MAX-PLANCK-INSTITUT FÜR KERNPHYSIK

Periodic table for highly charged ions

Chunhai Lyu

Max Planck Institute for Nuclear Physics (MPIK), Heidelberg, Germany

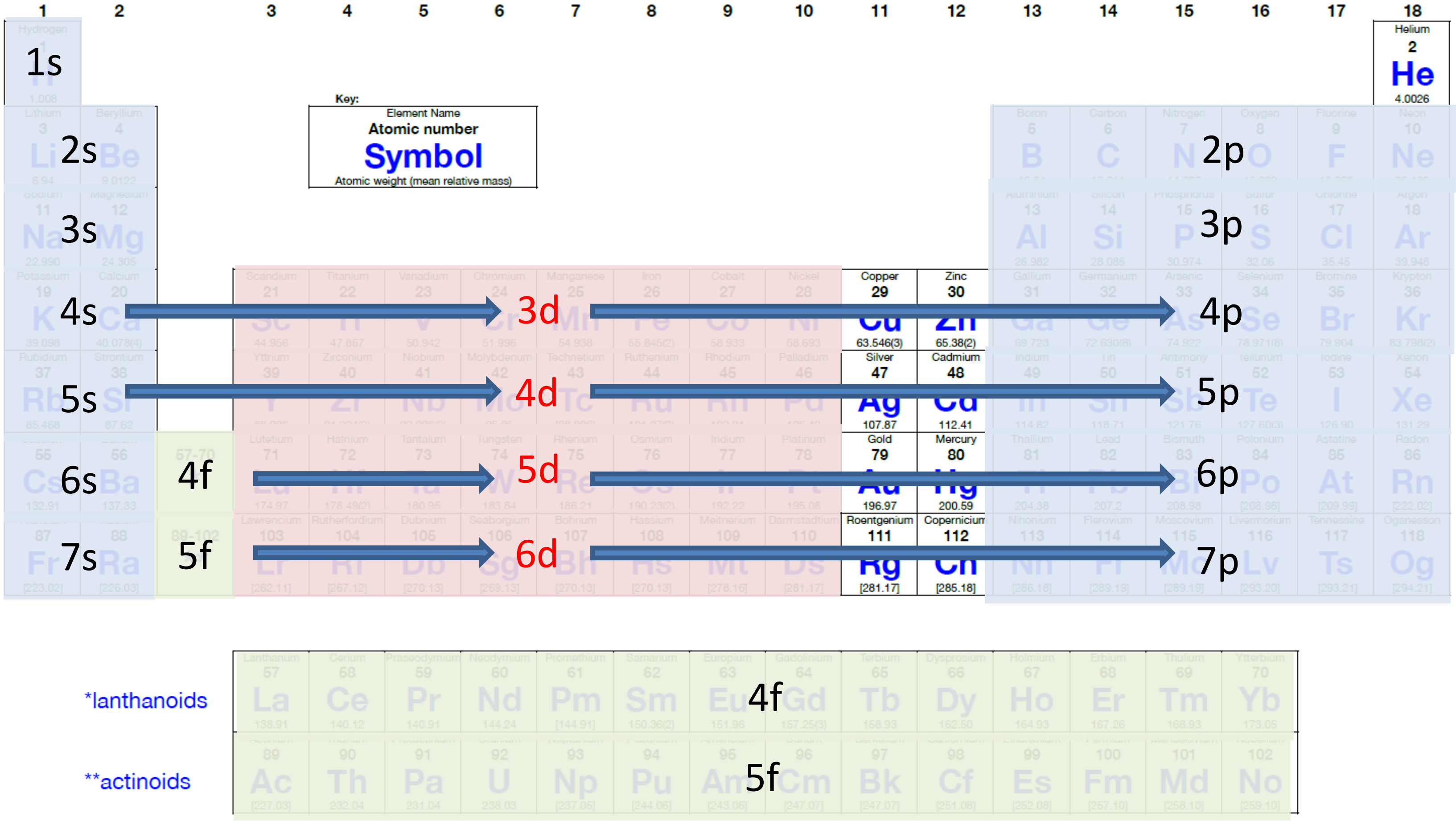
CompAS meeting, June 12, 2025, Lund, Sweden

Key:

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

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												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]	Meitnerium 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]	Tennessine 117 **Ts** [293.21]	Oganesson 118 **Og** [294.21]

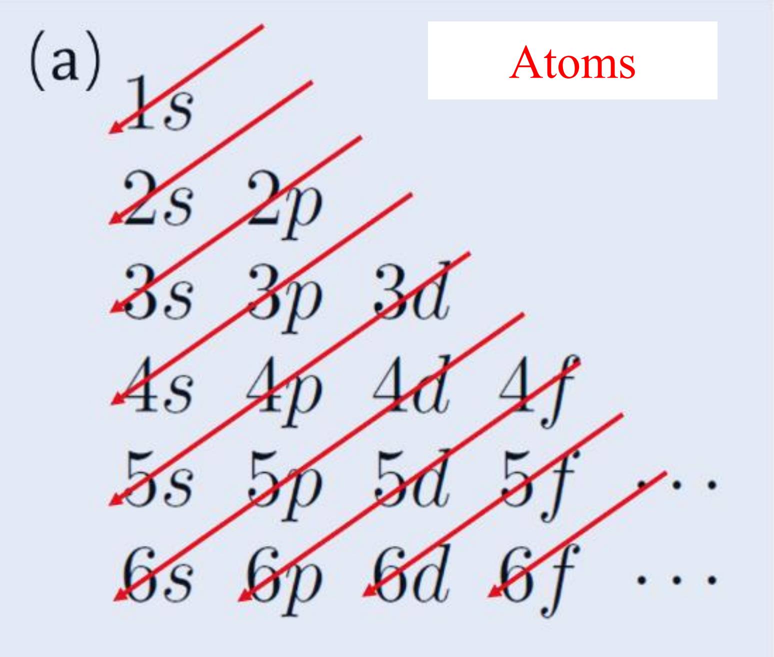
*lanthanoids	Lanthanum 57 **La** 138.91	Cerium 58 **Ce** 140.12	Praseodymium 59 **Pr** 140.91	Neodymium 60 **Nd** 144.24	Promethium 61 **Pm** [144.91]	Samarium 62 **Sm** 150.36(2)	Europium 63 **Eu** 151.96	Gadolinium 64 **Gd** 157.25(3)	Terbium 65 **Tb** 158.93	Dysprosium 66 **Dy** 162.50	Holmium 67 **Ho** 164.93	Erbium 68 **Er** 167.26	Thulium 69 **Tm** 168.93	Ytterbium 70 **Yb** 173.05
**actinoids	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** [252.08]	Fermium 100 **Fm** [257.10]	Mendelevium 101 **Md** [258.10]	Nobelium 102 **No** [259.10]



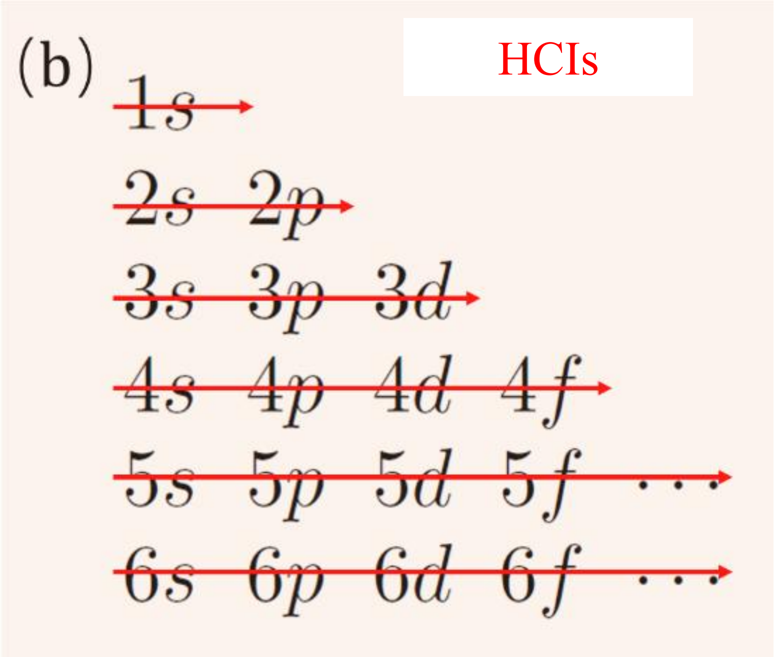
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18
1s
2s
3s
4s
5s
6s
7s
2p
3p
4p
5p
6p
7p
3d
4d
5d
6d
4f
5f
Key:
Element Name
Atomic number
Symbol
Atomic weight (mean relative mass)
Helium
2
He
4.0026
Copper
29
Cu
63.546(3)
Zinc
30
Zn
65.38(2)
Silver
47
Ag
107.87
Cadmium
48
Cd
112.41
Gold
79
Au
196.97
Mercury
80
Hg
200.59
Roentgenium
111
Rg
[281.17]
Copernicium
112
Cn
[285.18]
*lanthanoids
**actinoids

Aufbau Principle

Madelung-Janet filling rule



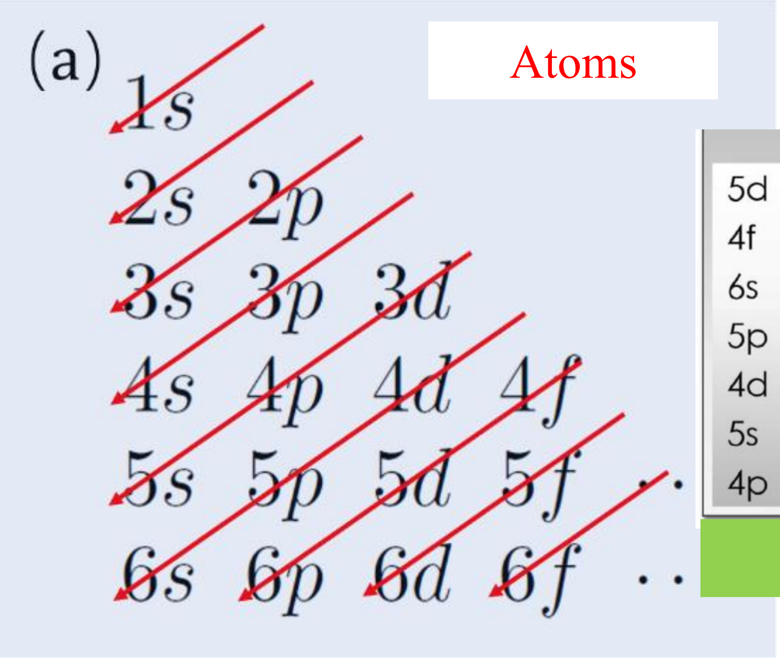
Coulomb filling rule

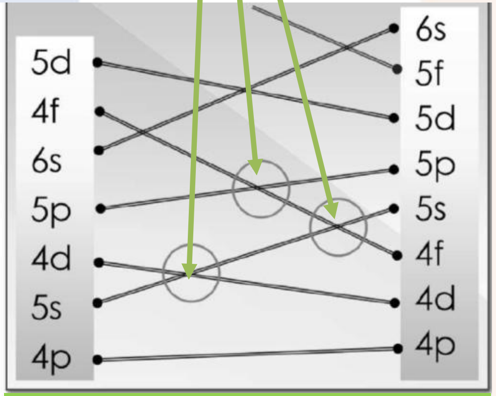


Aufbau Principle

- Optical transitions
- Variation of the fine-structure constant

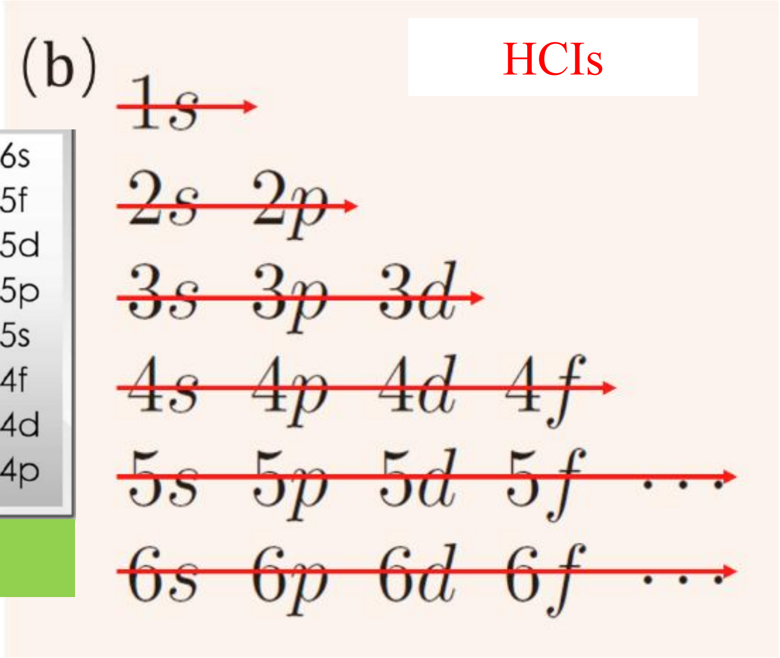
Madelung-Janet filling rule





Orbital crossing

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
			3 4
		5··10	11 12
		13··18	19 20
	21···30	31··36	37 38
	39···48	49··54	55 56
57····70	71···80	81··86	87 88
89····102	etc.		
f^{14}	d^{10}	p^6	s^2

a. NEUTRAL ATOMS

1 2				
3 4	5··10			
11 12	13··18	19···28		
29 30	31··36	37···46	47····60	
61 62	63··68	69···78	79····92	93·····110
111 112	etc.			
s^2	p^6	d^{10}	f^{14}	g^{18}

b. HIGHLY IONIZED ATOMS

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

Periodic table for HCI

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;
- ....

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 $4d_+^3$ Tc-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+	53 $4f_+^1$ I-like Au26+	54 $4f_+^2$ Xe-like Au25+	55 $4f_+^3$ Cs-like Tl26+	56 $4f_+^4$ Ba-like Po28+	57 $4f_+^5$ La-like Hg23+	58 $4f_+^6$ Ce-like Ir19+	59 $4f_+^7$ Pr-like Ir18+	60 $4f_+^8$ Nd-like Ir17+
					66 $5p_+^2$ Dy-like W08+	67 $5p_+^3$ Ho-like Re08+	68 $5p_+^4$ Er-like W06+														
					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 Tl06+	76 $5d_+^4$ Os-like Au03+	77 $5d_+^5$ Ir-like Au02+	78 $5d_+^6$ Pt-like Au01+								
								79 $5f_-^1$ Au-like Sg25+	80 $5f_-^2$ Hg-like Sg24+	81 $5f_-^3$ Tl-like Hs27+	82 $5f_-^4$ Pb-like Ds28+	83 $5f_-^5$ Bi-like Ds27+	84 $5f_-^6$ Po-like Nh29+	87 $5f_+^1$ Fr-like Sg19+	88 $5f_+^2$ Ra-like Hs20+	89 $5f_+^3$ Ac-like Mt20+	90 $5f_+^4$ Th-like Cn22+	91 $5f_+^5$ Pa-like Nh22+	92 $5f_+^6$ U-like Lv24+	93 $5f_+^7$ Np-like Og25+	94 $5f_+^8$ Pu-like Ubu27+

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

M_J \ 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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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 Tl06+	76 $5d_+^4$ Os-like Au03+	77 $5d_+^5$ Ir-like Au02+	78 $5d_+^6$ Pt-like Au01+								
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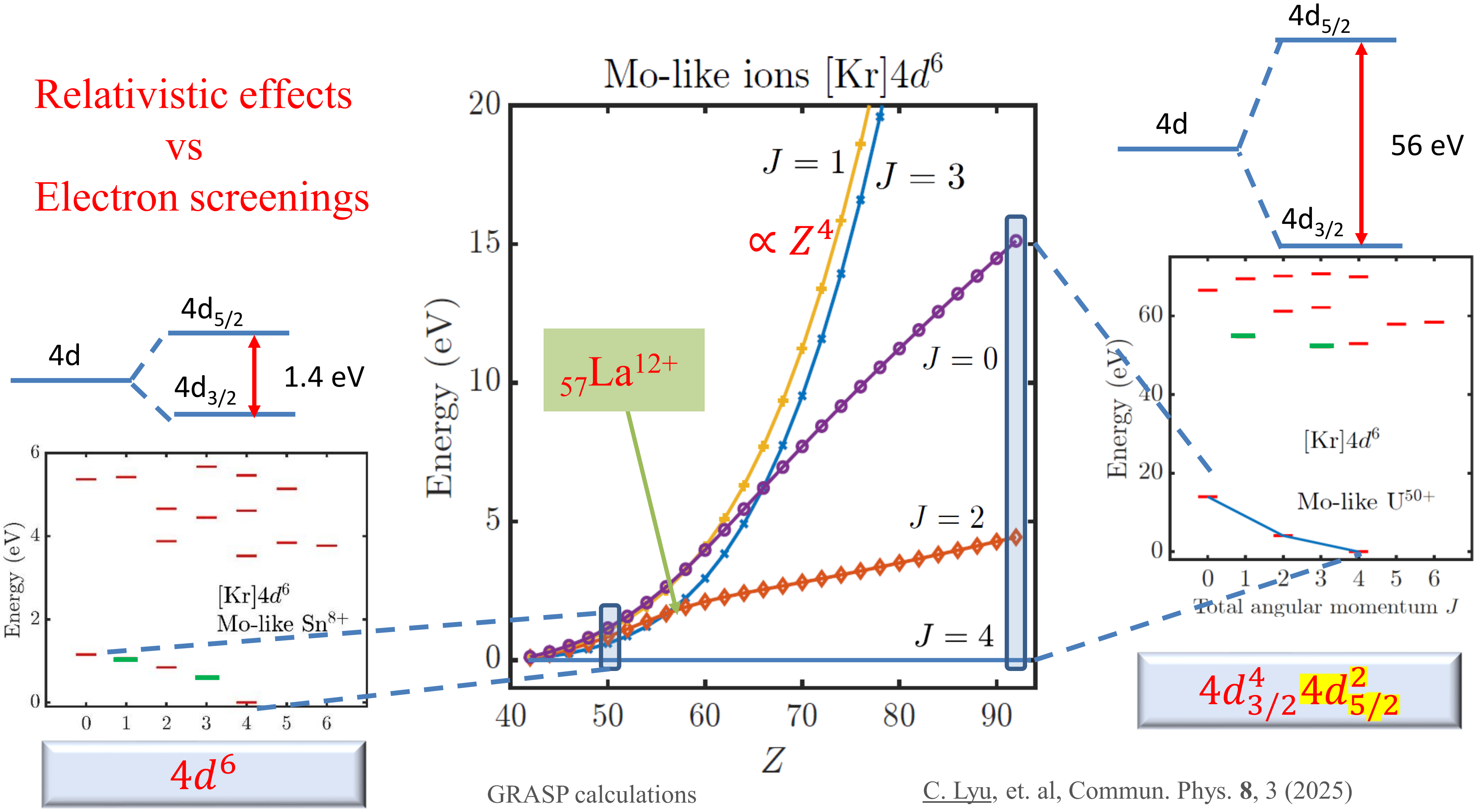
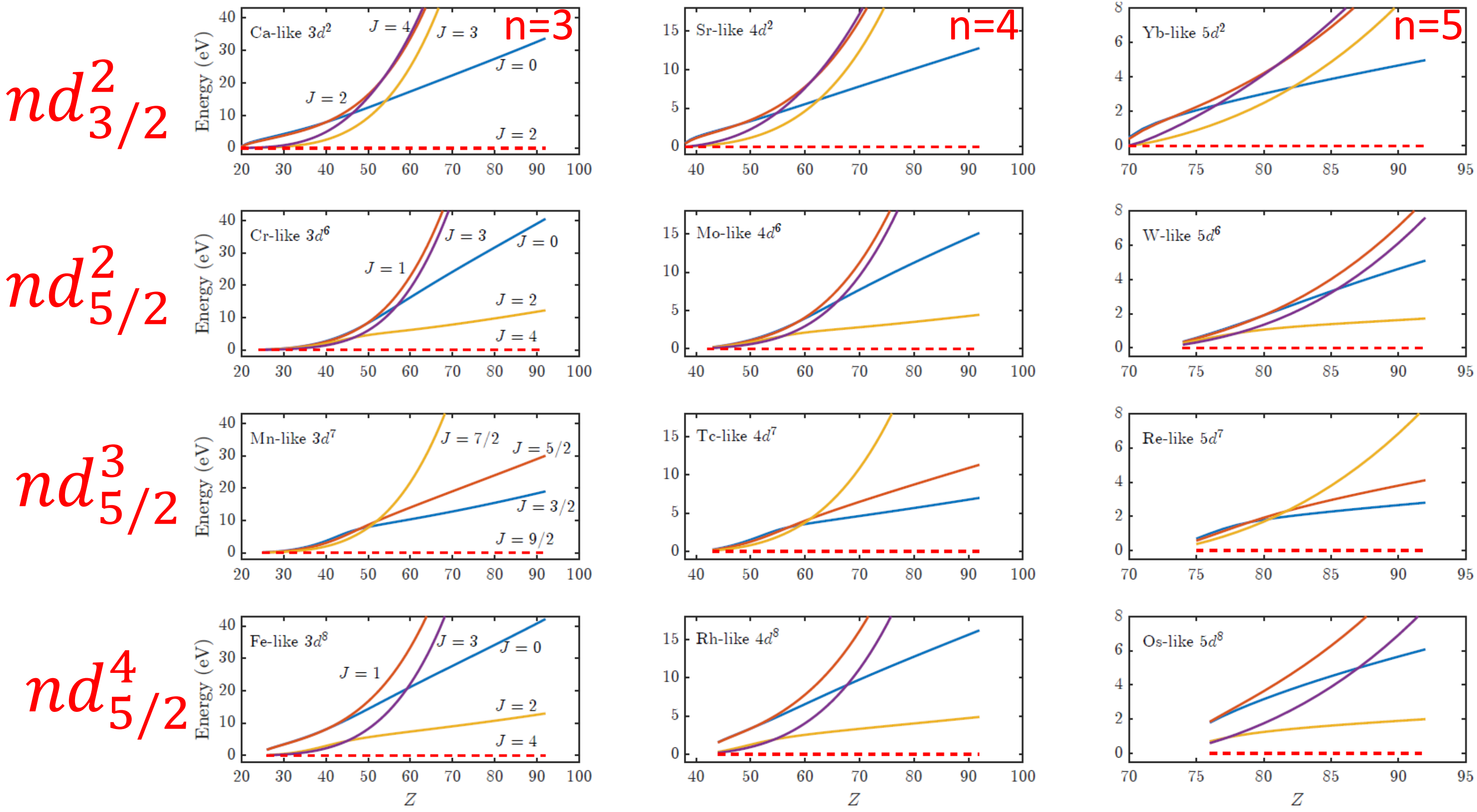


GRASP calculations

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



GRASP calculations

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

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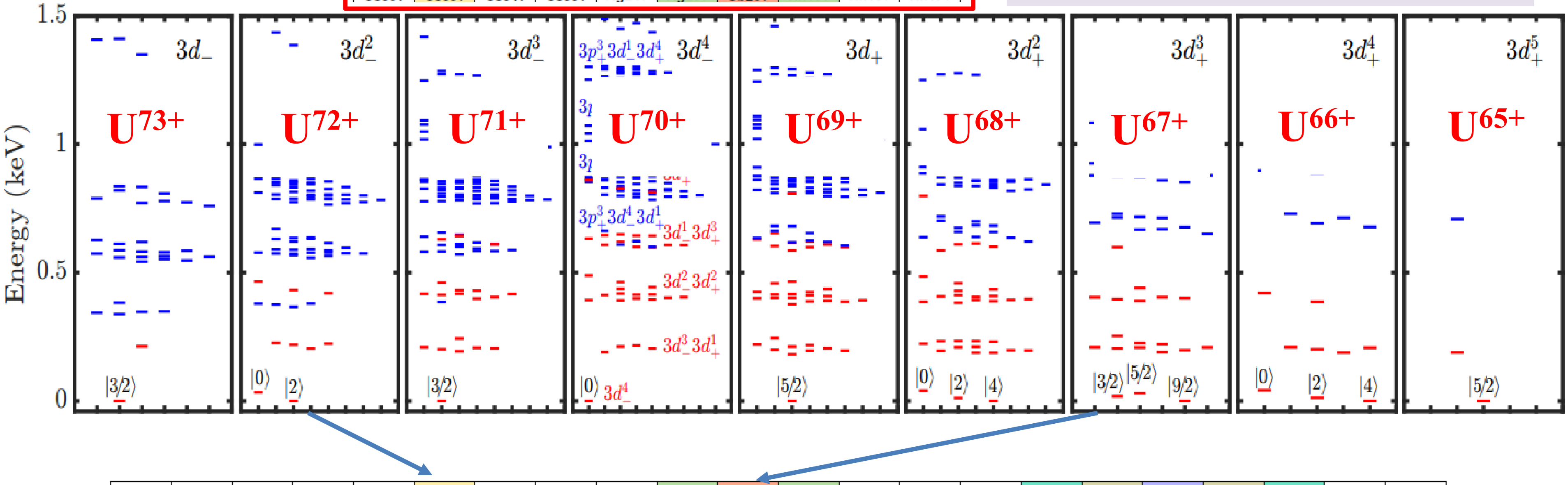
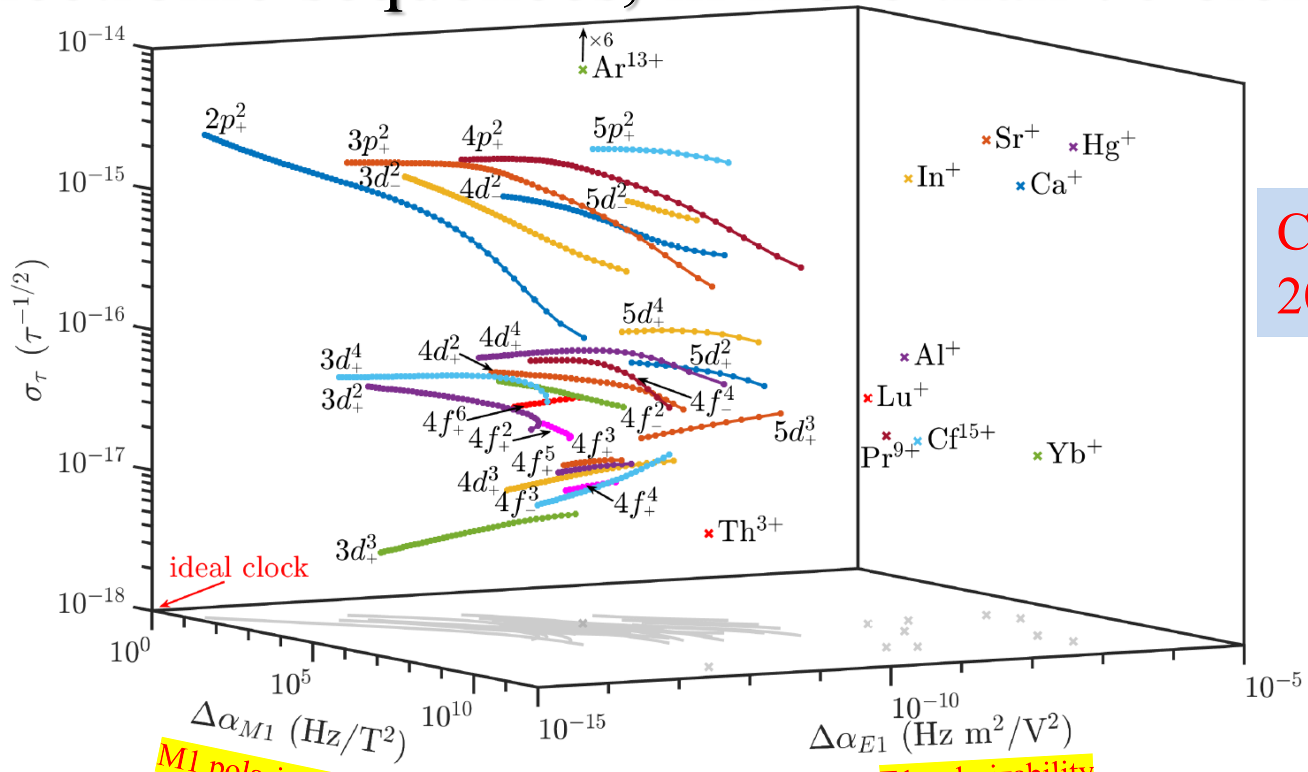


$\frac{1}{2}$	0	$\frac{1}{2}$	0	$\frac{3}{2}$	2,0	$\frac{3}{2}$	0	$\frac{5}{2}$	4,2,0	$\frac{9}{2},\frac{3}{2},\frac{5}{2}$	4,2,0	$\frac{5}{2}$	0	$\frac{7}{2}$	6,4, 2,0	(15,9, 11,3, 7,5)/2	8,5,2, 6,4,4, 2,0	(15,9, 11,3, 7,5)/2	6,4, 2,0	$\frac{7}{2}$	0

More than 700 HCI clock transitions in 24 isolelectronic sequences, in more than 70 elements

Instability



M1 polarizability

E1 polarizability

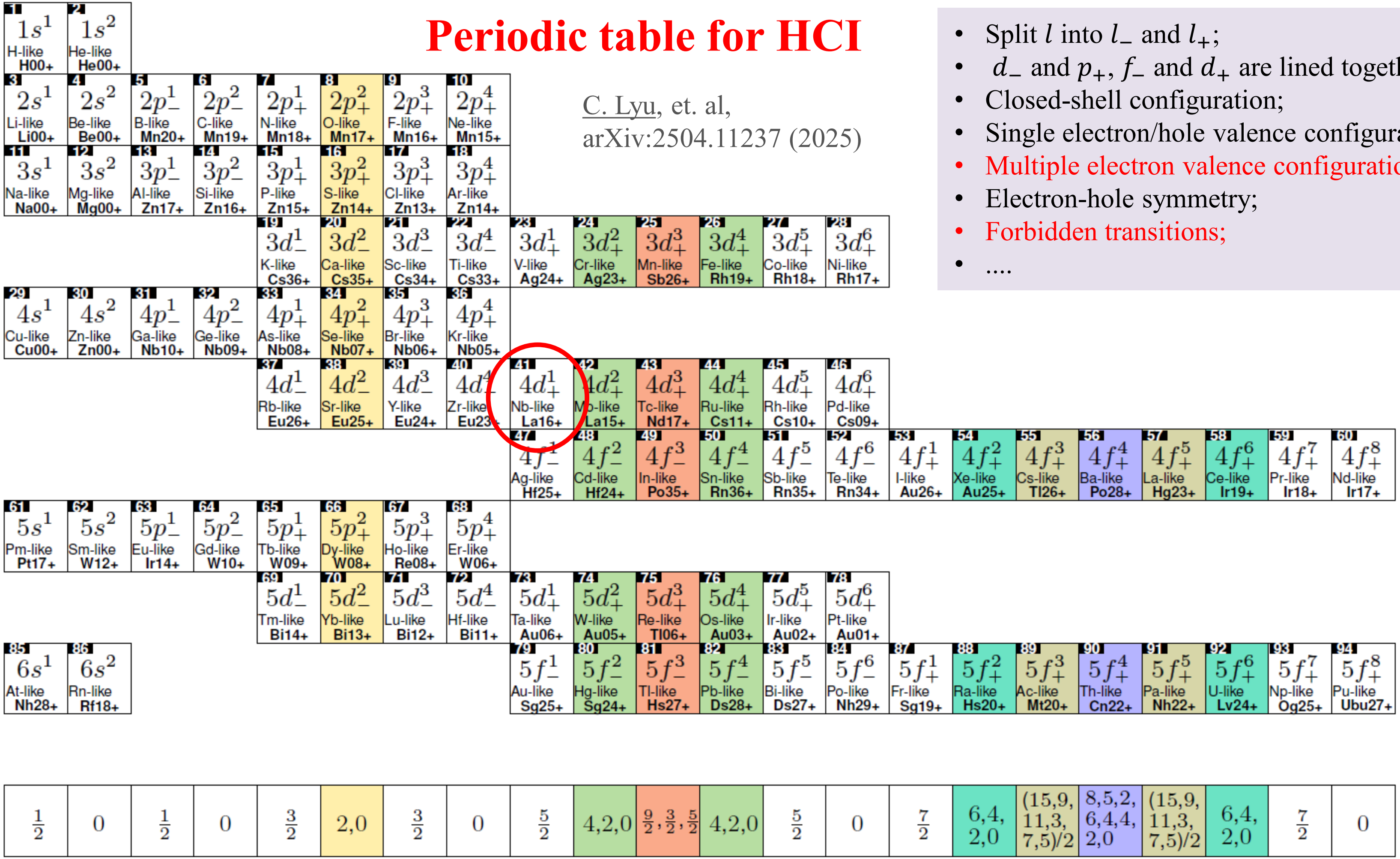
Currently 20+ clocks

Transition energies, lifetimes, and transition matrix elements are calculated with the GRASP2018 code.

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

Periodic table for HCI

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



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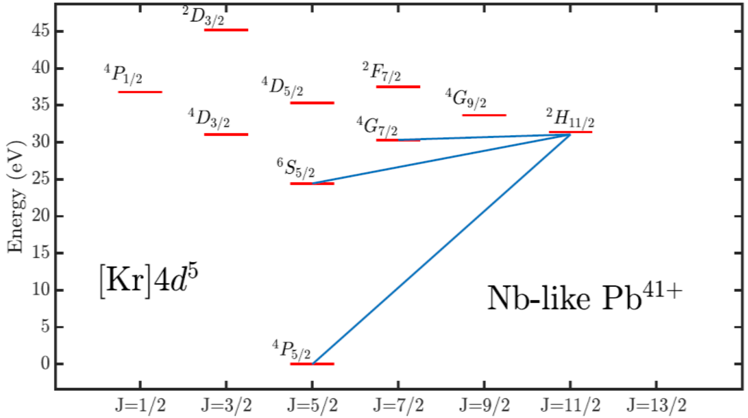
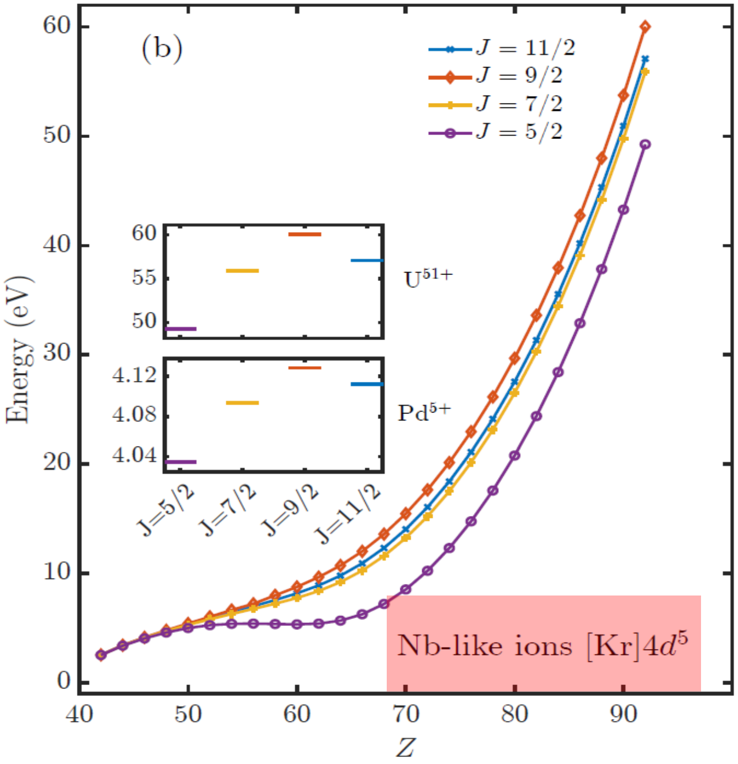
Theoretical predictions: many XUV **clock transitions** in HCIs

$4d^1_+$



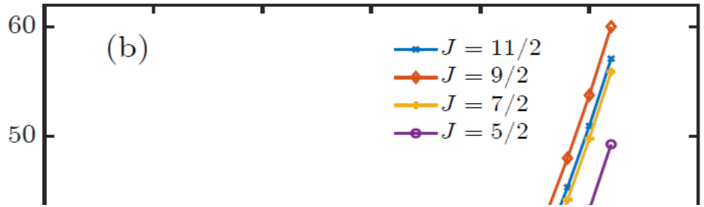


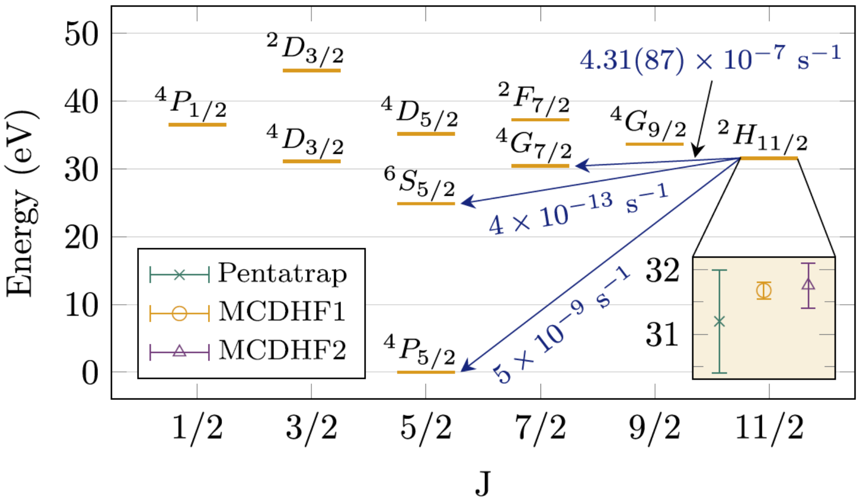
Multiconfiguration Dirac-Hatree-Fock calculations with the **GRASP2018 codes**

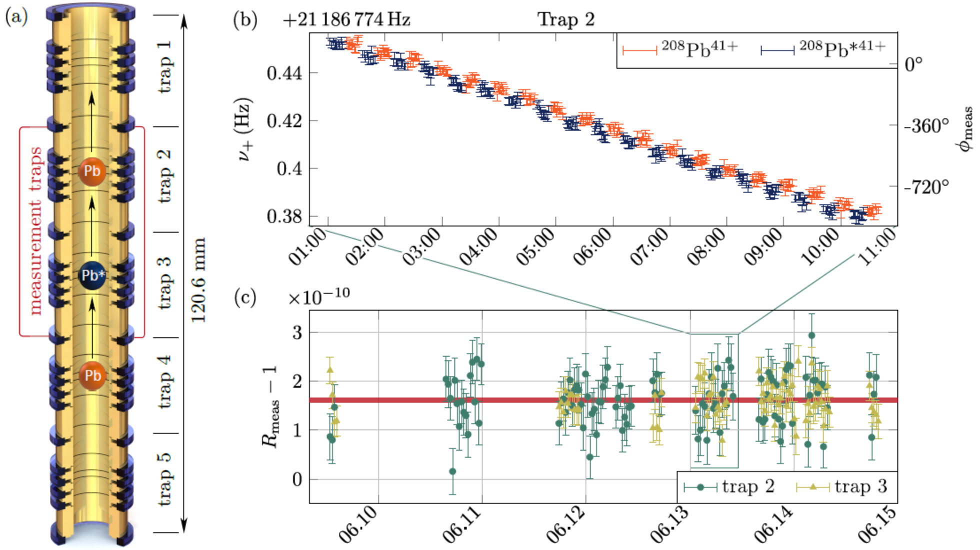
C. Lyu, et. al, Commun. Phys. **8**, 3 (2025)

Theoretical predictions: many XUV **clock transitions** in HCIs

Pb^{41+}







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

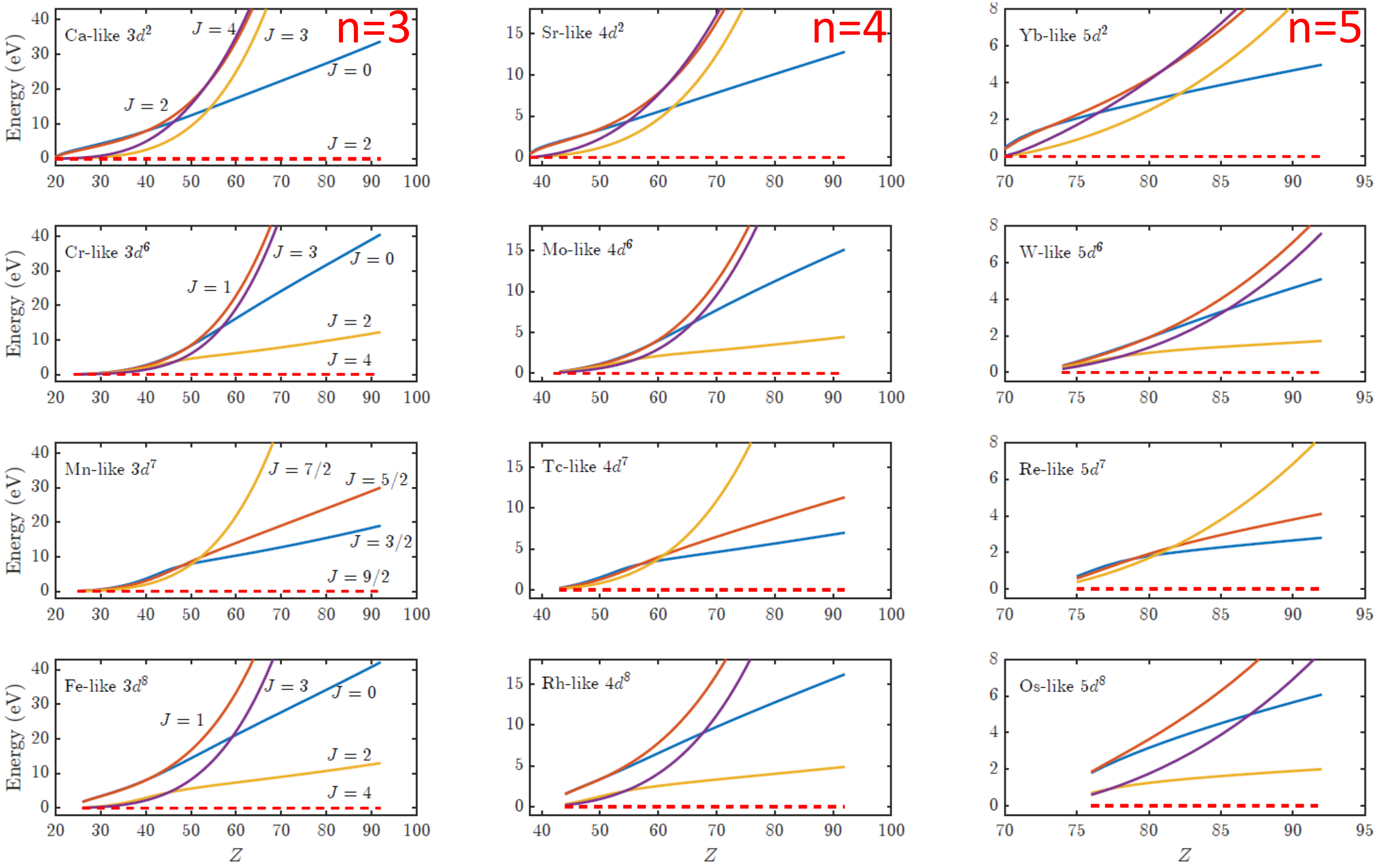
K. Kromer, C. Lyu, et. al, PRL.131.223002(2023)

$nd_{3/2}^2$

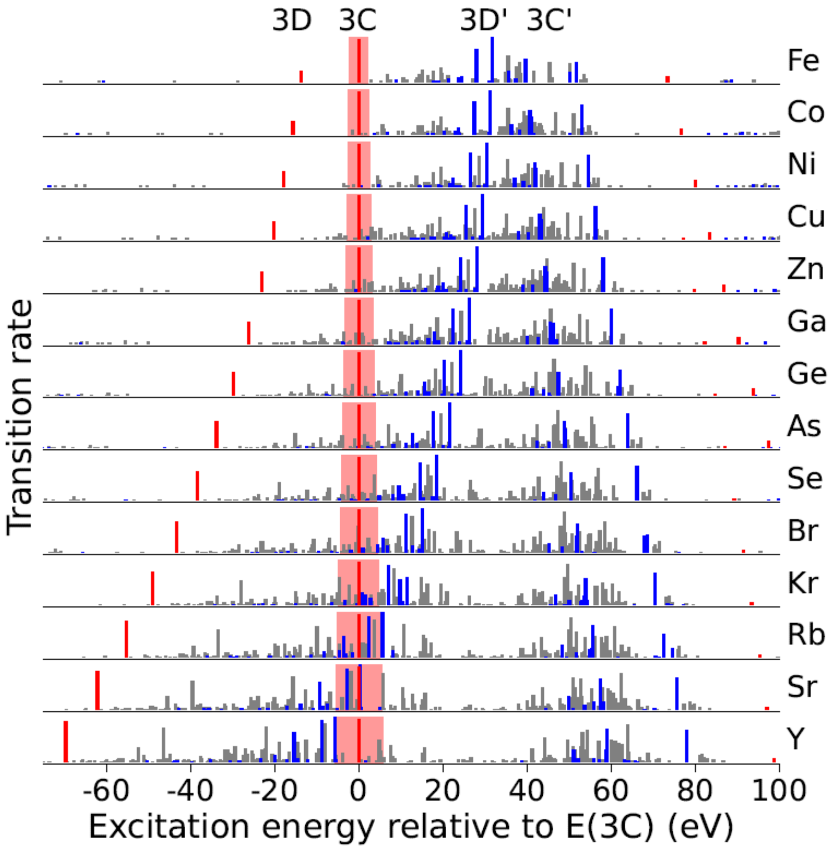
$nd_{5/2}^2$

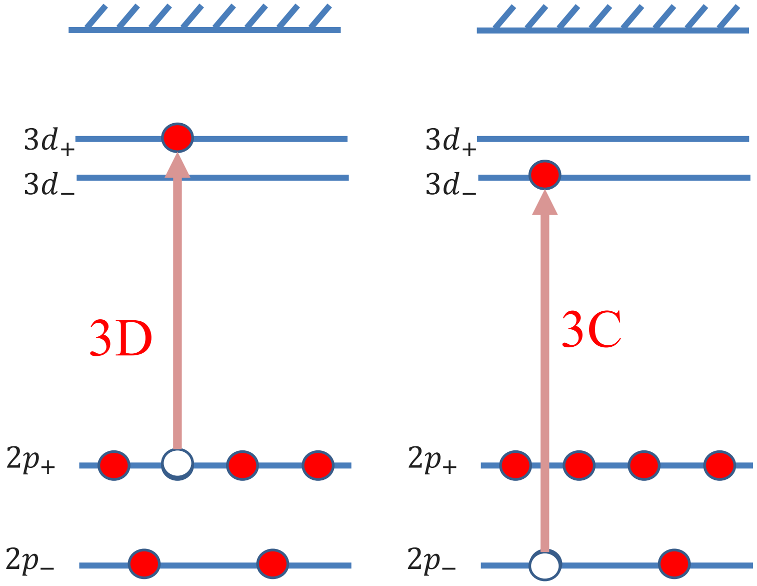
$nd_{5/2}^3$

$nd_{5/2}^4$



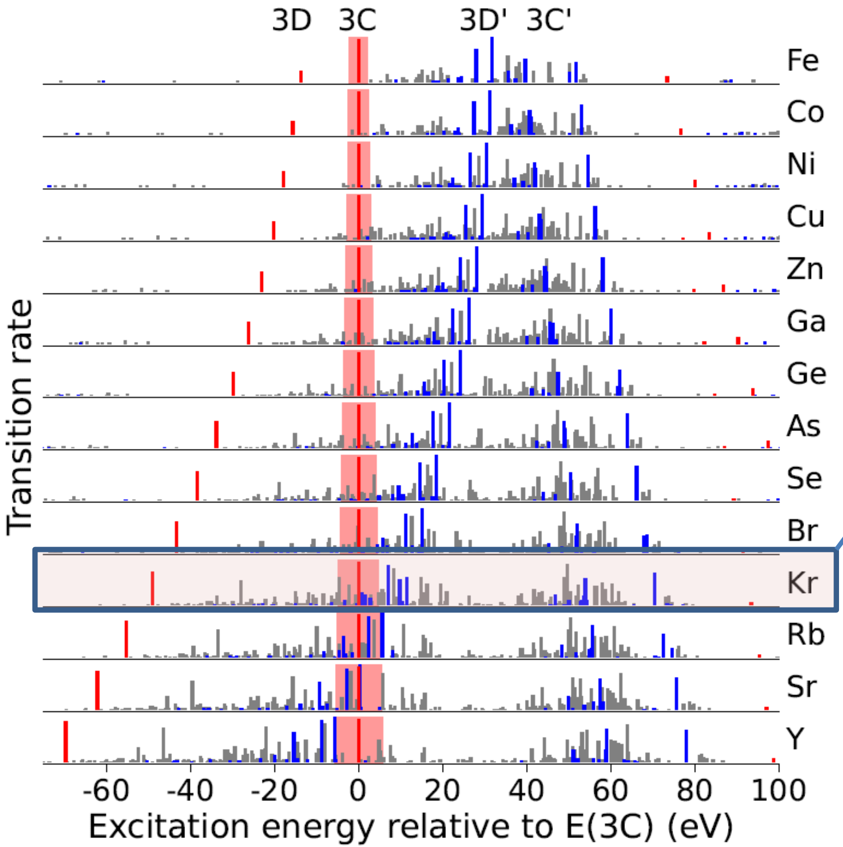
Two different scaling law in Ne-like ions

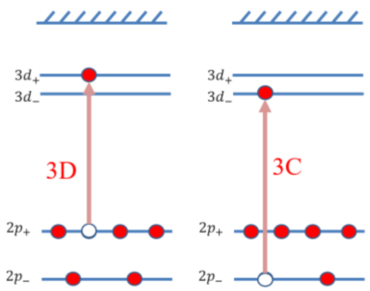


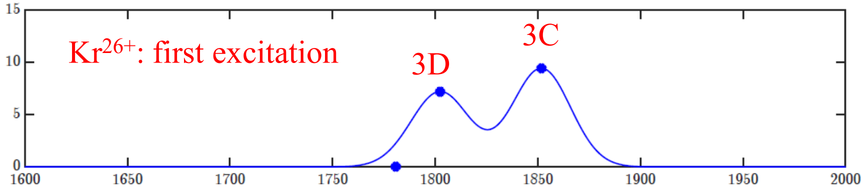


M. Tagawa, C. Lyu, et. al, under review

Two different scaling law in Ne-like ions







Spectrum calculated with the **GRASP2018 codes**

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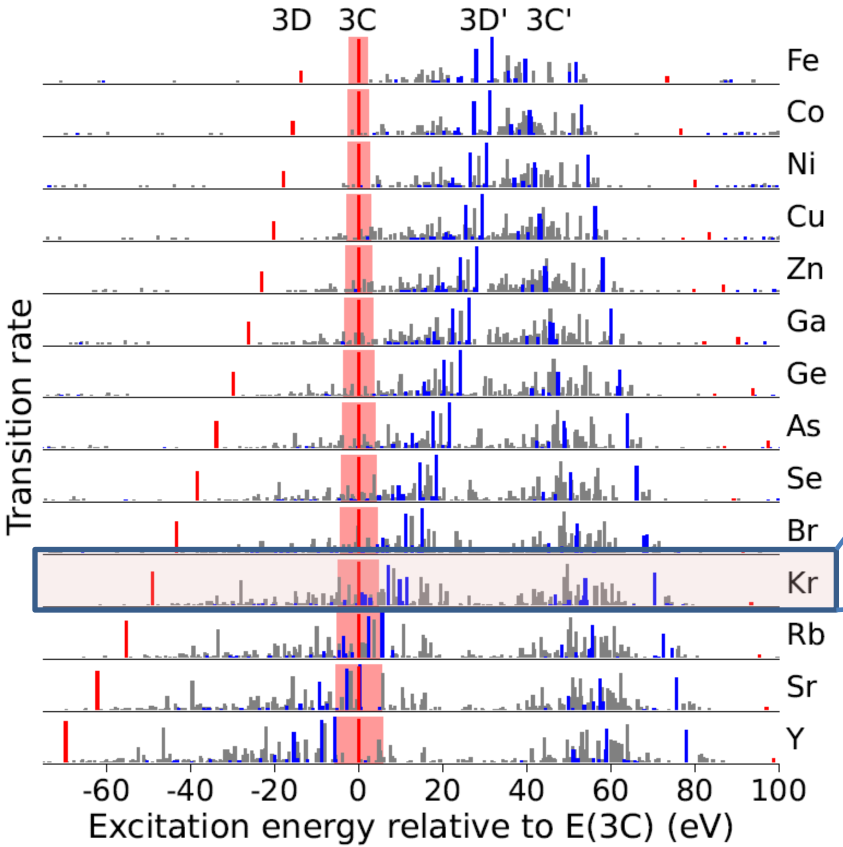
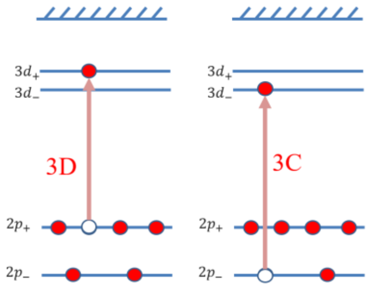
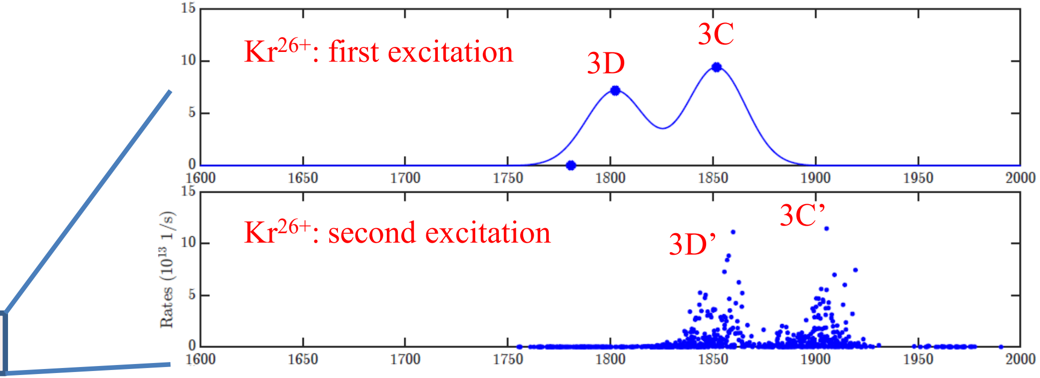
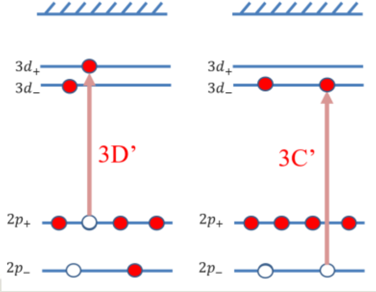
Two different scaling law in Ne-like ions







Spectrum calculated with the **GRASP2018 codes**



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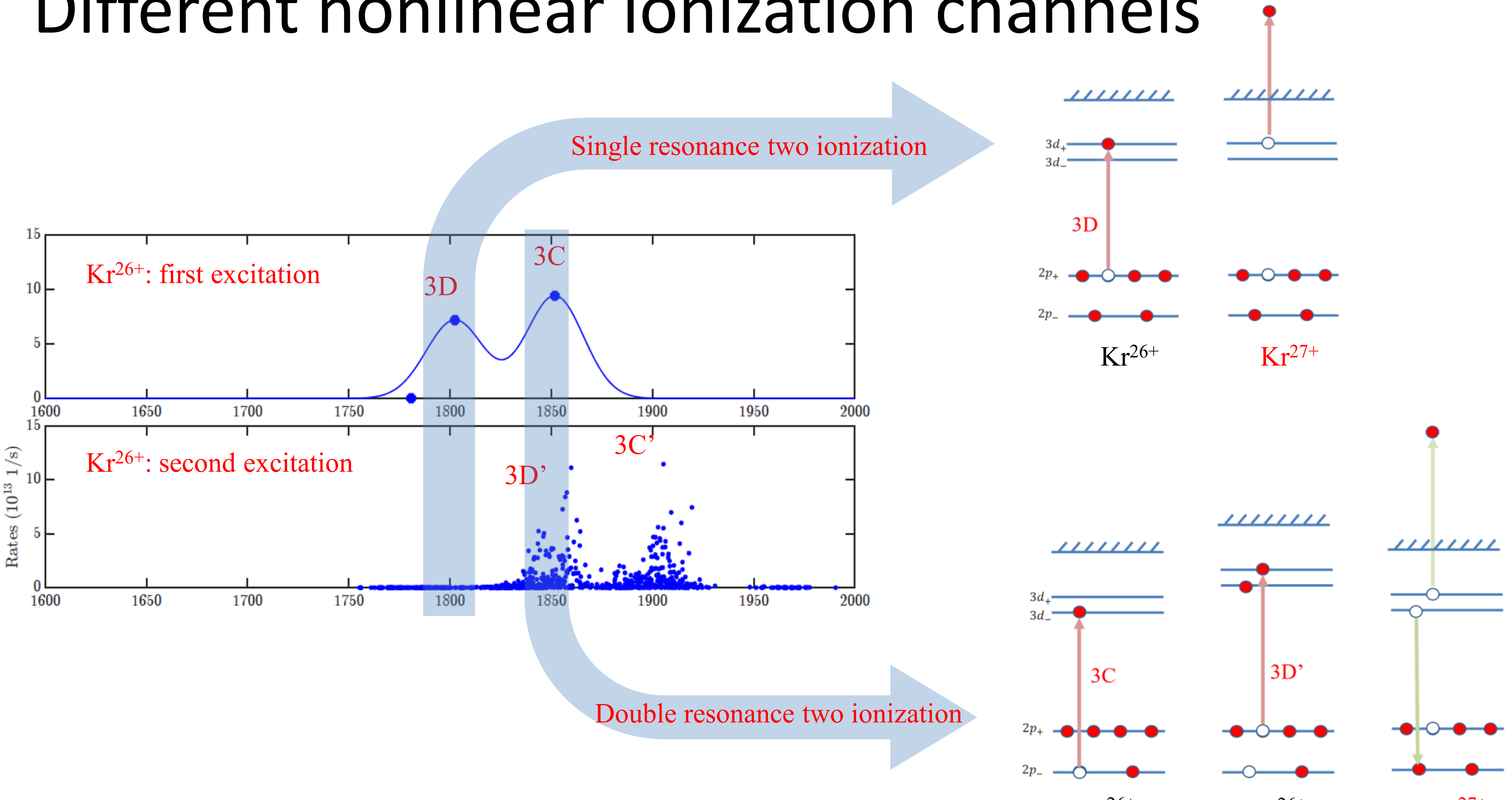
Different nonlinear ionization channels



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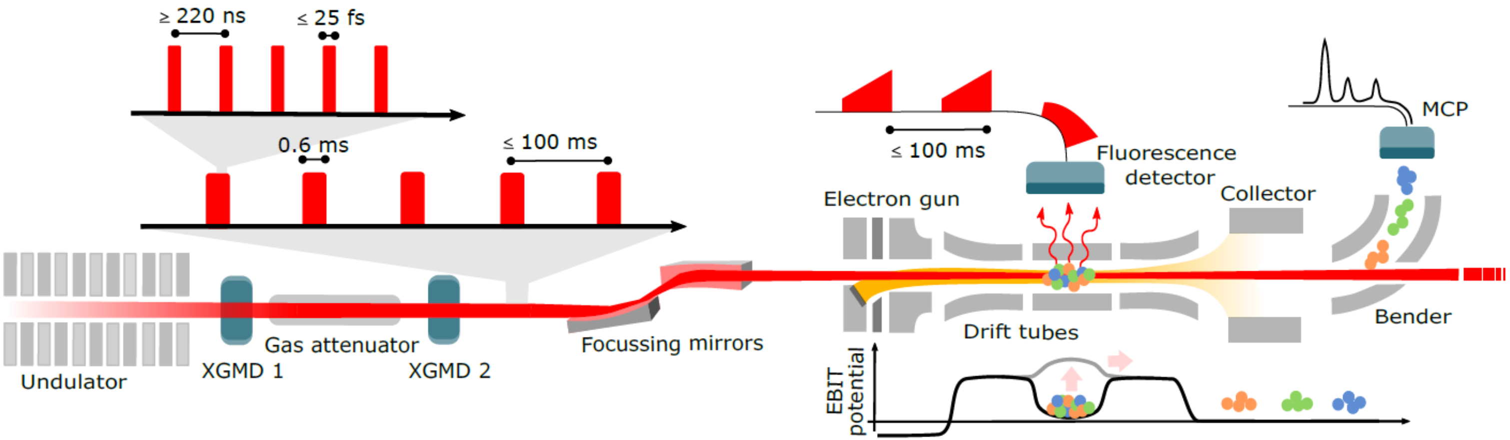
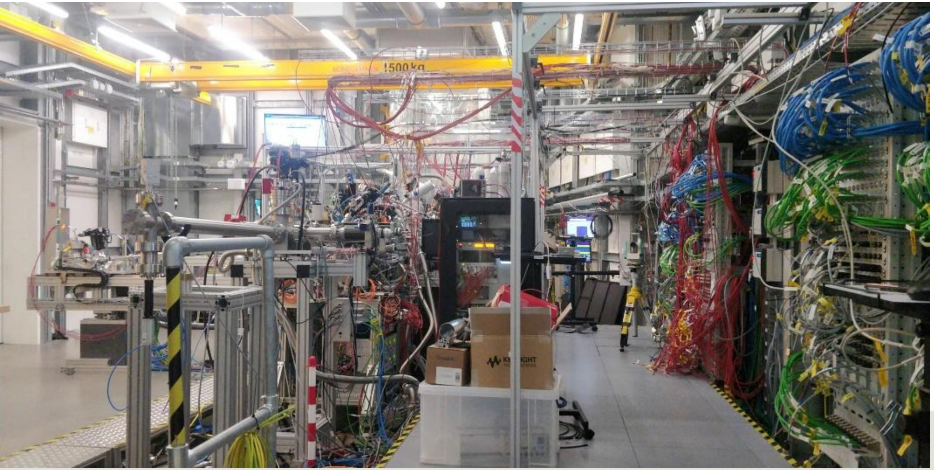
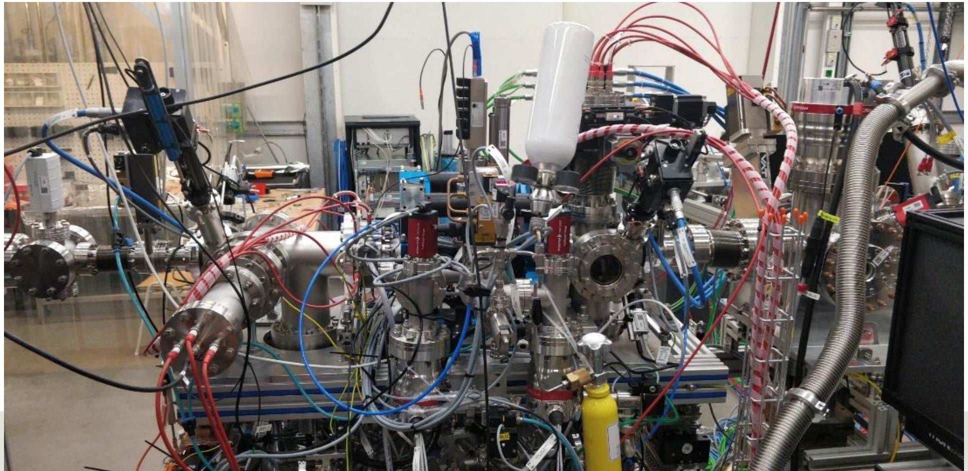
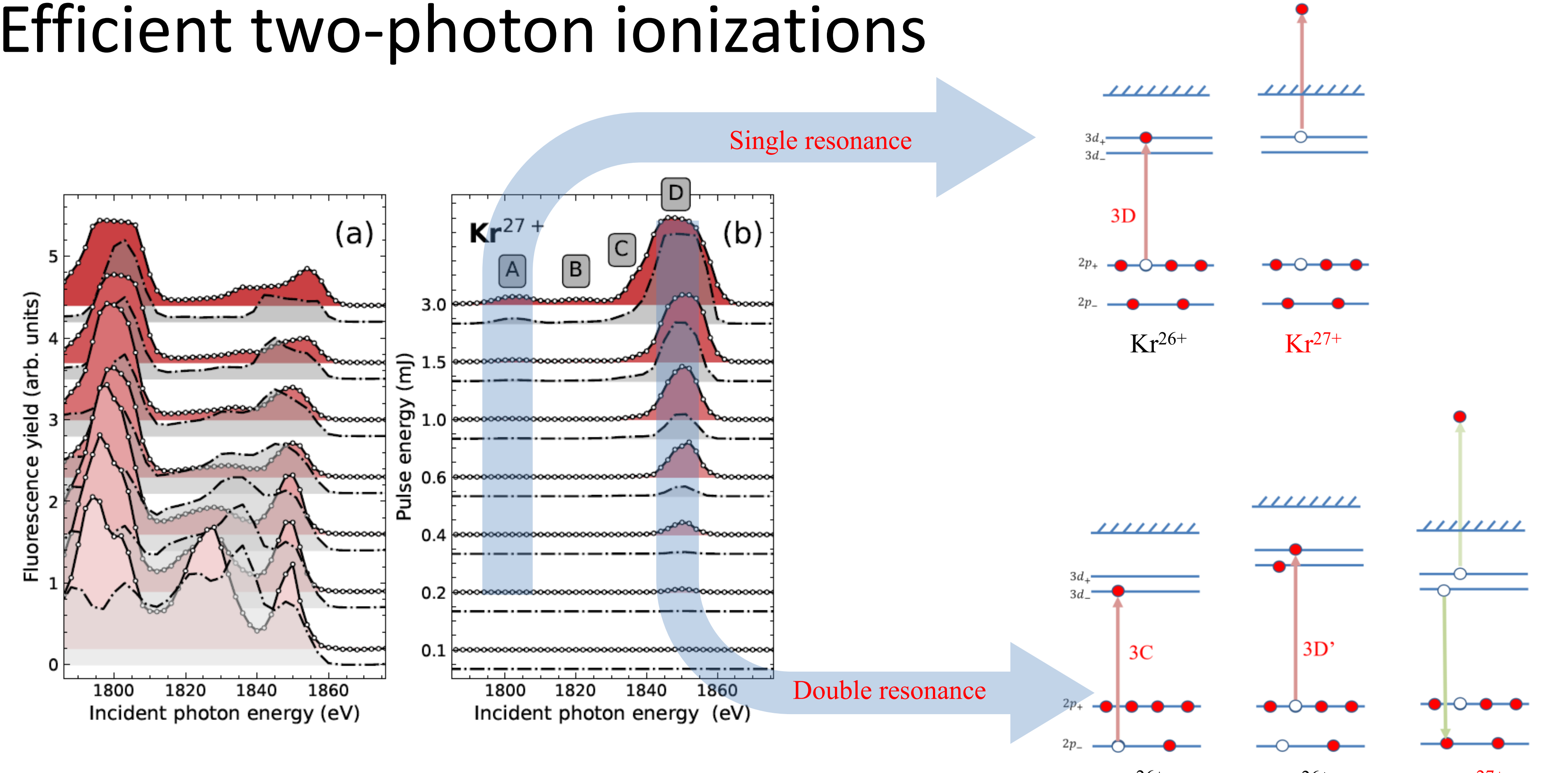
Experiment at European XFEL Facility







Efficient two-photon ionizations



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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.

Acknowledgement

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GRASP code developers

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K. Kromer, M. Tagawa, ….

Thank you for your attention!