute of Modern Physics and Key Laboratory of Nuclear Physics and Ion-beam Applic... Fudan University, Shanghai, China 200433*
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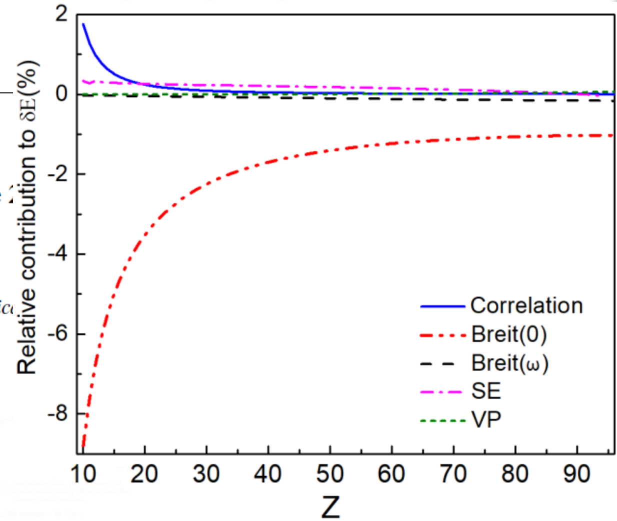
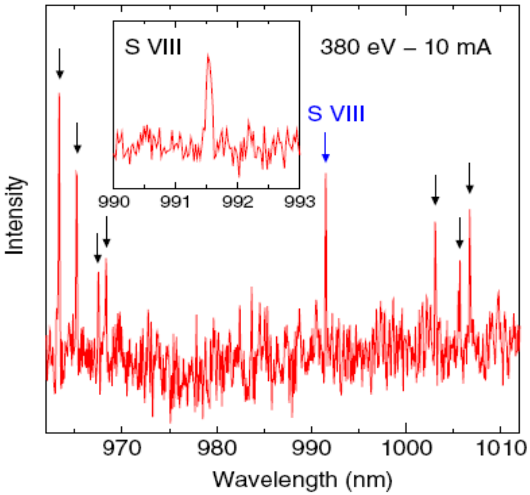


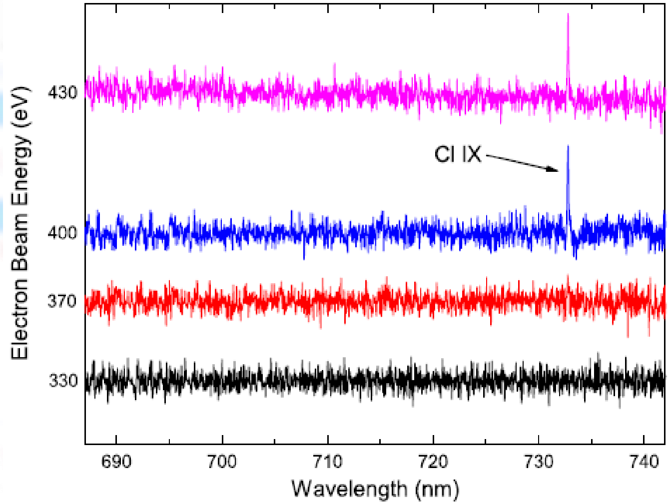
Single hole in outermost subshell of a shell (SHOSS)
e.g. $1s^2 2s^2 2p^5$ (F-like) or $1s^2 2s^2 2p^6 3s^2 3p^6 3d^9$ (Co-like)

Inspired by R.Hutton, Collaborated with N.Nakamura & A.Volotka

the Fine Structure Splitting of : $2p^5$

S^{7+} and Cl^{8+} $2p^5$: $^2P_{1/2} - {}^2P_{3/2}$



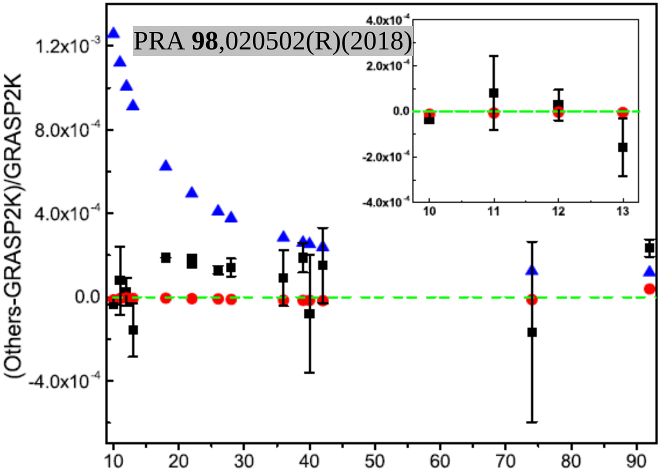


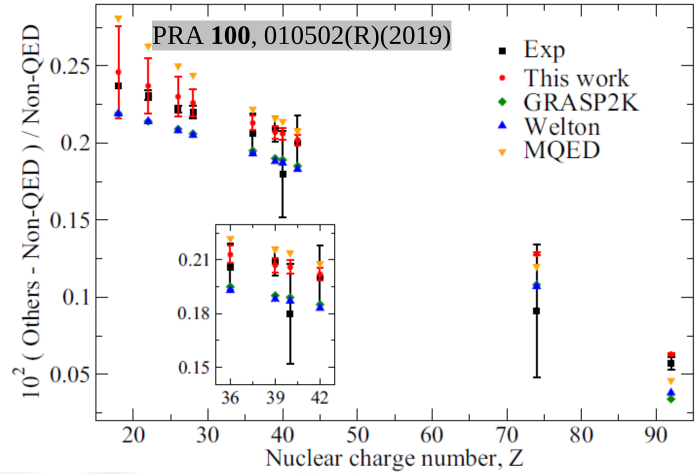
S^{7+} : λ=991.532 ±0.020 nm @Cobit

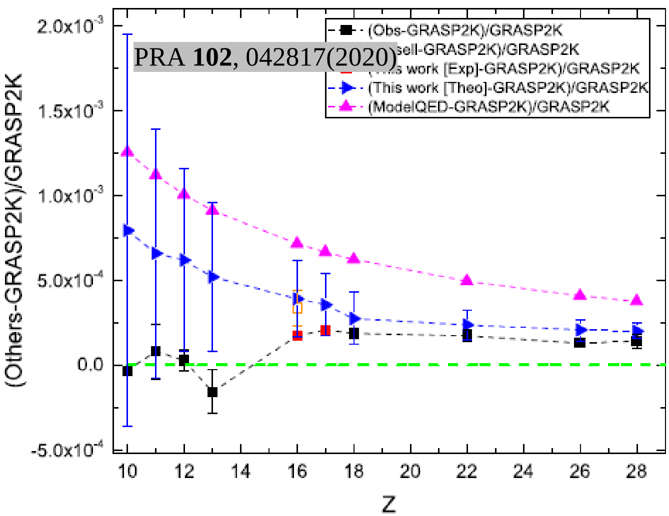
Cl^{8+} : λ=732.757 ±0.017 nm@SH-HtscEBIT

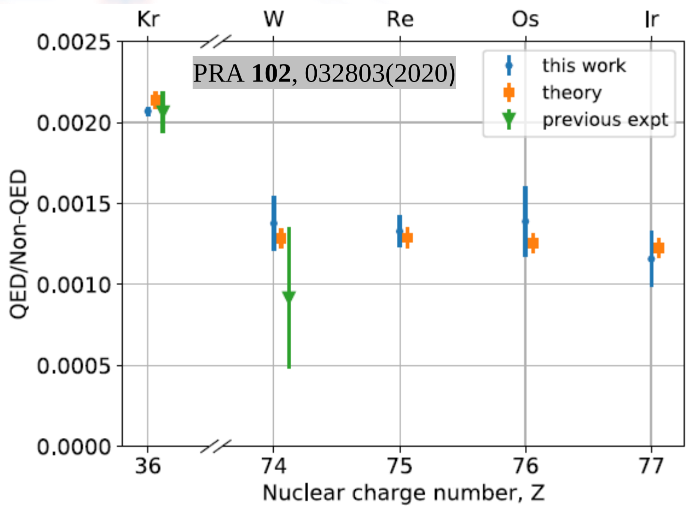
Q. Lu, *et al*. PRA **102**, 042817(2020)

the Fine Structure Splitting of : $2p^5$



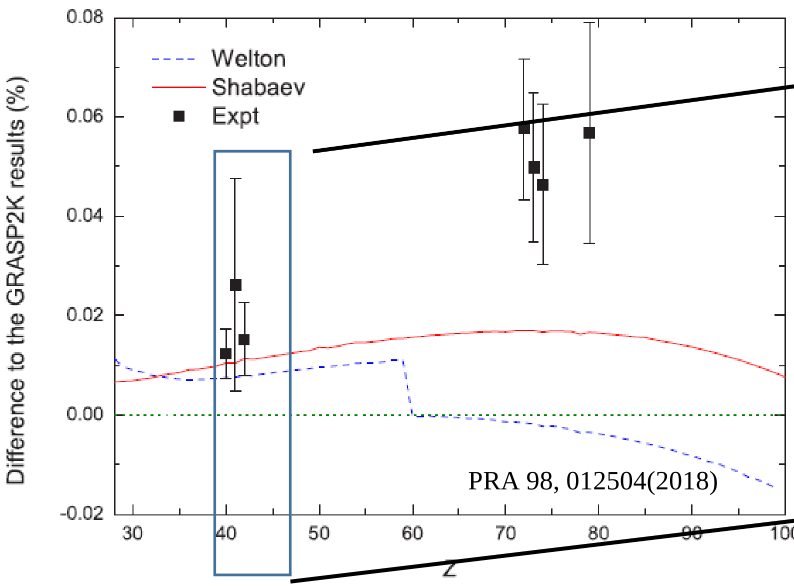


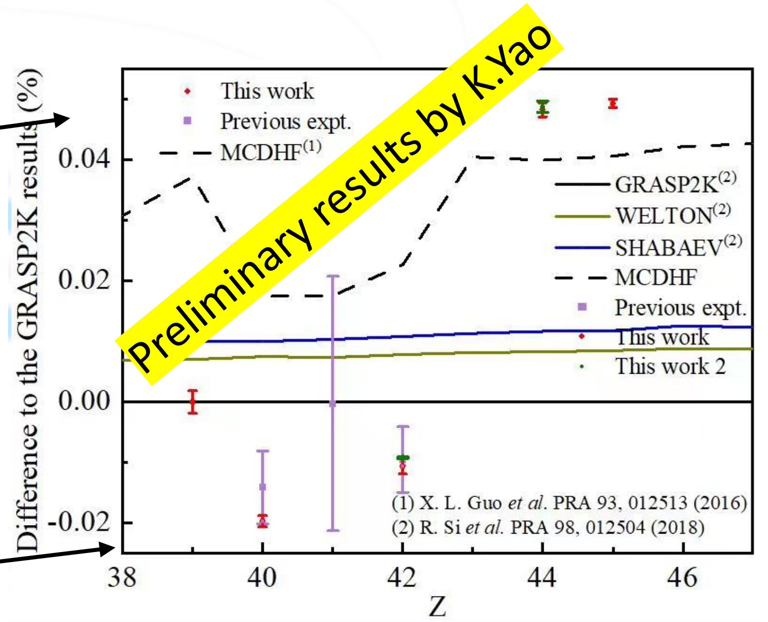




the Fine Structure Splitting of : $3d^9$

$3d^9\,{}^2D_{5/2,3/2}$





Z=41, 428 nm
Z=74, 18.567(3) nm

Summary

- Background
- Tungsten Spectroscopy
- Chlorine& Sulfur Spectroscopy
- Summary

Provide data for fusion

Open 4f electrons

Calculate more accurately

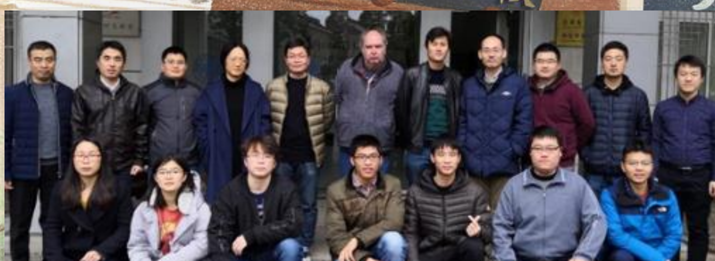
B-like ions

Fine structure/2p5

QED Test

Thanks for your attention!

C. Y. Chen, R.Si,
R. Hutton, Y. Yang, K. Yao,
B. Tu, B. Wei, Y. Zou…



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