



Periodic table for highly charged ions

Chunhai Lyu

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1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	
Hydrogen 1 H 1.008																	Helium 2 He 4.0026	
Lithium 3 Li 6.94	Beryllium 4 Be 9.0122	Key: Element Name Atomic number Symbol Atomic weight (mean relative mass)											Boron 5 B 10.81	Carbon 6 C 12.011	Nitrogen 7 N 14.007	Oxygen 8 O 15.999	Fluorine 9 F 18.998	Neon 10 Ne 20.180
Sodium 11 Na 22.990	Magnesium 12 Mg 24.305											Aluminium 13 Al 26.982	Silicon 14 Si 28.085	Phosphorus 15 P 30.974	Sulfur 16 S 32.06	Chlorine 17 Cl 35.45	Argon 18 Ar 39.948	
Potassium 19 K 39.098	Calcium 20 Ca 40.078(4)	Scandium 21 Sc 44.956	Titanium 22 Ti 47.867	Vanadium 23 V 50.942	Chromium 24 Cr 51.996	Manganese 25 Mn 54.938	Iron 26 Fe 55.845(2)	Cobalt 27 Co 58.933	Nickel 28 Ni 58.693	Copper 29 Cu 63.546(3)	Zinc 30 Zn 65.38(2)	Gallium 31 Ga 69.723	Germanium 32 Ge 72.630(8)	Arsenic 33 As 74.922	Selenium 34 Se 78.971(8)	Bromine 35 Br 79.904	Krypton 36 Kr 83.798(2)	
Rubidium 37 Rb 85.468	Strontium 38 Sr 87.62	Yttrium 39 Y 88.906	Zirconium 40 Zr 91.224(2)	Niobium 41 Nb 92.906(2)	Molybdenum 42 Mo 95.95	Technetium 43 Tc [98.906]	Ruthenium 44 Ru 101.07(2)	Rhodium 45 Rh 102.91	Palladium 46 Pd 106.42	Silver 47 Ag 107.87	Cadmium 48 Cd 112.41	Indium 49 In 114.82	Tin 50 Sn 118.71	Antimony 51 Sb 121.76	Tellurium 52 Te 127.60(3)	Iodine 53 I 126.90	Xenon 54 Xe 131.29	
Caesium 55 Cs 132.91	Barium 56 Ba 137.33	57-70 *	Lutetium 71 Lu 174.97	Hafnium 72 Hf 178.49(2)	Tantalum 73 Ta 180.95	Tungsten 74 W 183.84	Rhenium 75 Re 186.21	Osmium 76 Os 190.23(2)	Iridium 77 Ir 192.22	Platinum 78 Pt 195.08	Gold 79 Au 196.97	Mercury 80 Hg 200.59	Thallium 81 Tl 204.38	Lead 82 Pb 207.2	Bismuth 83 Bi 208.98	Polonium 84 Po [208.98]	Astatine 85 At [209.99]	Radon 86 Rn [222.02]
Francium 87 Fr [223.02]	Radium 88 Ra [226.03]	89-102 **	Lawrencium 103 Lr [262.11]	Rutherfordium 104 Rf [267.12]	Dubnium 105 Db [270.13]	Seaborgium 106 Sg [269.13]	Bohrium 107 Bh [270.13]	Hassium 108 Hs [270.13]	Mtnerium 109 Mt [278.16]	Darmstadtium 110 Ds [281.17]	Roentgenium 111 Rg [281.17]	Copernicium 112 Cn [285.18]	Nihonium 113 Nh [286.18]	Flerovium 114 Fl [289.19]	Moscovium 115 Mc [289.19]	Livermorium 116 Lv [293.20]	Tennesine 117 Ts [293.21]	Oganesson 118 Og [294.21]

*lanthanoids

**actinoids

Lanthanum 57 La 138.91	Cerium 58 Ce 140.12	Praseodymium 59 Pr 140.91	Neodymium 60 Nd 144.24	Promethium 61 Pm [144.91]	Samarium 62 Sm 150.36(2)	Europium 63 Eu 151.96	Gadolinium 64 Gd 157.25(3)	Terbium 65 Tb 158.93	Dysprosium 66 Dy 162.50	Holmium 67 Ho 164.93	Erbium 68 Er 167.26	Thulium 69 Tm 168.93	Ytterbium 70 Yb 173.05
Actinium 89 Ac [227.03]	Thorium 90 Th 232.04	Protactinium 91 Pa 231.04	Uranium 92 U 238.03	Neptunium 93 Np [237.05]	Plutonium 94 Pu [244.06]	Americium 95 Am [243.06]	Curium 96 Cm [247.07]	Berkelium 97 Bk [247.07]	Californium 98 Cf [251.08]	Einsteinium 99 Es [262.08]	Fermium 100 Fm [267.10]	Mendelevium 101 Md [268.10]	Nobelium 102 No [269.10]

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
Hydrogen 1 1.008 1s																	Helium 2 4.0026 He
Lithium 3 6.94 Li	Beryllium 4 9.0122 Be											Boron 5 10.81 B	Carbon 6 12.011 C	Nitrogen 7 14.0064 N	Oxygen 8 15.999 O	Fluorine 9 18.998 F	Neon 10 20.18 Ne
Sodium 11 22.990 Na	Magnesium 12 24.305 Mg											Aluminum 13 26.982 Al	Silicon 14 28.085 Si	Phosphorus 15 30.974 P	Sulfur 16 32.06 S	Chlorine 17 35.45 Cl	Argon 18 39.948 Ar
Potassium 19 39.098 K	Calcium 20 40.078(4) Ca	Scandium 21 44.956 Sc	Titanium 22 47.867 Ti	Vanadium 23 50.942 V	Chromium 24 51.996 Cr	Manganese 25 54.938 Mn	Iron 26 55.845(2) Fe	Cobalt 27 58.933 Co	Nickel 28 58.693 Ni	Copper 29 63.546(3) Cu	Zinc 30 65.38(2) Zn	Gallium 31 69.723 Ga	Germanium 32 72.630(8) Ge	Arsenic 33 74.922 As	Selenium 34 78.971(8) Se	Bromine 35 79.904 Br	Krypton 36 83.798(2) Kr
Rubidium 37 85.468 Rb	Sr 38 87.62 Sr	Yttrium 39 88.906 Y	Zirconium 40 91.224 Zr	Niobium 41 92.906 Nb	Molybdenum 42 95.94 Mo	Technetium 43 [98] Tc	Ruthenium 44 101.07 Ru	Rhodium 45 102.905 Rh	Palladium 46 106.42 Pd	Silver 47 107.87 Ag	Cadmium 48 112.41 Cd	Indium 49 114.82 In	Tin 50 118.71 Sn	Antimony 51 121.76 Sb	Tellurium 52 127.60(3) Te	Iodine 53 126.90 I	Xenon 54 131.29 Xe
Cesium 55 132.91 Cs	Barium 56 137.33 Ba	Lanthanum 57 138.91 La	Cerium 58 140.12 Ce	Praseodymium 59 140.91 Pr	Neodymium 60 144.24 Nd	Promethium 61 [144.91] Pm	Samarium 62 150.36(2) Sm	Europium 63 151.96 Eu	Gadolinium 64 157.25(3) Gd	Terbium 65 158.93 Tb	Dysprosium 66 162.50 Dy	Holmium 67 164.93 Ho	Erbium 68 167.26 Er	Thulium 69 168.93 Tm	Ytterbium 70 173.05 Yb		
Francium 87 [223.02] Fr	Radium 88 [226.03] Ra	Actinium 89 [227.03] Ac	Thorium 90 232.04 Th	Protactinium 91 231.04 Pa	Uranium 92 238.03 U	Np 93 [237.05] Np	Pu 94 [244.06] Pu	Am 95 [243.06] Am	Cm 96 [247.07] Cm	Bk 97 [247.07] Bk	Cf 98 [251.08] Cf	Es 99 [252.08] Es	Fm 100 [257.10] Fm	Md 101 [258.10] Md	No 102 [259.10] No		

Key:

Element Name
Atomic number
Symbol
Atomic weight (mean relative mass)

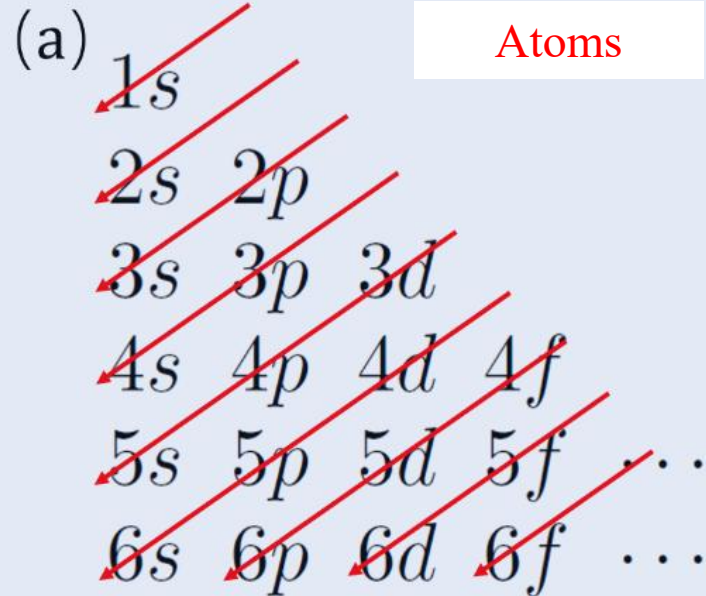
*lanthanoids

**actinoids

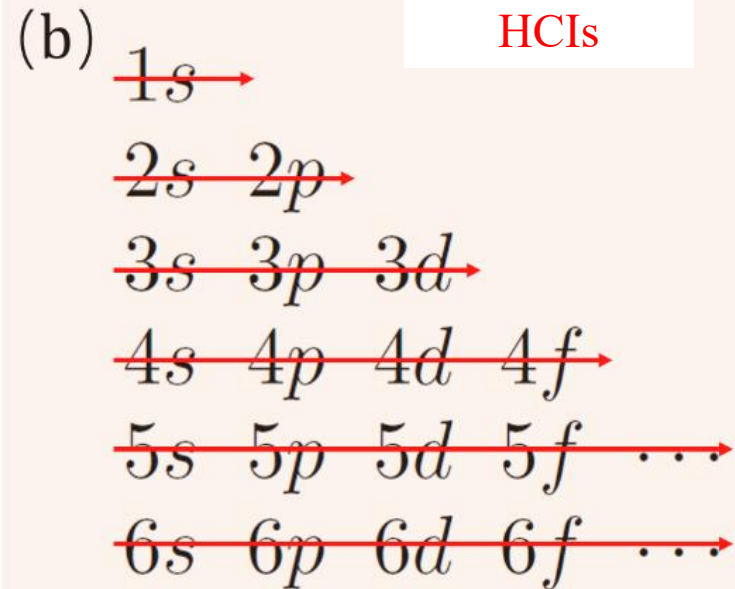
Lanthanum 57 138.91 La	Cerium 58 140.12 Ce	Praseodymium 59 140.91 Pr	Neodymium 60 144.24 Nd	Promethium 61 [144.91] Pm	Samarium 62 150.36(2) Sm	Europium 63 151.96 Eu	Gadolinium 64 157.25(3) Gd	Terbium 65 158.93 Tb	Dysprosium 66 162.50 Dy	Holmium 67 164.93 Ho	Erbium 68 167.26 Er	Thulium 69 168.93 Tm	Ytterbium 70 173.05 Yb
Actinium 89 [227.03] Ac	Thorium 90 232.04 Th	Protactinium 91 231.04 Pa	Uranium 92 238.03 U	Np 93 [237.05] Np	Pu 94 [244.06] Pu	Am 95 [243.06] Am	Cm 96 [247.07] Cm	Bk 97 [247.07] Bk	Cf 98 [251.08] Cf	Es 99 [252.08] Es	Fm 100 [257.10] Fm	Md 101 [258.10] Md	No 102 [259.10] No

Aufbau Principle

Madelung-Janet filling rule



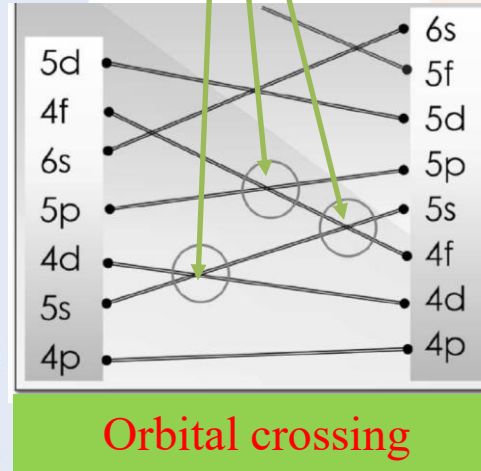
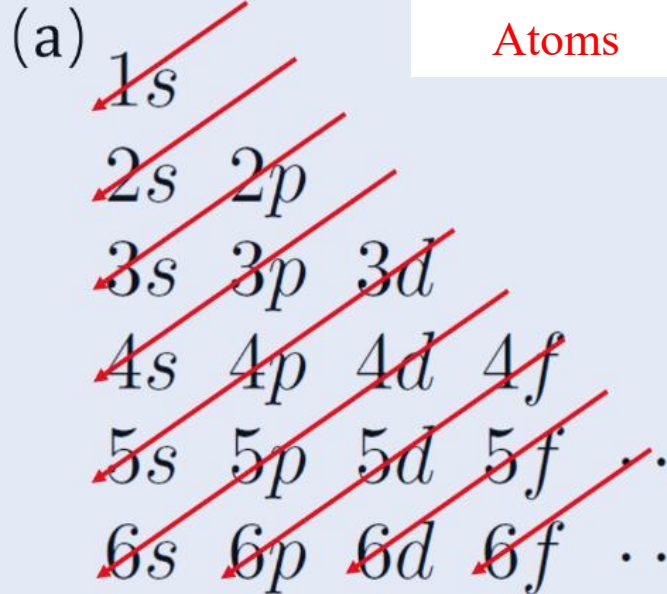
Coulomb filling rule



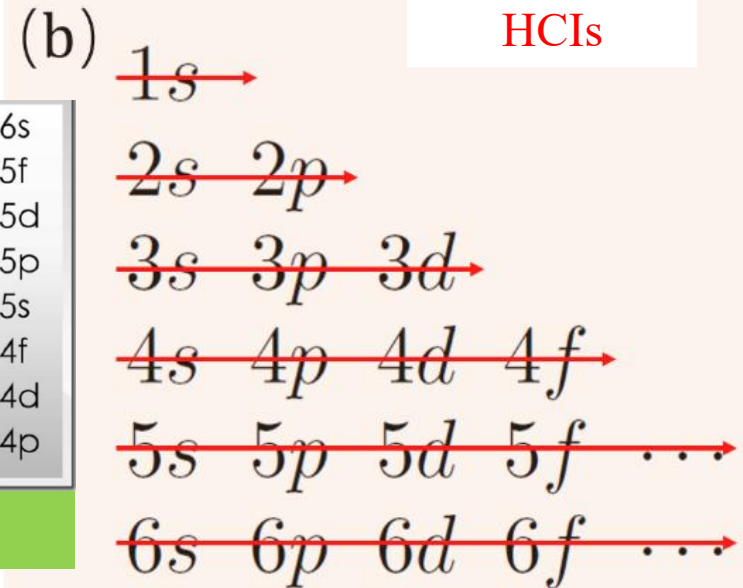
Aufbau Principle

- Optical transitions
- Variation of the fine-structure constant

Madelung-Janet filling rule



Coulomb filling rule



J. C. Berengut et. al, PRL **105**, 120801 (2010)

Periodic table based on Coulomb filling?

THE ORDER OF ELECTRON SHELLS IN IONIZED ATOMS*

By S. A. GOUDSMIT AND PAUL I. RICHARDS

BROOKHAVEN NATIONAL LABORATORY, UPTON, NEW YORK, AND
TECHNICAL OPERATIONS, INCORPORATED, BURLINGTON, MASSACHUSETTS

Communicated February 17, 1964

				1 2	1 2							
				3 4	3 4	5..10						
				5..10	11 12	11 12	13..18	19...28				
				13..18	19 20	29 30	31..36	37...46				
21...30	31..36	37 38	61 62	63..68	69...78	79....92	93.....110					
39...48	49..54	55 56	111 112	etc.								
57....70	71...80	81..86	87 88									
89....102	etc.											
f^{14}	d^{10}	p^6	s^2	s^2	p^6	d^{10}	f^{14}	g^{18}				
a. NEUTRAL ATOMS				b. HIGHLY IONIZED ATOMS								

FIG. 1.—The “Periodic System” for (a) neutral and (b) highly ionized atoms.

Periodic table for HCl

C. Lyu, et. al,
arXiv:2504.11237 (2025)

- Split l into l_- and l_+ ;
- d_- and p_+ , f_- and d_+ are lined together;
- Closed-shell configuration;
- Single electron/hole valence configuration;
- **Multiple electron valence configuration;**
- Electron-hole symmetry;
- **Forbidden transitions;**
-

- 2 electron, 4 orbitals
- In total $C_4^2=6$ occupations
- The 6 magnetic states for $J=0,2$

$M_J \backslash m_j$	3/2	1/2	-1/2	-3/2
2	×	×		
1	×		×	
0	×			×
0		×	×	
-1		×		×
-2			×	×

$\frac{1}{2}$	0	$\frac{1}{2}$	0	$\frac{3}{2}$	2,0	$\frac{3}{2}$	0	$\frac{5}{2}$	4,2,0	$\frac{9}{2}, \frac{3}{2}, \frac{5}{2}$	4,2,0	$\frac{5}{2}$	0	$\frac{7}{2}$	6,4,2,0	(15,9,11,3,7,5)/2	8,5,2,6,4,4,2,0	(15,9,11,3,7,5)/2	6,4,2,0	$\frac{7}{2}$	0
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66 5p ₊ ² Dy-like W08+	67 5p ₊ ³ Ho-like Re08+	68 5p ₊ ⁴ Er-like W06+	74 5d ₊ ¹ Ta-like Au06+	75 5d ₊ ² W-like Au05+	76 5d ₊ ³ Re-like Ti06+	77 5d ₊ ⁴ Os-like Au03+	78 5d ₊ ⁵ Ir-like Au02+	79 5d ₊ ⁶ Pt-like Au01+	80 5f ₋ ¹ Au-like Sg25+	81 5f ₋ ² Hg-like Sg24+	82 5f ₋ ³ Tl-like Hs27+	83 5f ₋ ⁴ Pb-like Ds28+	84 5f ₋ ⁵ Bi-like Ds27+	85 5f ₋ ⁶ Po-like Nh29+	86 5f ₊ ¹ Fr-like Sg19+	87 5f ₊ ² Ra-like Hs20+	88 5f ₊ ³ Ac-like Mt20+	89 5f ₊ ⁴ Th-like Cn22+	90 5f ₊ ⁵ Pa-like Nh22+	91 5f ₊ ⁶ U-like Lv24+	92 5f ₊ ⁷ Np-like Og25+	93 5f ₊ ⁸ Pu-like Ubu27+
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Periodic table for HCl

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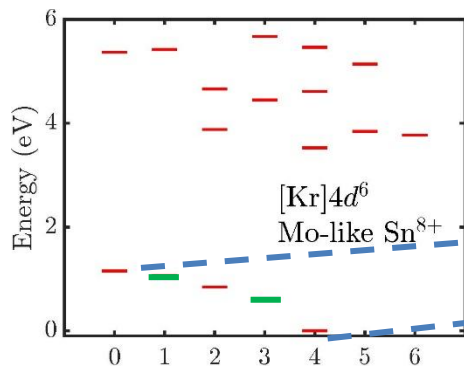
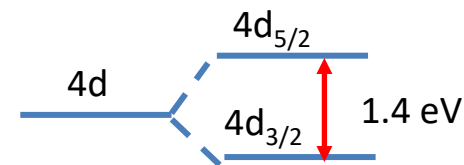
1 $1s^1$ H-like H00+	2 $1s^2$ He-like He00+																
3 $2s^1$ Li-like Li00+	4 $2s^2$ Be-like Be00+	5 $2p^1$ B-like Mn20+	6 $2p^2$ C-like Mn19+	7 $2p^1_+$ N-like Mn18+	8 $2p^2_+$ O-like Mn17+	9 $2p^3_+$ F-like Mn16+	10 $2p^4_+$ Ne-like Mn15+										
11 $3s^1$ Na-like Na00+	12 $3s^2$ Mg-like Mg00+	13 $3p^1$ Al-like Zn17+	14 $3p^2$ Si-like Zn16+	15 $3p^1_+$ P-like Zn15+	16 $3p^2_+$ S-like Zn14+	17 $3p^3_+$ Cl-like Zn13+	18 $3p^4_+$ Ar-like Zn14+										
				19 $3d^1$ K-like Cs36+	20 $3d^2$ Ca-like Cs35+	21 $3d^3$ Sc-like Cs34+	22 $3d^4$ Ti-like Cs33+	23 $3d^1_+$ V-like Ag24+	24 $3d^2_+$ Cr-like Ag23+	25 $3d^3_+$ Mn-like Sb26+	26 $3d^4_+$ Fe-like Rh19+	27 $3d^5_+$ Co-like Rh18+	28 $3d^6_+$ Ni-like Rh17+				
29 $4s^1$ Cu-like Cu00+	30 $4s^2$ Zn-like Zn00+	31 $4p^1$ Ga-like Nb10+	32 $4p^2$ Ge-like Nb09+	33 $4p^1_+$ As-like Nb08+	34 $4p^2_+$ Se-like Nb07+	35 $4p^3_+$ Br-like Nb06+	36 $4p^4_+$ Kr-like Nb05+										
				37 $4d^1$ Rb-like Eu26+	38 $4d^2$ Sr-like Eu25+	39 $4d^3$ Y-like Eu24+	40 $4d^4$ Zr-like Eu23+	41 $4d^1_+$ Nb-like La16+	42 $4d^2_+$ Mo-like La15+	43 $4d^3_+$ Tl-like Nd17+	44 $4d^4_+$ Ru-like Cs11+	45 $4d^5_+$ Rh-like Cs10+	46 $4d^6_+$ Pd-like Cs09+				
								47 $4f^1$ Ag-like Hf25+	48 $4f^2$ Cd-like Hf24+	49 $4f^3$ In-like Po35+	50 $4f^4$ Sn-like Rn36+	51 $4f^5$ Sb-like Rn35+	52 $4f^6$ Te-like Rn34+				
61 $5s^1$ Pm-like Pt17+	62 $5s^2$ Sm-like W12+	63 $5p^1$ Eu-like Ir14+	64 $5p^2$ Gd-like W10+	65 $5p^1_+$ Tb-like W09+	66 $5p^2_+$ Dy-like W08+	67 $5p^3_+$ Ho-like Re08+	68 $5p^4_+$ Er-like W06+										
				69 $5d^1$ Tm-like Bi14+	70 $5d^2$ Yb-like Bi13+	71 $5d^3$ Lu-like Bi12+	72 $5d^4$ Hf-like Bi11+	73 $5d^1_+$ Ta-like Au06+	74 $5d^2_+$ W-like Au05+	75 $5d^3_+$ Re-like Ti06+	76 $5d^4_+$ Os-like Au03+	77 $5d^5_+$ Ir-like Au02+	78 $5d^6_+$ Pt-like Au01+				
84 $6s^1$ At-like Nh28+	85 $6s^2$ Rn-like Rn18+																
								89 $5f^1$ Au-like Sa25+	90 $5f^2$ Hg-like Sa24+	91 $5f^3$ Tl-like Hs27+	92 $5f^4$ Pb-like Ds28+	93 $5f^5$ Bi-like Ds27+	94 $5f^6$ Po-like Nh29+				

- Split l into l_- and l_+ ;
- d_- and p_+ , f_- and d_+ are lined together;
- Closed-shell configuration;
- Single electron/hole valence configuration;
- Multiple electron valence configuration;
- Electron-hole symmetry;
- Forbidden transitions;
- ...

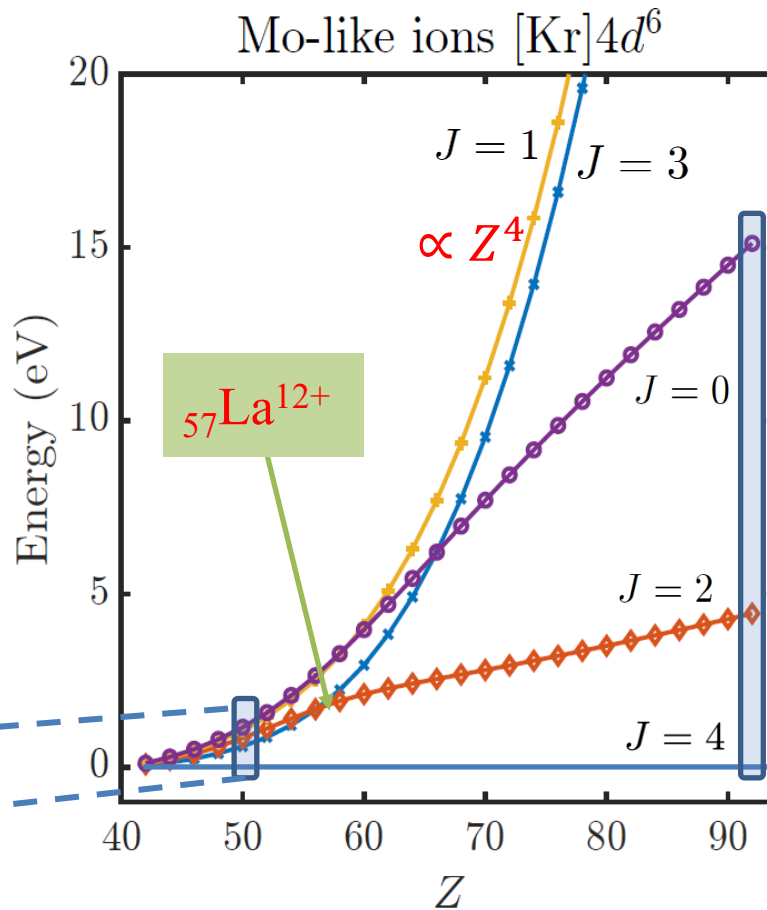
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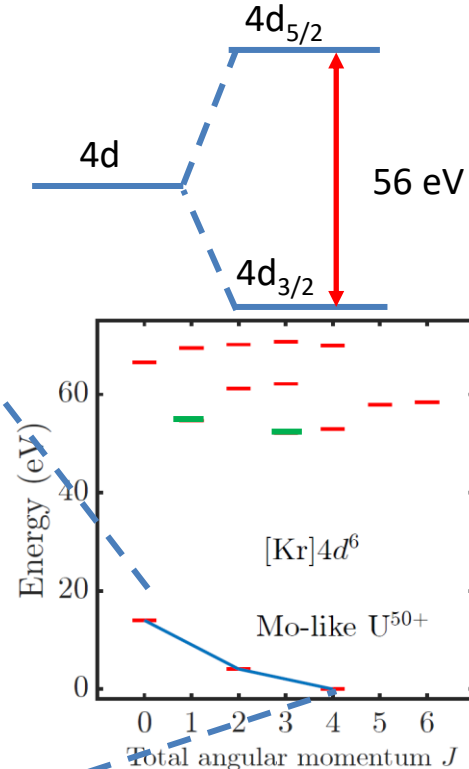
Relativistic effects vs Electron screenings



$4d^6$



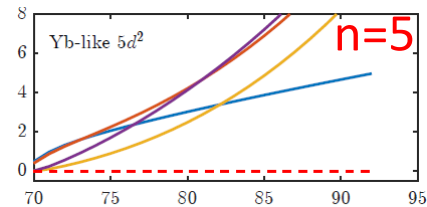
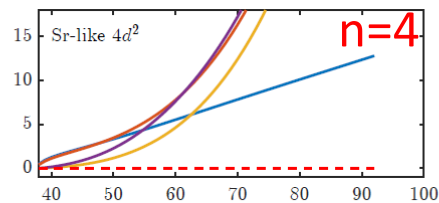
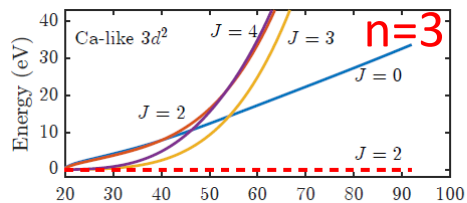
GRASP calculations



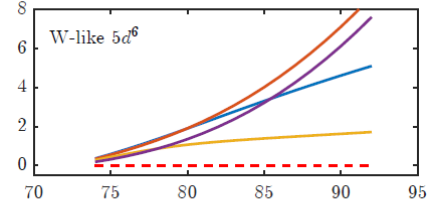
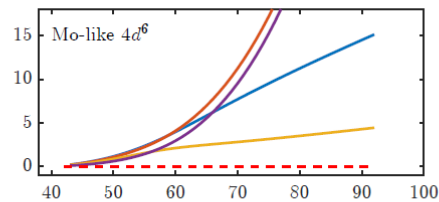
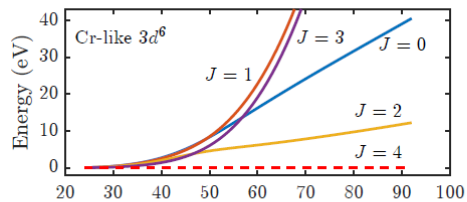
$4d_{3/2}^4 4d_{5/2}^2$

C. Lyu, et. al, Commun. Phys. **8**, 3 (2025)

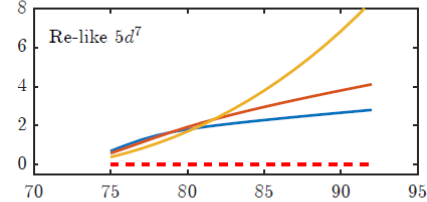
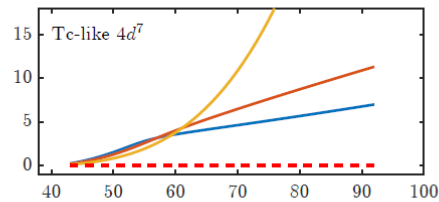
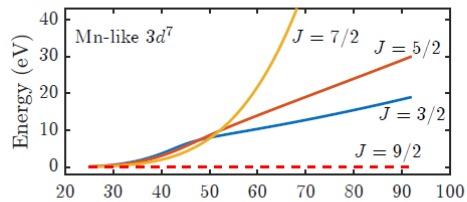
$nd_{3/2}^2$



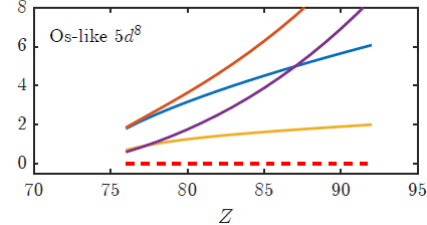
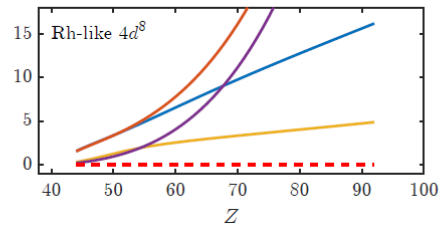
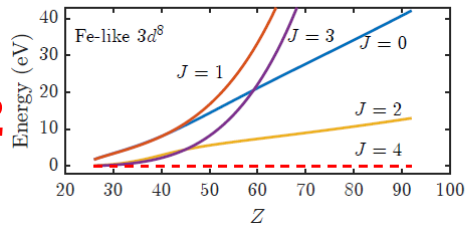
$nd_{5/2}^2$



$nd_{5/2}^3$



$nd_{5/2}^4$



GRASP calculations

C. Lyu, et. al, arXiv:2504.11237 (2025)

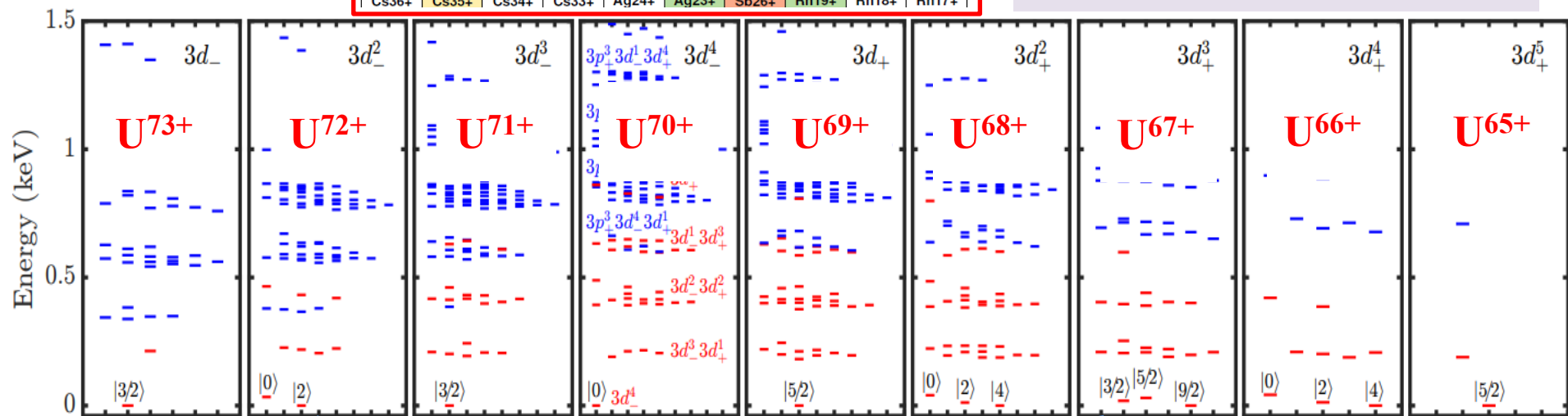
Periodic table for HCI

C. Lyu, et. al,
arXiv:2504.11237 (2025)

- Split l into l_- and l_+ ;
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- Closed-shell configuration;
- Single electron/hole valence configuration;
- Multiple electron valence configuration;
- Electron-hole symmetry;
- Forbidden transitions;
-

1 $1s^1$ H-like H00+	2 $1s^2$ He-like He00+								
3 $2s^1$ Li-like Li00+	4 $2s^2$ Be-like Be00+	5 $2p_1^-$ B-like Mn20+	6 $2p_2^-$ C-like Mn19+	7 $2p_3^+$ N-like Mn18+	8 $2p_4^+$ O-like Mn17+	9 $2p_5^+$ F-like Mn16+	10 $2p_6^+$ Ne-like Mn15+		
11 $3s^1$ Na-like Na00+	12 $3s^2$ Mg-like Mg00+	13 $3p_1^-$ Al-like Zn17+	14 $3p_2^-$ Si-like Zn16+	15 $3p_3^+$ P-like Zn15+	16 $3p_4^+$ S-like Zn14+	17 $3p_5^+$ Cl-like Zn13+	18 $3p_6^+$ Ar-like Zn12+		

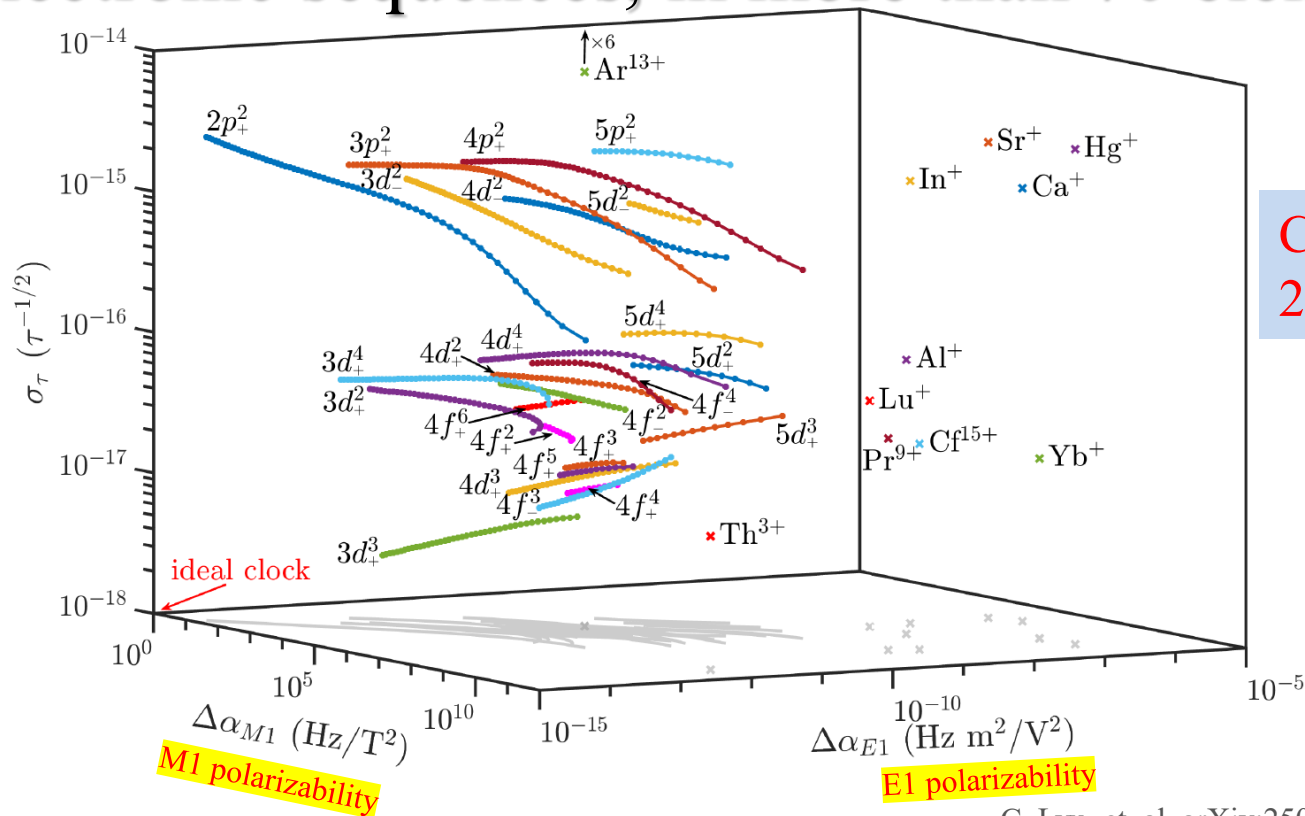
19 $3d_1^-$ K-like Cs36+	20 $3d_2^-$ Ca-like Cs35+	21 $3d_3^-$ Sc-like Cs34+	22 $3d_4^-$ Ti-like Cs33+	23 $3d_5^+$ V-like Ag24+	24 $3d_6^+$ Cr-like Ag23+	25 $3d_7^+$ Mn-like Sb26+	26 $3d_8^+$ Fe-like Rh19+	27 $3d_9^+$ Co-like Rh18+	28 $3d_{10}^+$ Ni-like Rh17+
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$\frac{1}{2}$	0	$\frac{1}{2}$	0	$\frac{3}{2}$	2,0	$\frac{3}{2}$	0	$\frac{5}{2}$	4,2,0	$\frac{9}{2}, \frac{3}{2}, \frac{5}{2}$	4,2,0	$\frac{5}{2}$	0	$\frac{7}{2}$	6,4,2,0	(15,9,11,3,7,5)/2	8,5,2,6,4,4,2,0	(15,9,11,3,7,5)/2	6,4,2,0	$\frac{7}{2}$	0
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More than 700 HCI clock transitions in 24 isoelectronic sequences, in more than 70 elements

Instability



C. Lyu, et. al, arXiv:2504.11237 (2025)

Periodic table for HCl

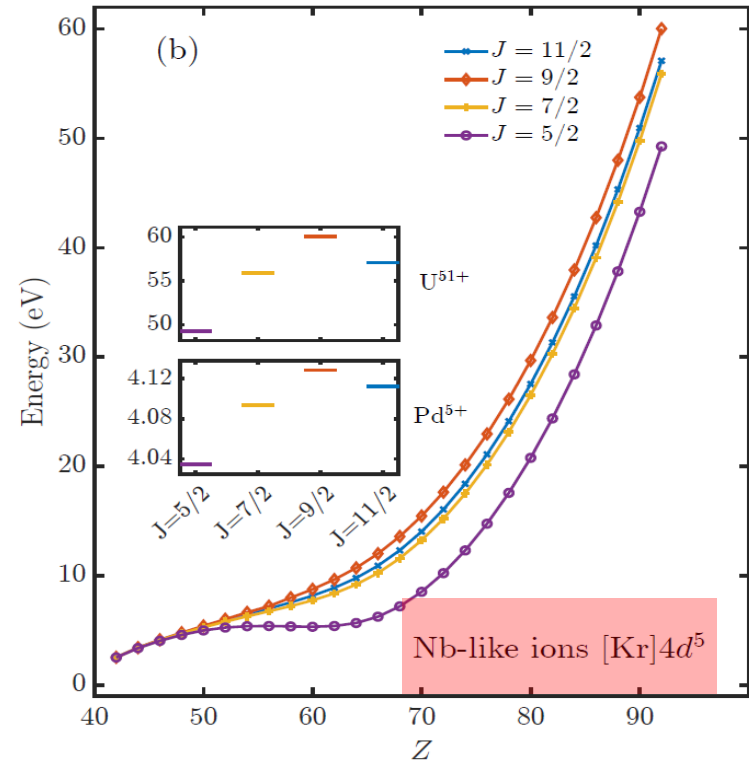
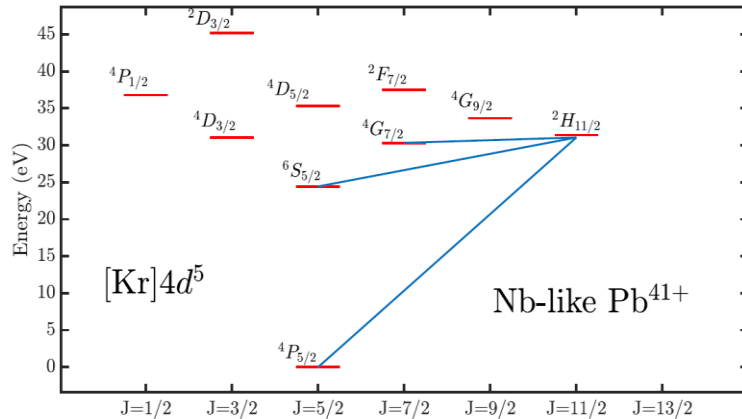
C. Lyu, et. al,
arXiv:2504.11237 (2025)

- Split l into l_- and l_+ ;
- d_- and p_+ , f_- and d_+ are lined together;
- Closed-shell configuration;
- Single electron/hole valence configuration;
- **Multiple electron valence configuration;**
- Electron-hole symmetry;
- **Forbidden transitions;**
-

Periodic table for HCI																		- Split l into l_- and l_+; d_- and p_+, f_- and d_+ are lined together; - Closed-shell configuration; - Single electron/hole valence configuration; - Multiple electron valence configuration; - Electron-hole symmetry; - Forbidden transitions; 																																																																																																																																																																																																																							
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Theoretical predictions: many XUV clock transitions in HCIs

$$4d_{+}^1$$

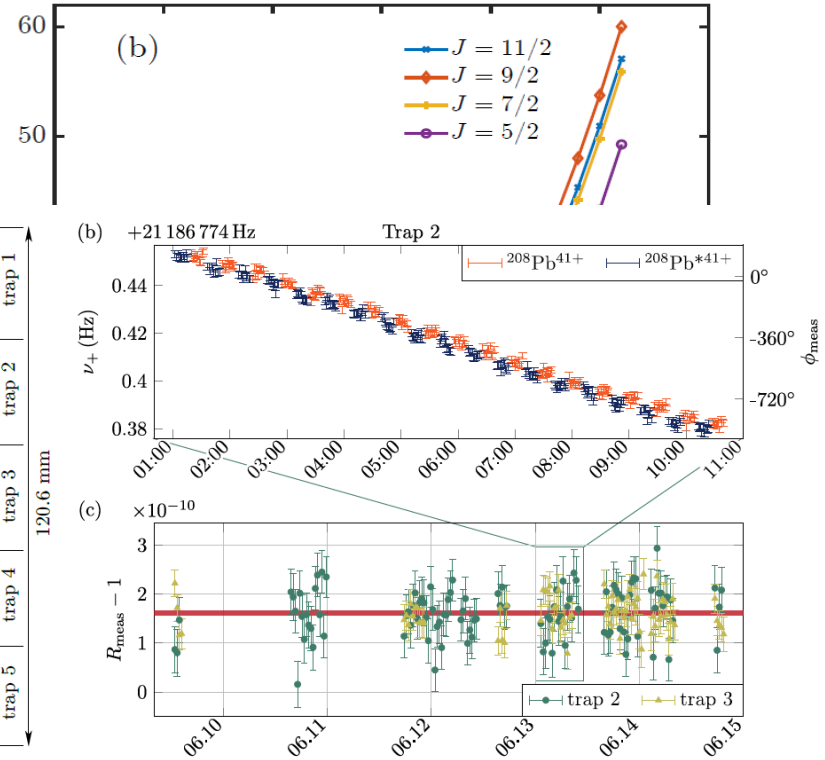
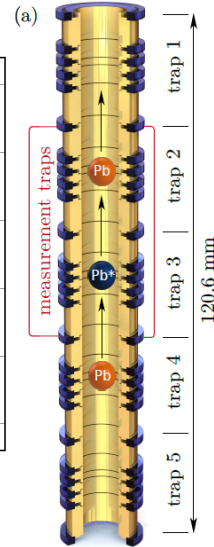
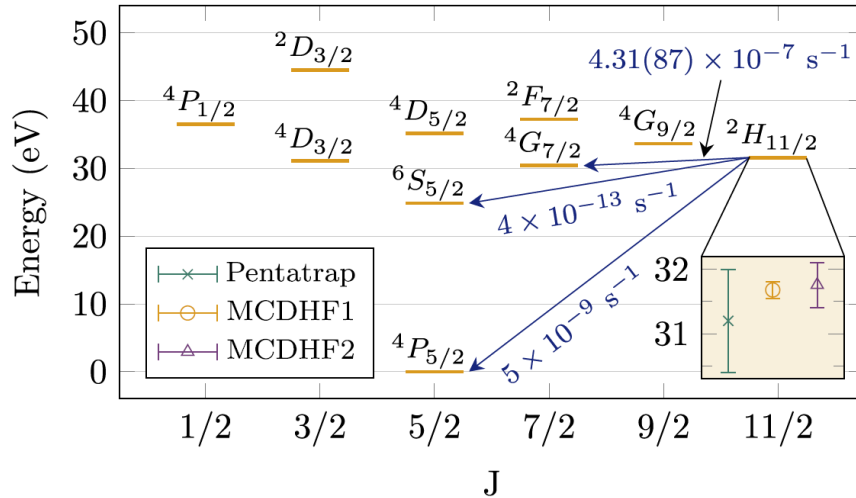


Multiconfiguration Dirac-Hatree-Fock calculations with the **GRASP2018** codes

C. Lyu, et. al, Commun. Phys. **8**, 3 (2025)

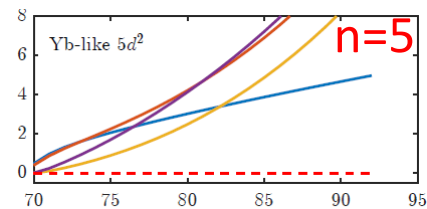
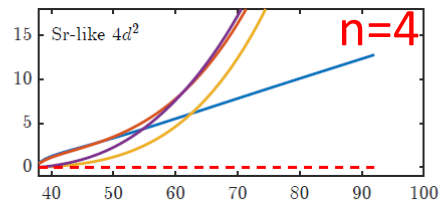
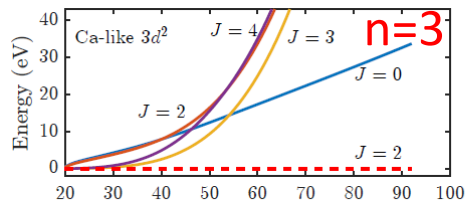
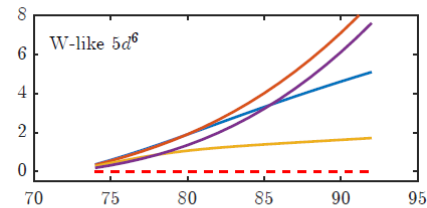
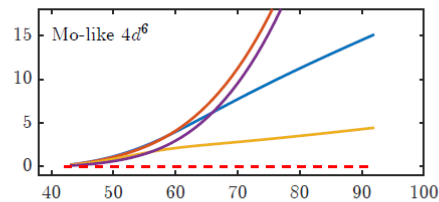
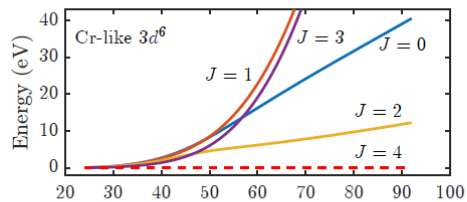
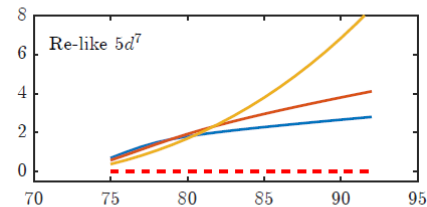
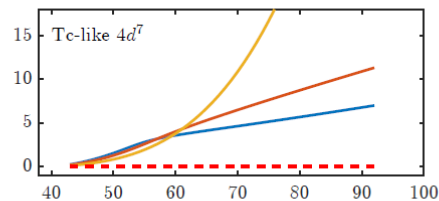
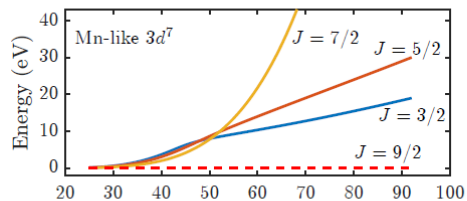
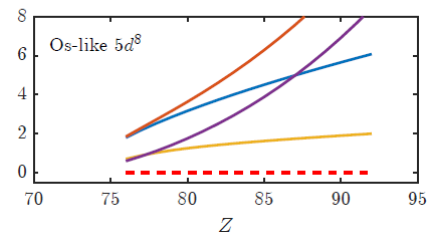
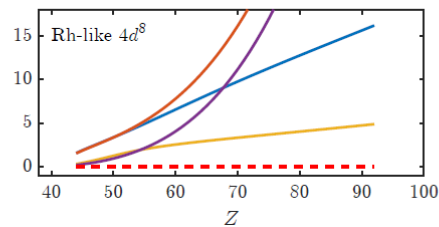
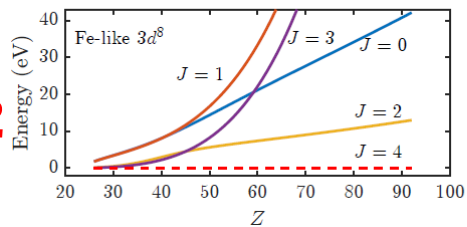
Theoretical predictions: many XUV clock transitions in HClIs

Pb⁴¹⁺

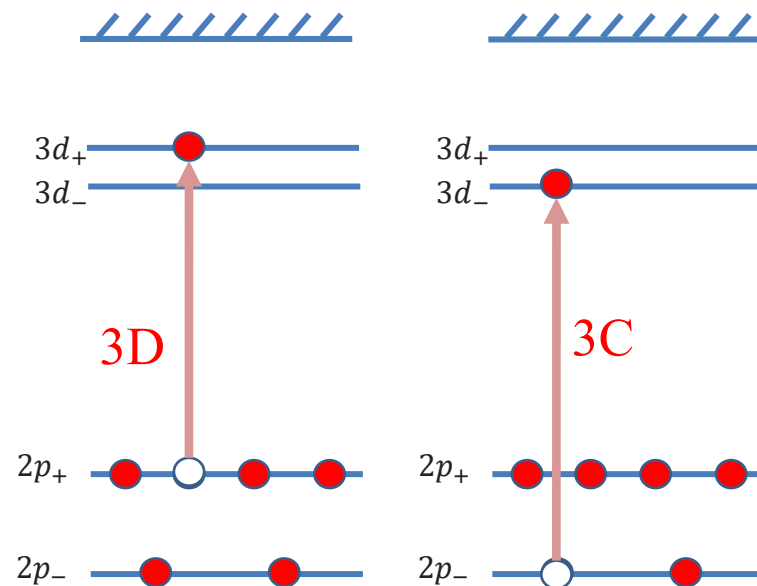
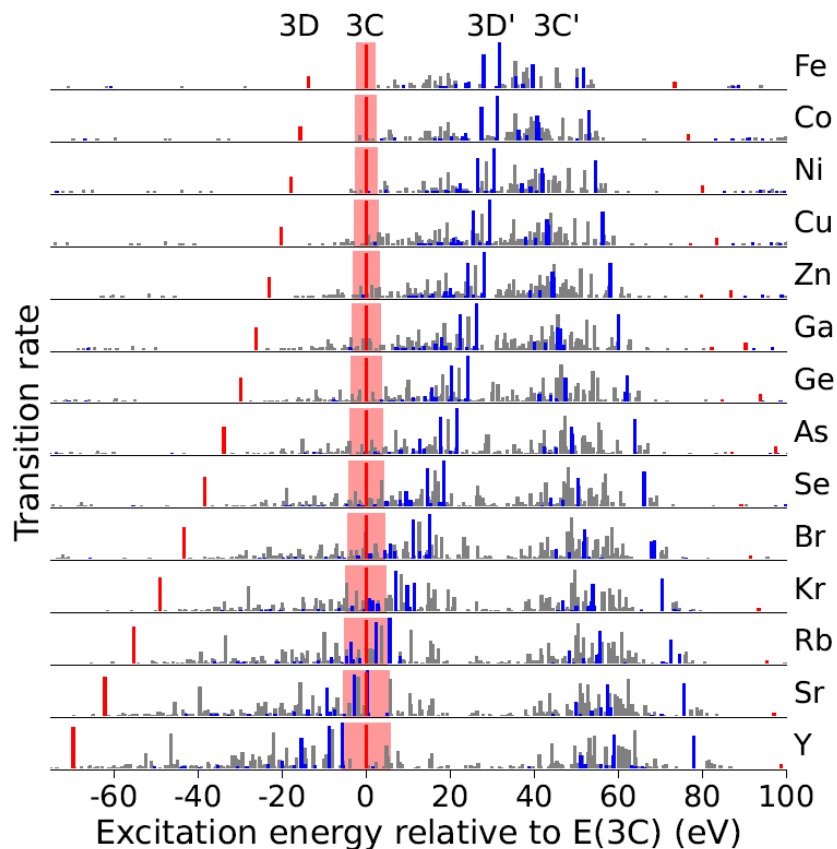


Multiconfiguration Dirac-Hatree-Fock calculations with the **GRASP2018 codes**

K. Kromer, C. Lyu, et. al, PRL.131.223002(2023)

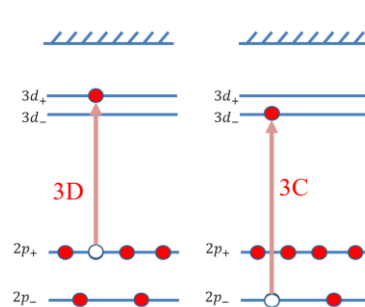
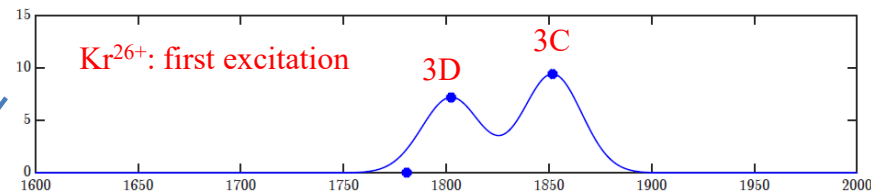
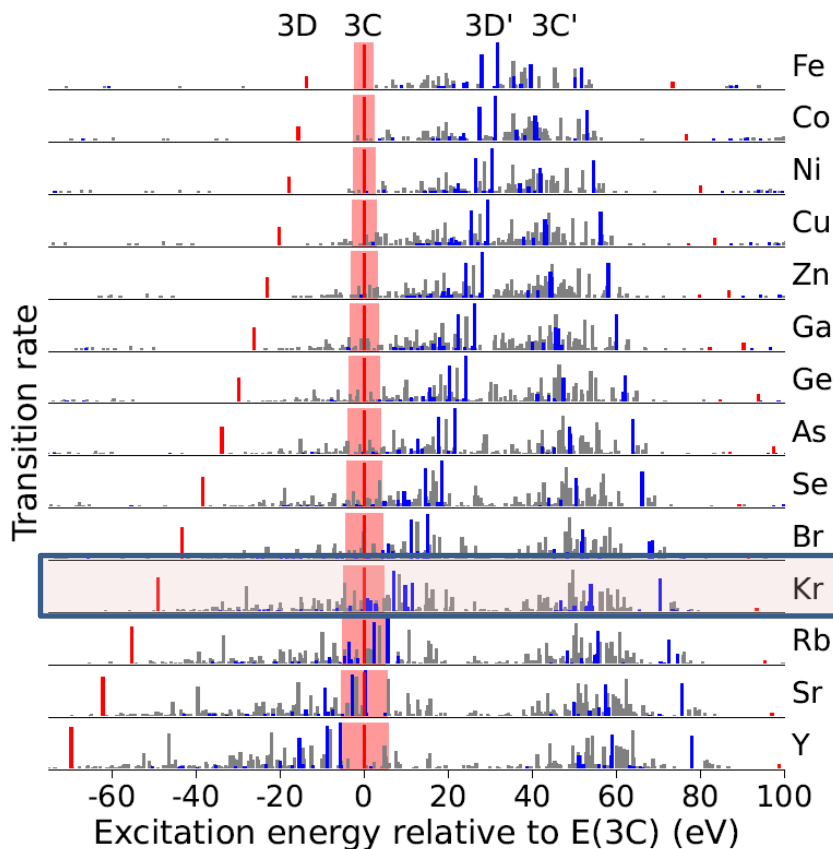
$nd_{3/2}^2$  $nd_{5/2}^2$  $nd_{5/2}^3$  $nd_{5/2}^4$ 

Two different scaling law in Ne-like ions



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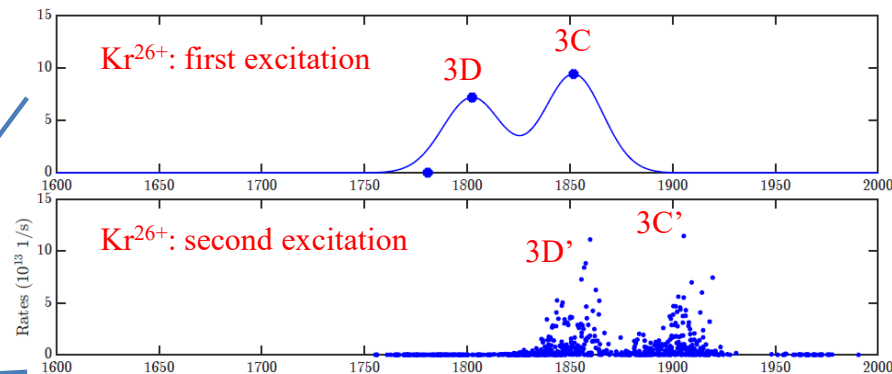
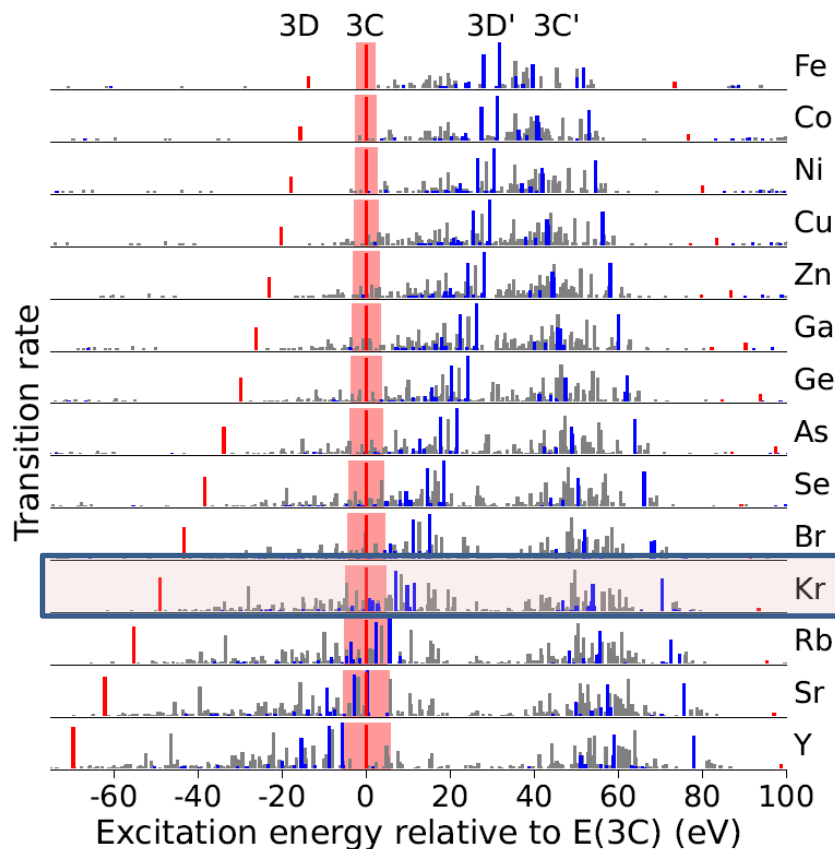
Two different scaling law in Ne-like ions



Spectrum calculated with
the **GRASP2018** codes

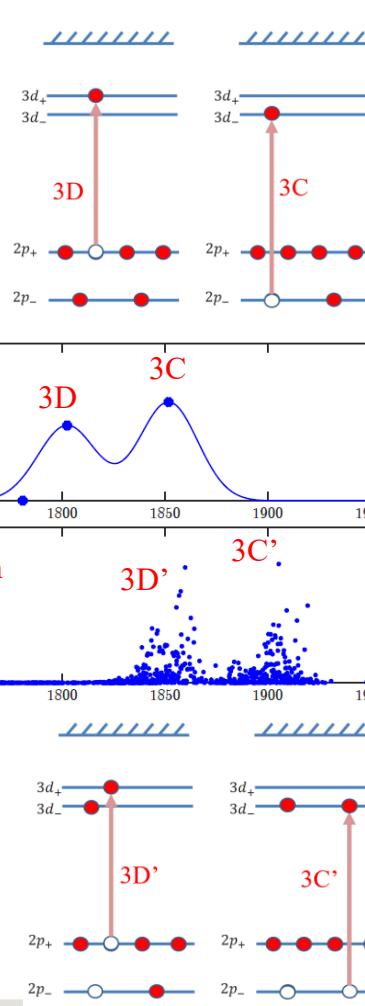
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Two different scaling law in Ne-like ions

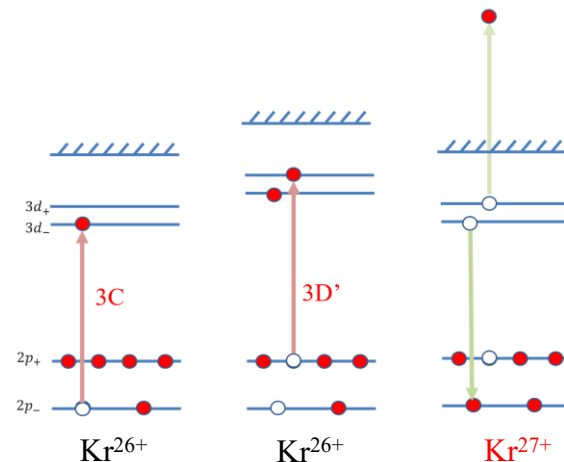
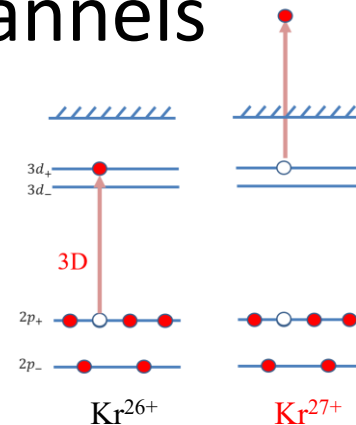
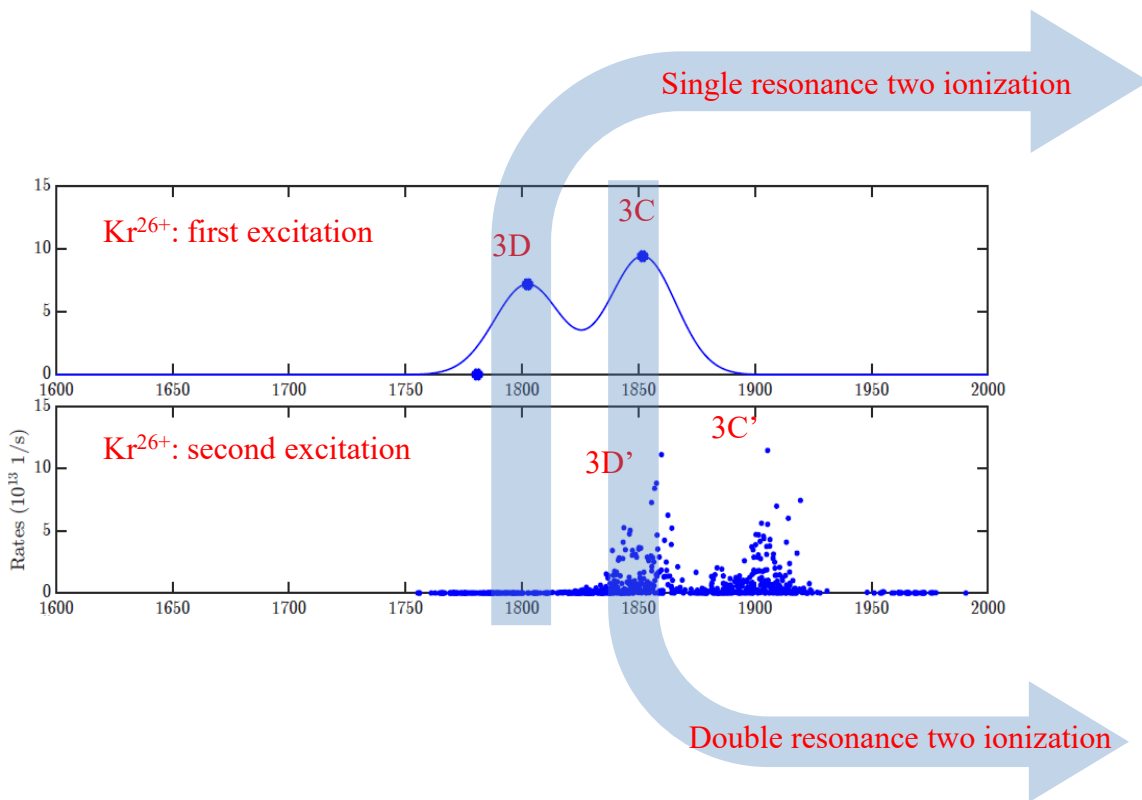


Spectrum calculated with the **GRASP2018** codes

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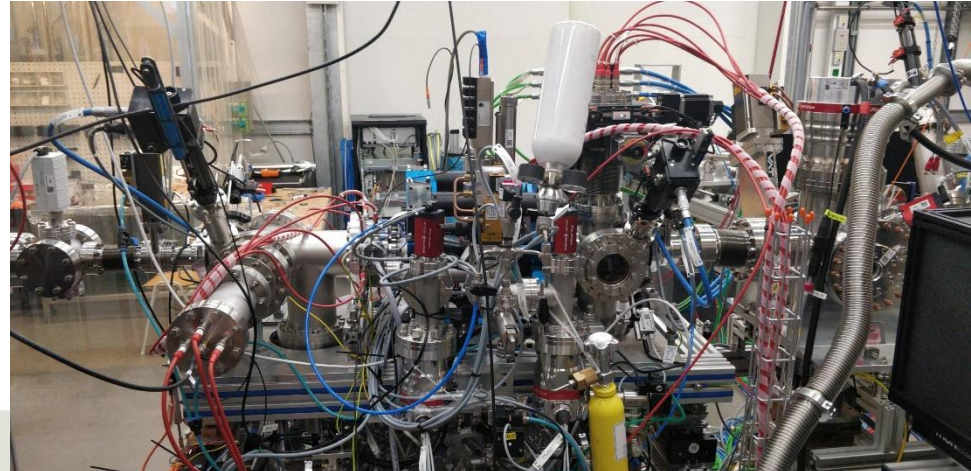
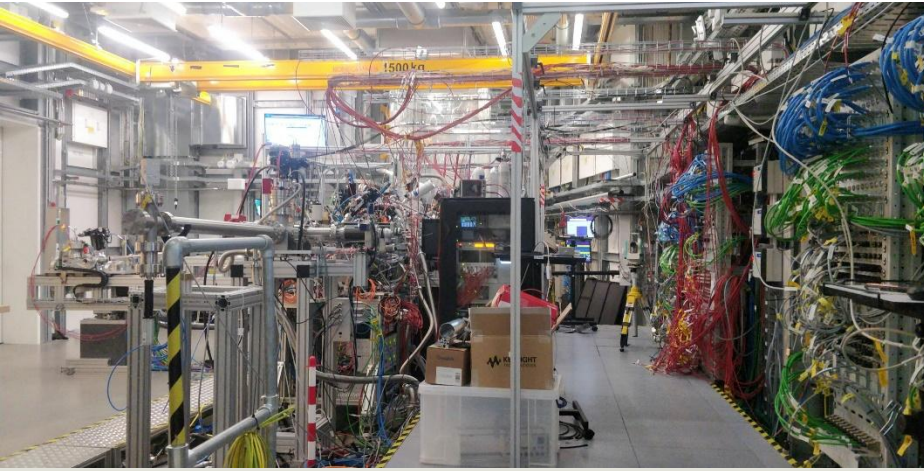
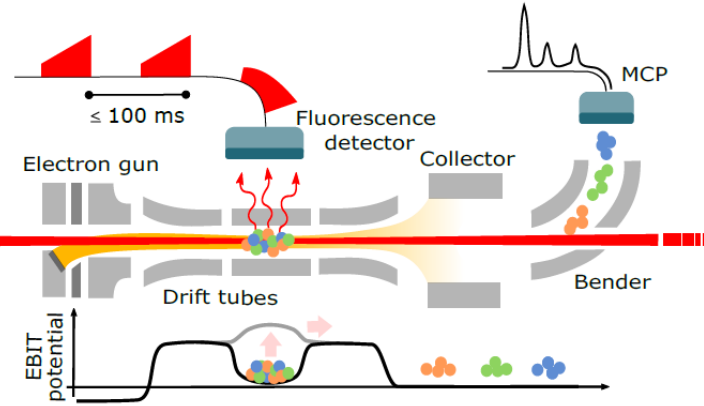
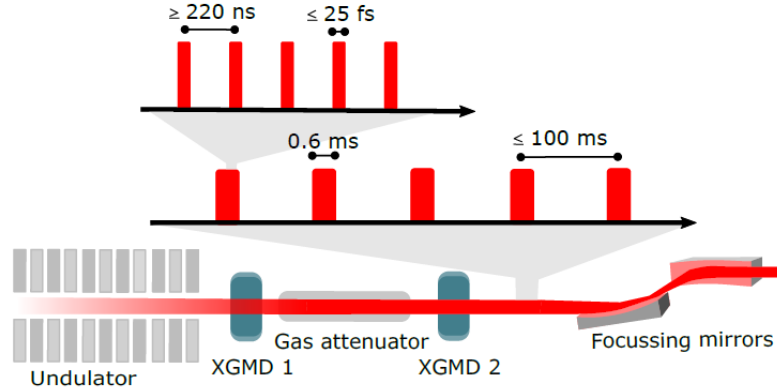


Different nonlinear ionization channels

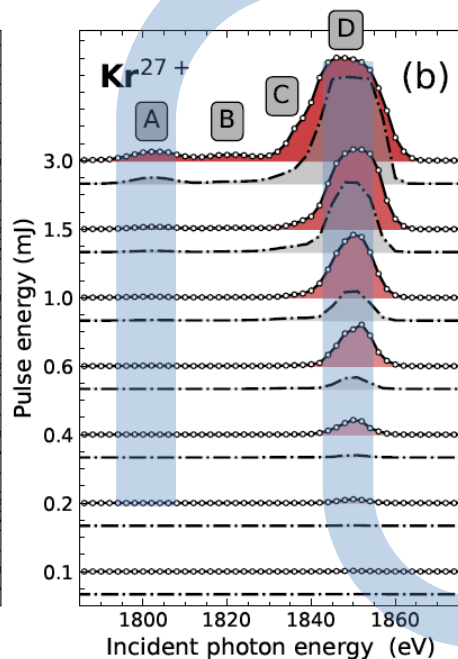
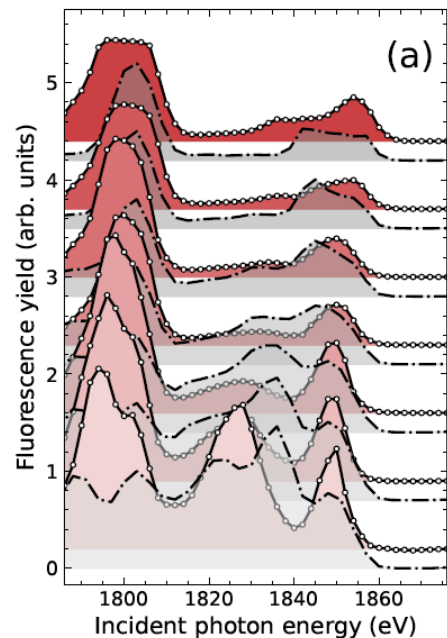


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Experiment at European XFEL Facility

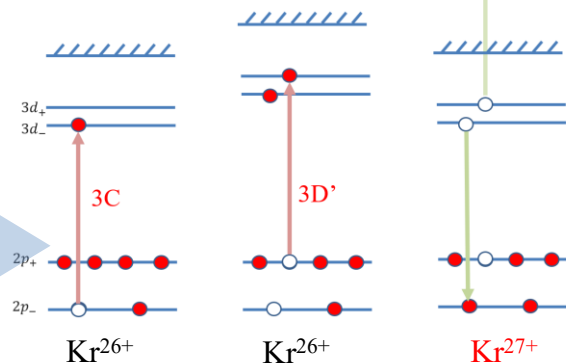
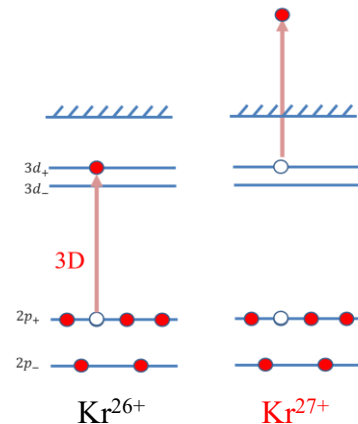


Efficient two-photon ionizations



Single resonance

Double resonance



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Summary

The new periodic table enables novel applications of highly charged ions:

- clocks,
- mass spectrometry,
- x-ray optics, plasma physics
-

Outlook

- Looking for more applications.

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GRASP code developers

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K. Kromer, M. Tagawa,

Thank you for your attention!