

2020 NSF CYBERINFRASTRUCTURE FOR SUSTAINED SCIENTIFIC INNOVATION (CSSI) PRINCIPAL INVESTIGATOR MEETING

ELEMENTS: COMMUNITY PORTAL FOR HIGH-PRECISION ATOMIC PHYSICS DATA AND COMPUTATION

PI: Marianna Safronova, Co-PI: Rudolf Eigenmann, University of Delaware



University of Delaware project team and collaborators

C. Cheung¹, P. Barakhshan², A. Marrs¹, S. G. Porsev^{1,3}, M. G. Kozlov^{3,4}

¹*Department of Physics and Astronomy, University of Delaware,*

²*Department of Electrical & Computer Engineering, University of Delaware,*

³*Petersburg Nuclear Physics Institute, Gatchina 188300, Russia*

⁴*St. Petersburg Electrotechnical University “LETI”, St. Petersburg, Russia*

Award #1931339

Extraordinary progress in the control of atoms and ions

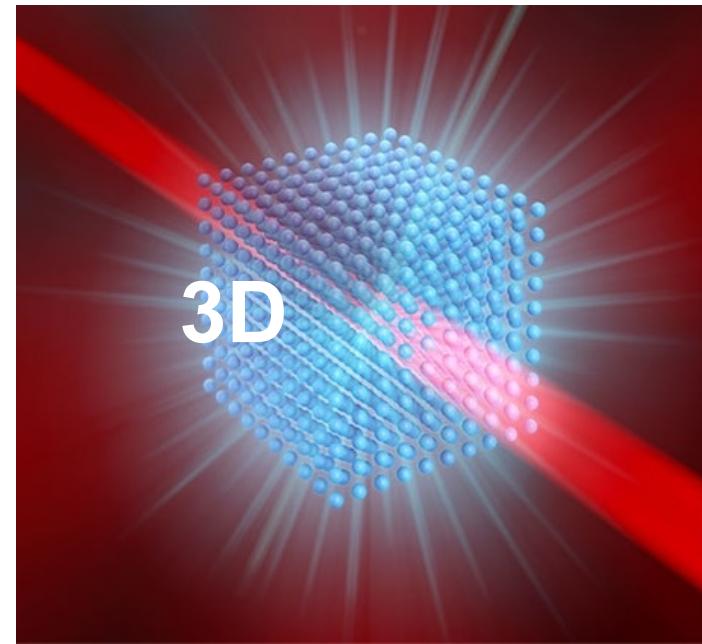
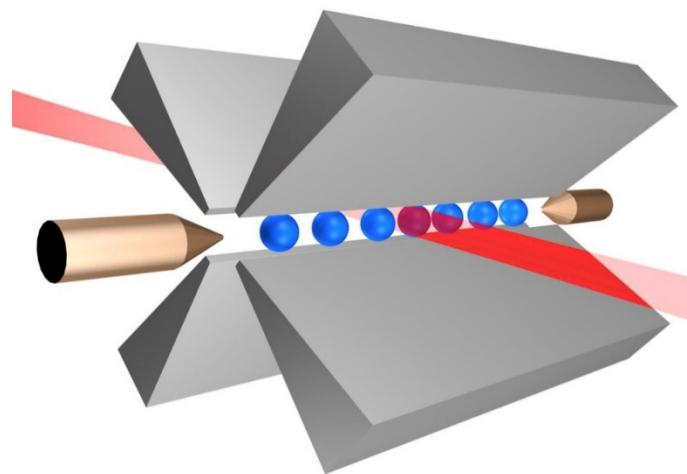
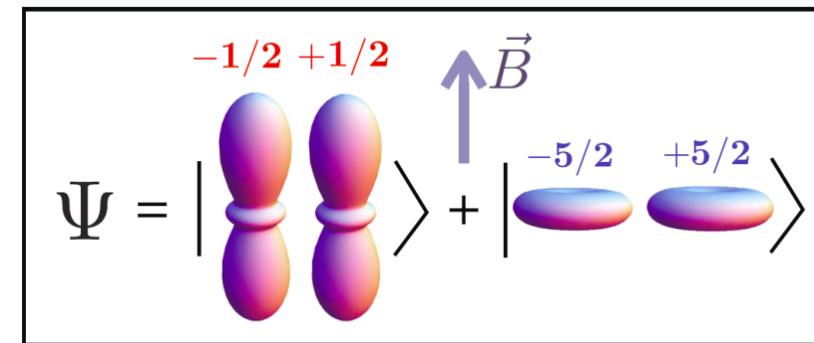
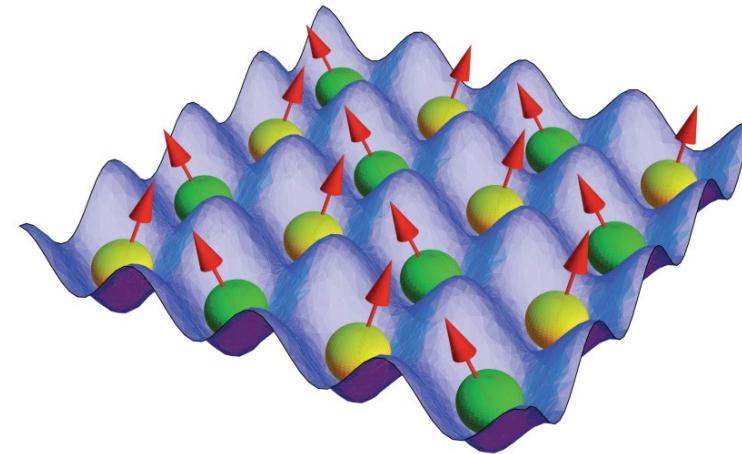
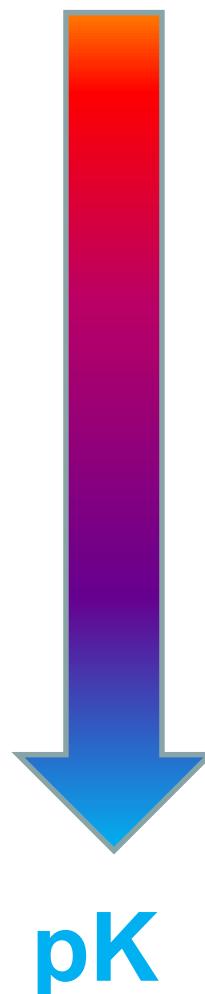
1997 Nobel Prize
Laser cooling and trapping

2001 Nobel Prize
Bose-Einstein Condensation

2005 Nobel Prize
Frequency combs

2012 Nobel prize
Quantum control

300K



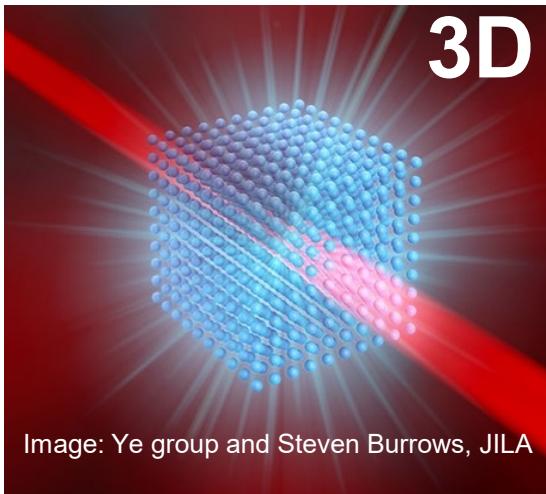
Atoms are now:

Ultracold

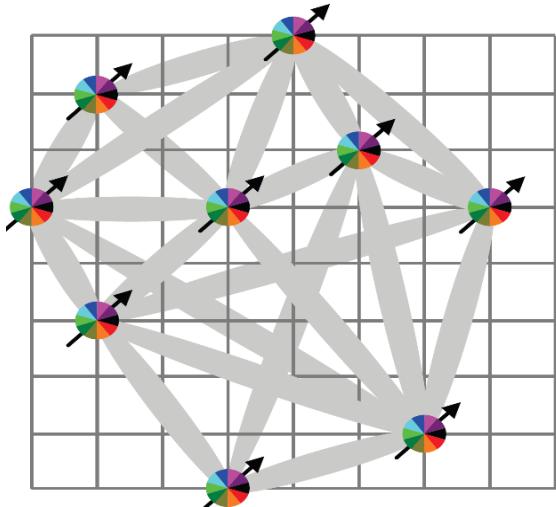
Trapped

Precisely controlled

Numerous applications that need precise atomic data

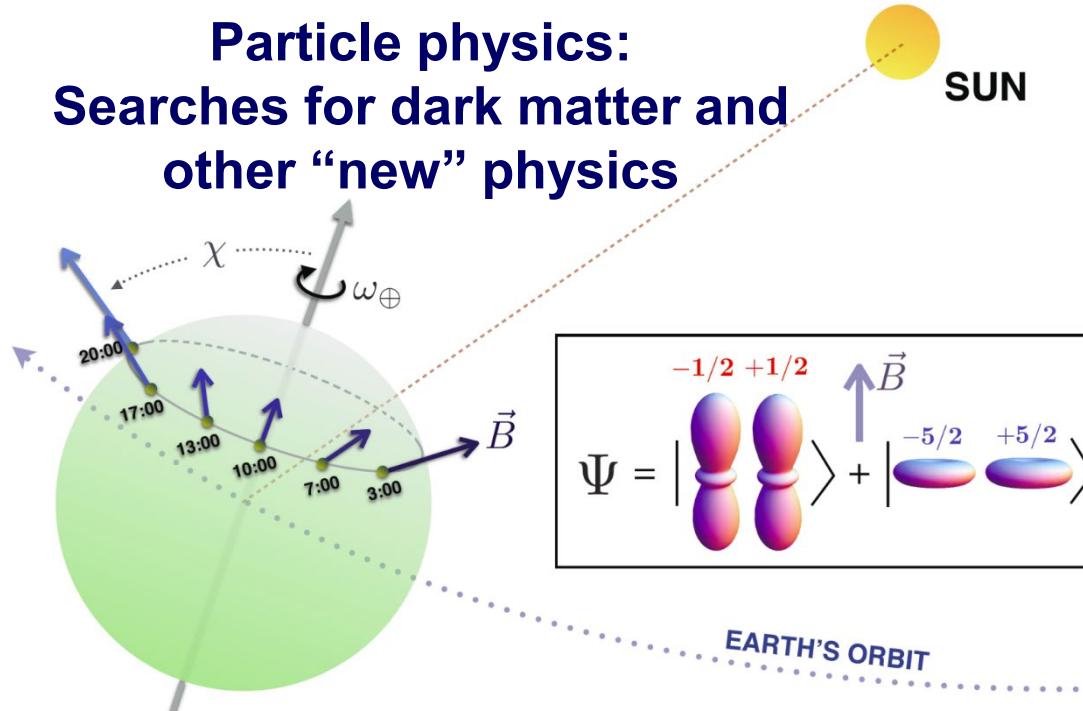


Atomic clocks

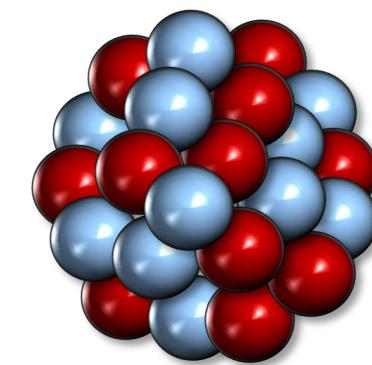


Ultracold atoms
Quantum computing and simulation

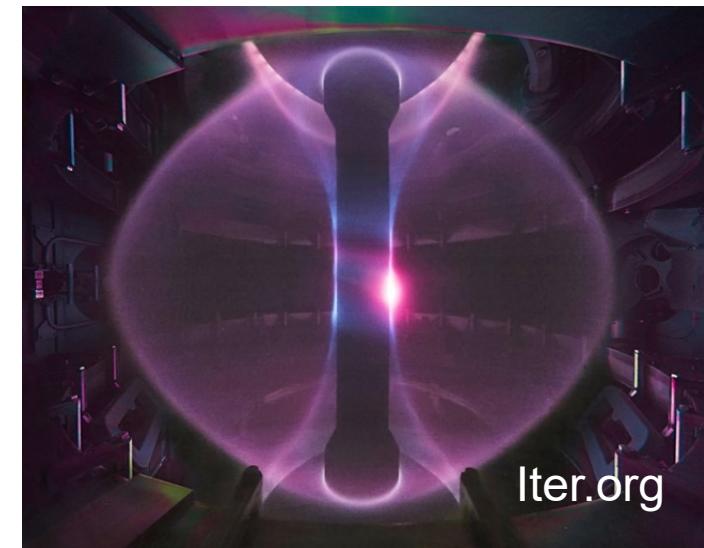
Particle physics:
Searches for dark matter and other “new” physics



Nuclear and hadronic physics - extracting nuclear properties



Astrophysics



Iter.org

Plasma physics

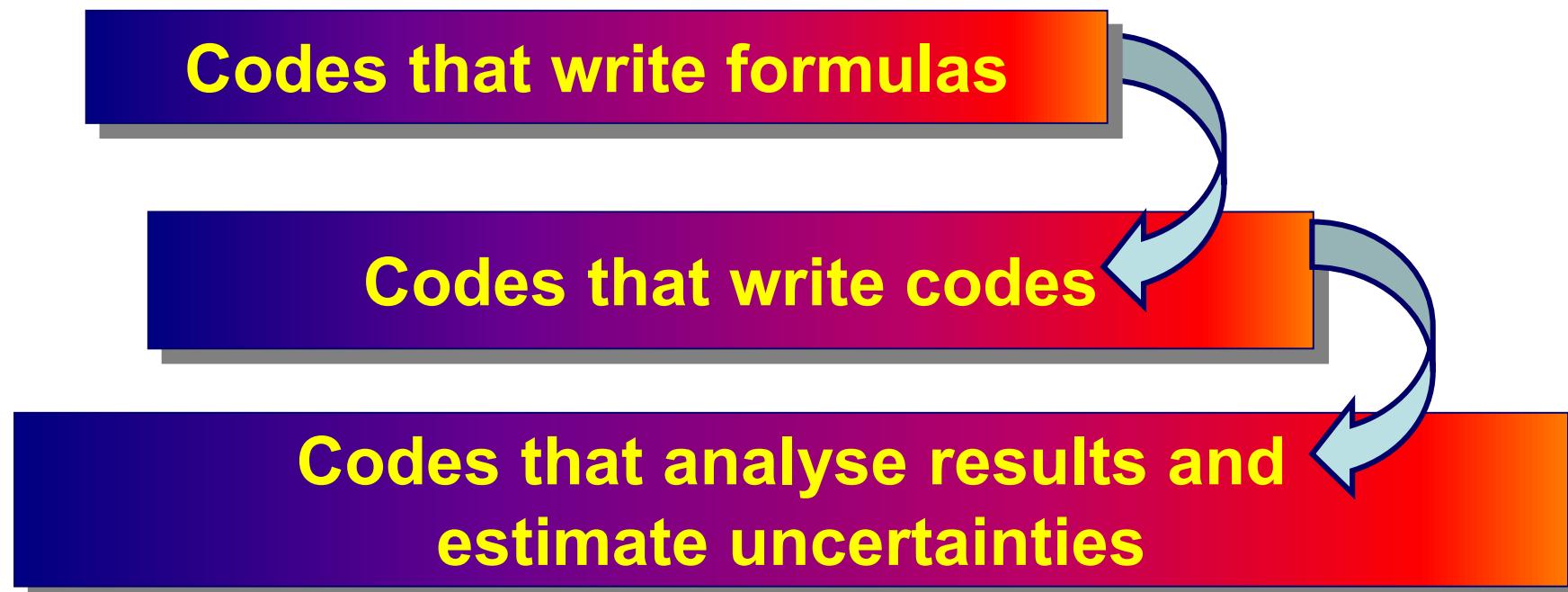
Problems with currently available atomic community codes

- Old - developed initially in 1980s and 1990s, with later updates
- Unsupported or unwieldy (too many updates by many people)
- Designed to produce large volumes of low-precision data
- Poorly documented and/or require expert knowledge to use
- No estimates of how accurate the results are
- Do not serve the need of the present community

There are very few groups in the world developing new atomic codes

University of Delaware team & collaborators

- We have been developing high precision atomic codes and applying them to solve completely different problems for over 20 years
- All codes are written by us
- Because we have several *ab initio* codes we can estimate how accurate numbers are – we are the only group to routinely publish reliable uncertainties
- Most accurate and versatile set of atomic code packages in the world



Numerous emails from experimental colleagues

We are building

atomic clock
degenerate quantum gas microscope
tweezer arrays
quantum simulator with atoms
precision measurement experiment
for new physics searches

...

with

Li, K, Rb,
Cs, Ca,
 Al^+ , Ca^+ ,
 Sr , Sr^+ ,
 Yb , Yb^+ ,
 Lu^+ ,
....

We need [*transition rates, branching ratios, lifetimes, polarizabilities, ...*]

We found some data in your papers – will it be possible to provide?

Would you collaborate with us on the interpretation of our measurements?

We have measured ... but the values differ strongly from the existing literature values.

Will it be possible for you to calculate these?

Variations: atoms are missing from the trap, no expected signal observed, ...

**We plan to measure [....]. Will these quantities be useful in testing your new codes?
What else will be useful to measure?**

NSF PIF: Physics at the Information Frontier Program



Contents lists available at [ScienceDirect](#)

Computer Physics Communications

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

CI-MBPT: A package of programs for relativistic atomic calculations based on a method combining configuration interaction and many-body perturbation theory[☆]

M.G. Kozlov^{a,b,*}, S.G. Porsev^{a,c,**}, M.S. Safronova^{c,d}, I.I. Tupitsyn^e

Comput. Phys. Commun. 195, 199 (2015).

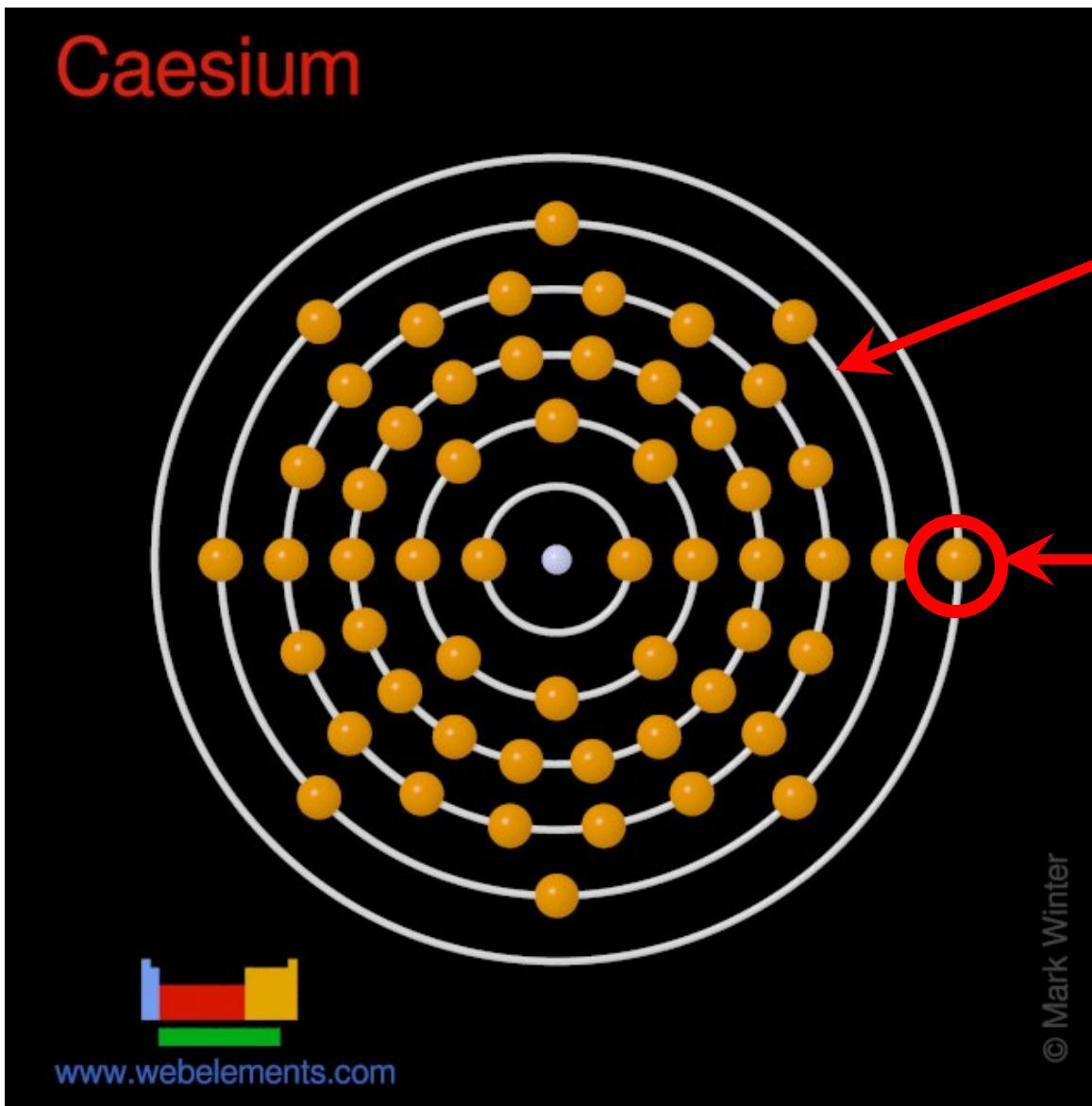
Used by theory rather than experimental groups

Observations: users, numbers, and codes

- Atomic physics has ~ 90% to 10% ratio of experiment vs. theory
- Very large number of users need **numbers**, preferably with error bars, rather than codes.
- The threshold to download, understand and run a complicated set of codes of high-precision codes without much support is extremely high – usually not done by experimental groups.
- Present high precision codes are complicated and requires expert knowledge to run successfully and access to significant computational resources.
- To develop even more accurate codes we need precision experimental benchmarks, so we need to support precision experiments!

PERIODIC TABLE Atomic Properties of the Elements																					
Group	Periodic Table of the Elements																				
1	IA																				
Period	1	H	² S _{1/2}	Hydrogen	1.00794	1s ¹	13.5984	2	Be	¹ S ₀	Beryllium	9.012182	1s ² s ²	9.3227	3	Li	Lithium	6.941	1s ² s ²	5.3917	
	2	Mg	¹ S ₀	Magnesium	24.3050	[Ne]3s ²	7.6462	3	Na	² S _{1/2}	Sodium	22.989770	[Ne]3s ²	5.1381	4	Ca	Calcium	40.078	[Ar]4s ²	6.1132	
	3	Sc	² D _{3/2}	Scandium	44.955910	[Ar]3d ¹ 4s ²	6.5615	4	Ti	³ F ₂	Titanium	47.867	[Ar]3d ² 4s ²	6.7462	5	V	Vanadium	50.9415	[Ar]3d ³ 4s ²	6.7665	
	4	Cr	⁴ F _{3/2}	Chromium	51.9961	[Ar]3d ⁵ 4s ¹	7.4340	6	Mn	⁵ S ₅	Manganese	54.93804	[Ar]3d ⁵ 4s ²	7.9024	7	Fe	Iron	55.845	55.933200	7.8810	
	5	Nb	⁶ S _{5/2}	Niobium	91.924	[Kr]4d ⁵ 5s ²	6.6339	8	Co	⁶ D ₄	Cobalt	59.933200	[Ar]3d ⁷ 4s ¹	7.6398	9	Ni	Nickel	58.6934	[Ar]3d ⁸ 4s ¹	7.6398	
	6	Zr	⁷ D _{3/2}	Zirconium	87.62	[Kr]4d ⁶ 5s ²	6.2173	10	Cu	⁷ F ₄	Copper	63.546	[Ar]3d ¹⁰ 4s ¹	7.7264	11	Zn	Zinc	65.409	[Ar]3d ¹⁰ 4s ²	9.3942	
	7	Rb	⁸ S _{1/2}	Rubidium	85.4678	[Kr]5s ²	4.1771	12	Ga	⁸ P _{1/2}	Gallium	69.723	[Ar]3d ¹⁰ 4s ²	7.8984	13	Ge	Germanium	72.64	[Ar]3d ¹⁰ 4s ²	5.9993	
	8	Sr	⁹ D _{5/2}	Strontium	88.90585	[Kr]4d ⁵ 5s ²	6.5694	14	As	⁹ S _{3/2}	Arsenic	74.92160	[Ar]3d ¹⁰ 4s ²	9.7524	15	Se	Selenium	78.96	[Ar]3d ¹⁰ 4s ²	11.8138	
Period	9	Y	¹⁰ F ₂	Yttrium	88.90585	[Kr]4d ⁵ 5s ²	6.5694	16	Br	¹⁰ P _{3/2}	Bromine	79.904	[Ar]3d ¹⁰ 4s ²	12.9966	17	Kr	Krypton	83.798	[Ar]3d ¹⁰ 4s ²	13.9996	
	10	Nb	¹¹ S _{1/2}	Niobium	92.90538	[Kr]4d ⁵ 5s ²	6.7589	18	Xe	¹¹ S ₀	Xenon	131.293	[Kr]4d ¹⁰ 5s ²	12.1298	19	Rf	Rutherfordium	(223)	[Rn]7s ²	4.0727	
Period	11	Mo	¹² D _{5/2}	Molybdenum	95.94	[Kr]4d ⁶ 5s ²	7.0924	20	Ag	¹² P _{1/2}	Silver	107.8682	[Kr]4d ¹⁰ 5s ²	8.3369	21	Sc	Scandium	40.078	[Ar]3d ¹ 4s ²	6.1132	
	12	Tc	¹³ F ₅	Technetium	(98)	[Kr]4d ⁵ 5s ²	7.28	22	Rh	¹³ F _{9/2}	Ruthenium	101.07	[Kr]4d ⁹ 5s ²	7.4589	23	Ti	Titanium	47.867	[Ar]3d ² 4s ²	6.7462	
Period	13	Ru	¹⁴ F _{9/2}	Ruthenium	101.07	[Kr]4d ⁹ 5s ²	7.3605	24	Pd	¹⁴ S ₀	Rhodium	102.90550	[Kr]4d ¹⁰ 5s ²	8.3369	25	Mn	Manganese	54.93804	[Ar]3d ⁵ 4s ²	7.9024	
	14	Pt	¹⁵ D ₄	Osmium	190.23	[Xe]4f ¹⁴ 5d ⁶ 6s ²	8.4382	26	Ir	¹⁵ F _{9/2}	Iridium	192.217	[Xe]4f ¹⁴ 5d ⁶ 6s ²	8.9570	27	Os	Osmium	190.23	[Xe]4f ¹⁴ 5d ⁶ 6s ²	7.6398	
Period	15	In	¹⁶ P _{1/2}	Cadmium	112.411	[Kr]4d ¹⁰ 5s ²	7.7349	28	Sn	¹⁶ S _{3/2}	Tin	118.710	[Kr]4d ¹⁰ 5s ²	9.7884	29	Ge	Gallium	69.723	[Ar]3d ¹⁰ 4s ²	5.9993	
	16	Sb	¹⁷ D _{5/2}	Antimony	121.760	[Kr]4d ¹⁰ 5s ²	9.0096	30	Te	¹⁷ F ₅	Tellurium	127.60	[Kr]4d ¹⁰ 5s ²	10.4513	31	Br	Bromine	79.904	[Ar]3d ¹⁰ 4s ²	11.8138	
Period	17	Te	¹⁸ S _{1/2}	Iodine	128.90447	[Kr]4d ¹⁰ 5s ²	12.9966	32	I	¹⁸ P _{3/2}	Iodine	128.90447	[Kr]4d ¹⁰ 5s ²	12.9966	33	At	Astatine	(210)	[Hg]6p ⁴	8.414	
	18	Xe	¹⁹ D _{5/2}	Xenon	131.293	[Kr]4d ¹⁰ 5s ²	12.1298	34	Rn	¹⁹ S ₀	Radon	(222)	[Hg]6p ⁴	10.7485	35	Rf	Rutherfordium	(223)	[Rn]7s ²	4.0727	
Period	19	Hf	²⁰ F ₂	Hafnium	178.49	[Xe]4f ¹⁴ 5d ⁶ 6s ²	6.8251	20	Ta	²¹ F ₅	Tantalum	180.9479	[Xe]4f ¹⁴ 5d ⁶ 6s ²	7.5495	21	W	Tungsten	183.84	[Xe]4f ¹⁴ 5d ⁶ 6s ²	7.8640	
	21	Re	²² S _{5/2}	Rhenium	186.207	[Xe]4f ¹⁴ 5d ⁶ 6s ²	7.8335	22	Os	²³ D ₄	Osmium	190.23	[Xe]4f ¹⁴ 5d ⁶ 6s ²	8.4382	23	Ir	Iridium	192.217	[Xe]4f ¹⁴ 5d ⁶ 6s ²	8.9570	
Period	22	Pt	²⁴ F _{9/2}	Platinum	195.078	[Xe]4f ¹⁴ 5d ⁶ 6s ²	8.9588	24	Au	²⁴ S _{1/2}	Gold	196.98655	[Xe]4f ¹⁴ 5d ⁶ 6s ²	9.2255	25	Tl	Thallium	204.3833	[Hg]6p ²	6.1082	
	23	Hg	²⁵ P _{1/2}	Mercury	200.59	[Xe]4f ¹⁴ 5d ⁶ 6s ²	10.4375	26	Pb	²⁵ D _{5/2}	Lead	207.2	[Hg]6p ²	7.4167	27	Bi	Bismuth	208.98038	[Hg]6p ³	7.2855	
Period	24	Tl	²⁶ F ₅	Thallium	204.3833	[Hg]6p ²	6.1082	28	Po	²⁶ P _{3/2}	Polonium	(209)	[Hg]6p ⁴	8.414	29	At	Astatine	(210)	[Hg]6p ⁵	10.7485	
	25	Uuu	²⁷ S _{1/2}	Ununtrium	(281)	[Rn]5f ¹⁴ 7s ²	11.8138	30	Uuh	²⁷ F _{9/2}	Ununhexium	(292)	[Rn]5f ¹⁴ 7s ²	12.9966	31	Uq	Ununquadium	(289)	[Rn]5f ¹⁴ 7s ²	13.9996	
Period	26	Uun	²⁸ S _{1/2}	Ununpentium	(282)	[Rn]5f ¹⁴ 7s ²	12.9966	32	Uub	²⁸ F ₅	Ununhexium	(285)	[Rn]5f ¹⁴ 7s ²	13.9996	33	Uq	Ununquadium	(289)	[Rn]5f ¹⁴ 7s ²	13.9996	
	27	Uuu	²⁹ F ₂	Ununhexium	(281)	[Rn]5f ¹⁴ 7s ²	12.9966	34	Uuh	²⁹ S _{1/2}	Ununhexium	(292)	[Rn]5f ¹⁴ 7s ²	13.9996	35	Uq	Ununquadium	(289)	[Rn]5f ¹⁴ 7s ²	13.9996	
Period	28	Fr	³⁰ S _{1/2}	Francium	(223)	[Rn]7s ²	4.0727	36	Lu	³⁰ D _{5/2}	Lutetium	174.967	[Xe]4f ¹⁴ 5d ⁶ 2	5.4259	37	Ra	Radium	(226)	[Rn]7s ²	5.2784	
	29	Ra	³¹ S ₀	Radium	(226)	[Rn]7s ²	5.2784	38	Ac	³² D _{3/2}	Actinium	(227)	[Rn]5f ¹⁴ 7s ²	5.17	40	Th	³² F ₂	Thorium	(232)	[Rn]5f ¹⁴ 7s ²	6.3067
Period	30	Db	³³ F ₂	Dubnium	(262)	[Rn]5f ¹⁴ 7s ²	6.3067	41	Pa	³⁴ K _{1/2}	Protactinium	231.03588	[Rn]5f ¹⁴ 7s ²	5.89	42	U	³⁴ L _{5/2}	Uranium	238.02891	[Rn]5f ¹⁴ 7s ²	6.1941
	31	Sg	³⁵ F ₂	Seaborgium	(265)	[Rn]5f ¹⁴ 7s ²	6.2657	43	Pu	³⁵ F _{9/2}	Plutonium	(244)	[Rn]5f ¹⁴ 7s ²	6.0260	44	Np	³⁶ L _{11/2}	Neptunium	(237)	[Rn]5f ¹⁴ 7s ²	6.9738
Period	32	Hs	³⁷ F ₅	Hassium	(277)	[Rn]5f ¹⁴ 7s ²	6.9738	45	Am	³⁷ F _{9/2}	Americium	(243)	[Rn]5f ¹⁴ 7s ²	5.9914	46	Gd	³⁸ S _{7/2}	Gadolinium	(145)	[Xe]4f ⁷ 6s ²	5.582
	33	Mt	³⁸ F _{9/2}	Methylmercury	(268)	[Rn]5f ¹⁴ 7s ²	6.9738	47	Tb	³⁹ D _{5/2}	Terbium	158.92534	[Xe]4f ⁷ 6s ²	6.1498	48	Dy	³⁹ P _{1/2}	Dysprosium	162.500	[Xe]4f ¹¹ 6s ²	6.0215
Period	34	Uun	⁴⁰ S _{1/2}	Ununpentium	(281)	[Rn]5f ¹⁴ 7s ²	6.1941	49	Bk	⁴⁰ H _{5/2}	Berkelium	(247)	[Rn]5f ¹⁴ 7s ²	6.1979	50	Ho	⁴⁰ I _{15/2}	Holmium	164.93032	[Xe]4f ¹¹ 6s ²	6.1843
	35	Uub	⁴¹ F ₅	Ununhexium	(285)	[Rn]5f ¹⁴ 7s ²	6.2855	51	Cf	⁴¹ P _{1/2}	Berkeleyium	(251)	[Rn]5f ¹⁴ 7s ²	6.2817	52	Es	⁴¹ I _{15/2}	Einsteinium	(257)	[Rn]5f ¹⁴ 7s ²	6.42
Period	36	Uq	⁴² S _{1/2}	Ununquadium	(289)	[Rn]5f ¹⁴ 7s ²	11.8138	53	Tm	⁴² F _{7/2}	Thulium	168.93421	[Xe]4f ¹⁴ 6s ²	6.2542	54	Yb	⁴² I _{15/2}	Ytterbium	173.04	[Xe]4f ¹⁴ 6s ²	5.4259
	37	Uuh	⁴³ F _{9/2}	Ununhexium	(292)	[Rn]5f ¹⁴ 7s ²	13.9996	55	Lu	⁴³ D _{5/2}	Lutetium	174.967	[Xe]4f ¹⁴ 6s ²	5.4259	56	Fr	⁴⁴ S _{1/2}	Francium	(223)	[Rn]7s ²	4.0727
Period	38	Uq	⁴⁴ F ₂	Ununquadium	(289)	[Rn]5f ¹⁴ 7s ²	13.9996	57	La	⁴⁵ D _{3/2}	Lanthanum	138.9055	[Xe]5d ⁶ 2	5.5387	58	Ce	⁴⁶ G ₄	Cerium	140.116	[Xe]5d ⁶ 2	5.5387
	39	Uuh	⁴⁵ F ₂	Ununhexium	(292)	[Rn]5f ¹⁴ 7s ²	13.9996	59	Pr	⁴⁷ I _{9/2}	Praseodymium	140.90765	[Xe]4f ⁵ 6s ²	5.4733	60	Nd	⁴⁸ H _{5/2}	Neodymium	144.24	[Xe]4f ⁵ 6s ²	5.5250
Period	40	Uq	⁴⁶ F ₂	Ununquadium	(289)	[Rn]5f ¹⁴ 7s ²	13.9996	61	Pm	⁴⁹ H _{9/2}	Promethium	(145)	[Xe]4f ⁵ 6s ²	5.5250	62	Sm	⁵⁰ L _{5/2}	Samarium	150.984	[Xe]4f ⁵ 6s ²	5.6437
	41	Uuh	⁴⁷ F ₂	Ununhexium	(285)	[Rn]5f<sup															

Classify atomic calculations by difficulty level



Closed shells

Can be approximated
by a mean field

Single
valence
electron

Classify atomic calculations by difficulty level

3	² S _{1/2}	4	¹ S ₀
Li	Boron	Be	Beryllium
Lithium	9.012182	9.012182	9.012182
6.941	1s ² 2s	1s ² 2s	1s ² 2s
5.3917	9.3227		
11	² S _{1/2}	12	¹ S ₀
Na	Sodium	Mg	Magnesium
22.989770	24.3050	[Ne]3s ²	[Ne]3s ²
5.1391	7.6462		
19	² S _{1/2}	20	¹ S ₀
K	Potassium	Ca	Calcium
39.0983	40.078	[Ar]4s ²	[Ar]4s ²
4.3407	6.1132		
37	² S _{1/2}	38	¹ S ₀
Rb	Rubidium	Sr	Strontium
85.4678	87.62	[Kr]5s ²	[Kr]5s ²
4.1771	5.6949		
55	² S _{1/2}	56	¹ S ₀
Cs	Cesium	Ba	Barium
132.90545	137.327	[Xe]6s ²	[Xe]6s ²
3.8839	5.2117		
87	² S _{1/2}	88	¹ S ₀
Fr	Franium	Ra	Radium
(223)	(226)	[Rn]7s ²	[Rn]7s ²
4.0727	5.2784		

Group 1
Calculations we
can do “routinely”,
with default
parameters

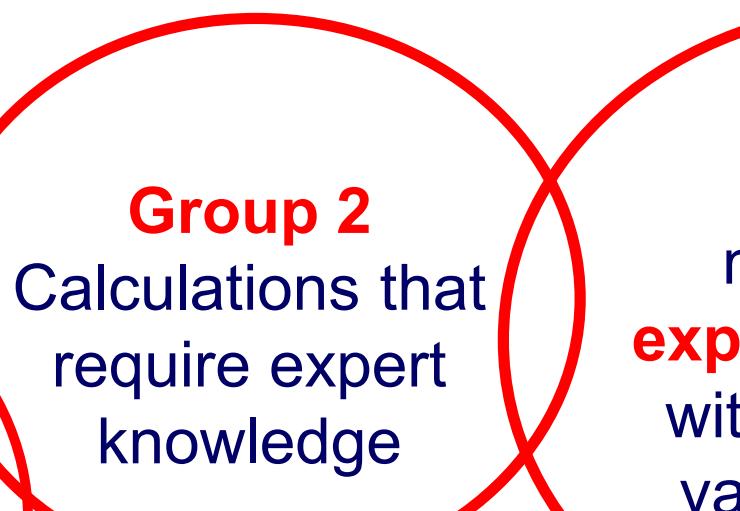
1 – 2(3) valence
electrons

Can automate

(3)/4-5 valence
electrons
or special cases
with more
valence electrons

**Only calculations of wave
functions requires expert
knowledge**

Group 2
Calculations that
require expert
knowledge



Group 3
No precision
methods exist:
exponential scaling
with the number of
valence electrons

25	⁶ S _{5/2}	26	⁵ D ₄	27	⁴ F _{9/2}	28	³ F ₄
Mn	Manganese	Fe	Iron	Co	Cobalt	Ni	Nickel
54.938049	[Ar]3d ⁵ 4s ²	55.845	[Ar]3d ⁵ 4s ²	58.933200	[Ar]3d ⁵ 4s ²	58.6934	[Ar]3d ⁵ 4s ²
7.4340		7.9024		7.8810		7.6398	
43	⁶ S _{5/2}	44	⁵ F ₅	45	⁴ F _{9/2}	46	¹ S ₀
Tc	Techneium	Ru	Ruthenium	Rh	Rhodium	Pd	Palladium
(98)	[Kr]4d ⁵ 5s ²	101.07	[Kr]4d ⁵ 5s ²	102.90550	[Kr]4d ⁵ 5s ²	106.42	[Kr]4d ¹⁰
7.28		7.3605		7.4589		8.3369	
75	⁶ S _{5/2}	76	⁵ D ₄	77	⁴ F _{9/2}	78	³ D ₃
Re	Rhenium	Os	Osmium	Ir	Iridium	Pt	Platinum
186.207	190.23	192.217	196.078				
[Xe]4f ¹⁴ 5d ⁶ s ²							
7.8336	8.4382	8.9670	8.9588				

60	⁵ I ₄	61	⁸ H _{5/2}	62	⁷ F ₀	63	⁸ S _{7/2}	64	⁹ D ₂	65	⁸ H _{15/2}	66	⁵ I ₈	67	⁴ I _{15/2}	68	³ H ₆	69	² F _{7/2}
Nd	Neodymium	Pm	Promethium	Sm	Samarium	Eu	Europium	Gd	Gadolinium	Tb	Terbium	Dy	Dysprosium	Ho	Holmium	Er	Erbium	Tm	Thulium
144.24	(144)	(145)	(145)	150.36	151.964	157.25	158.92534	167.259	164.93032	164.93032	167.259	168.93421	(252)	(252)	(252)	(252)	(252)	(252)	
[Xe]4f ¹⁰ 6s ²	[Xe]4f ⁹ 6s ²	[Xe]4f ⁹ 6s ²	[Xe]4f ⁹ 6s ²	[Xe]4f ⁹ 6s ²	[Xe]4f ⁸ 6s ²	[Xe]4f ¹⁰ 6s ²	[Xe]4f ¹⁰ 6s ²	[Xe]4f ¹⁰ 6s ²	[Xe]4f ¹⁰ 6s ²	[Xe]4f ¹⁰ 6s ²	[Xe]4f ¹⁰ 6s ²								
5.5250	5.5852	5.6437	6.1498	5.6838	5.9389	6.0215	6.0215	6.0215	6.0215	6.0215	6.0215	6.0215	6.0215	6.0215	6.0215	6.0215	6.0215		
92	⁵ L ₈	93	⁸ L _{11/2}	94	⁷ F ₀	95	⁸ S _{7/2}	96	⁹ D ₂	97	⁸ H _{15/2}	98	⁵ I ₈	99	⁴ I _{15/2}	100	³ H ₆	101	² F _{7/2}
U	Uranium	Np	Neptunium	Pu	Plutonium	Am	Americium	Cm	Curium	Bk	Berkelium	Cf	Californium	Es	Einsteinium	Fm	Fermium	Md	Mendelevium
238.02891	(237)	(237)	(244)	240.2657	(244)	243.9738	(247)	247.59738	(247)	247.61979	(247)	251.62817	(252)	(252)	(252)	(252)	(252)	(252)	
[Rn]5f ¹⁴ 6d ⁷ s ²																			
6.1941		6.2657		6.0260		5.9738		5.9914		6.1979		6.2817		6.42		6.50		6.58	

Half-filled shells
and holes in shells

**Method development in
progress, need new ideas –
machine learning**

Community – driven project: there is enormous need for data

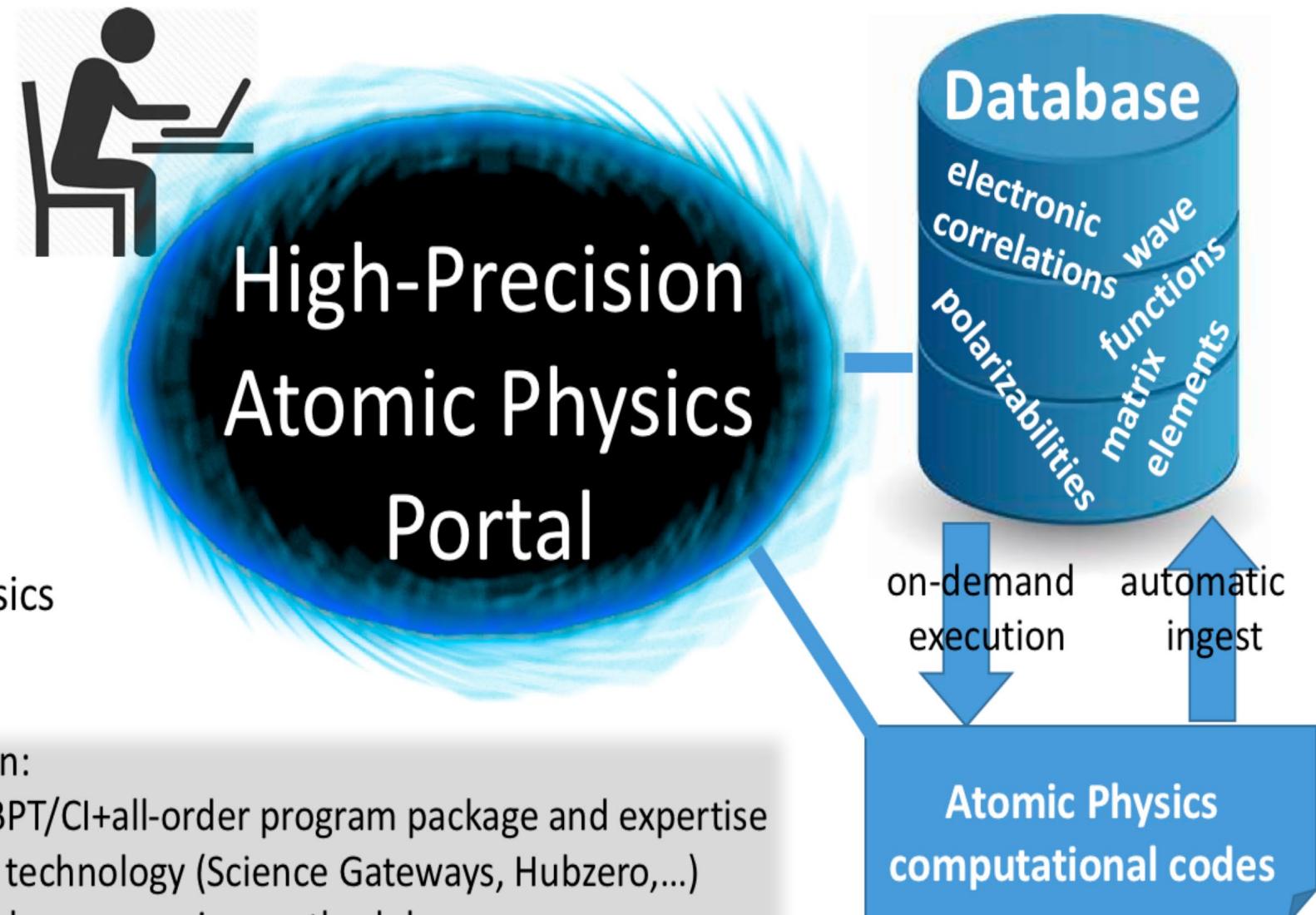
Applications in science and engineering

- quantum information
- degenerate quantum gases
- atomic clocks
- precision measurements
- plasma physics
- astrophysics
- studies of fundamental physics

Difficulty Groups 1 and 2

Building on:

- CI+MBPT/CI+all-order program package and expertise
- Portal technology (Science Gateways, Hubzero,...)
- Parallel programming methodology



COMPUTER, CALCULATE!

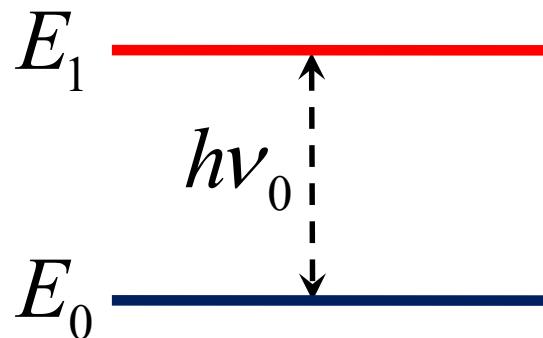
To boldly go where no one has gone before ...



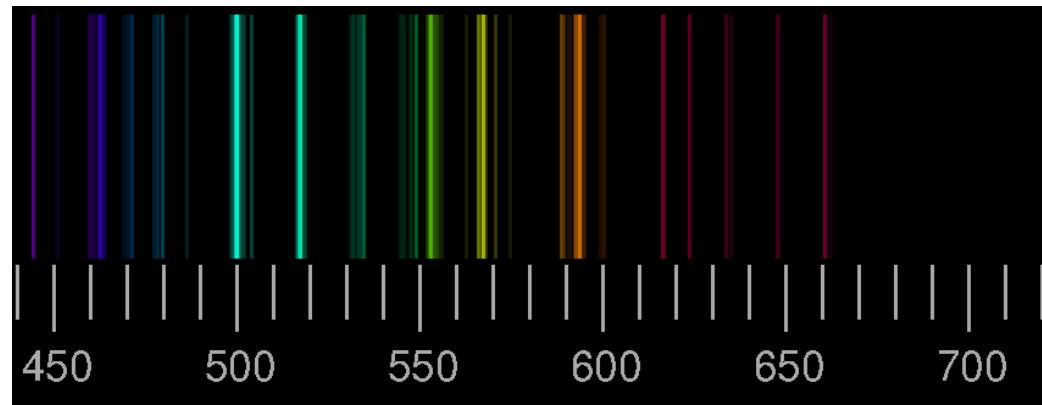
www.film.ru

How to serve the most diverse group of users?

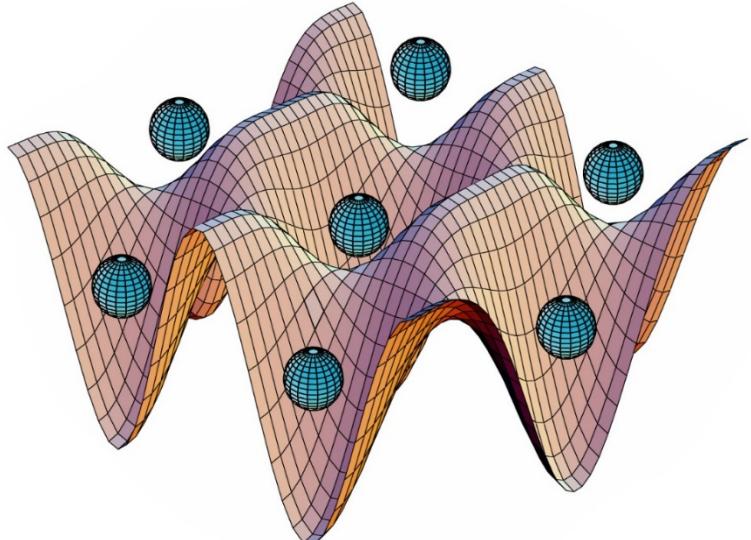
Most requested data:
transition matrix
elements and
polarizabilities



What is transition probability?



Atoms are now **trapped by light**



Need electric-dipole polarizability α to determine how deep the trap will be for specified laser wavelength

What is transition energy?

$$U \propto \alpha(\lambda)$$

How to serve the most diverse group of users?

Most requested data: transition matrix elements and polarizabilities will be pre-calculated for atoms/ions of most interest, Group 1 and some Group 2.

Uncertainty estimates will be provided for all data.

This will require vast computations so the code packages are being completely automated for such data production for Group 1 atoms/ions.

Users who need other data for these systems: all wave functions from runs above will be stored so other data can be requested – will be calculated automatically. Users do not need to know anything about codes.

Advanced users – frequent need of data and theory groups

All codes will be released to public – optimized and **very** user friendly.

We will have tutorials and workshops providing training to use the codes.

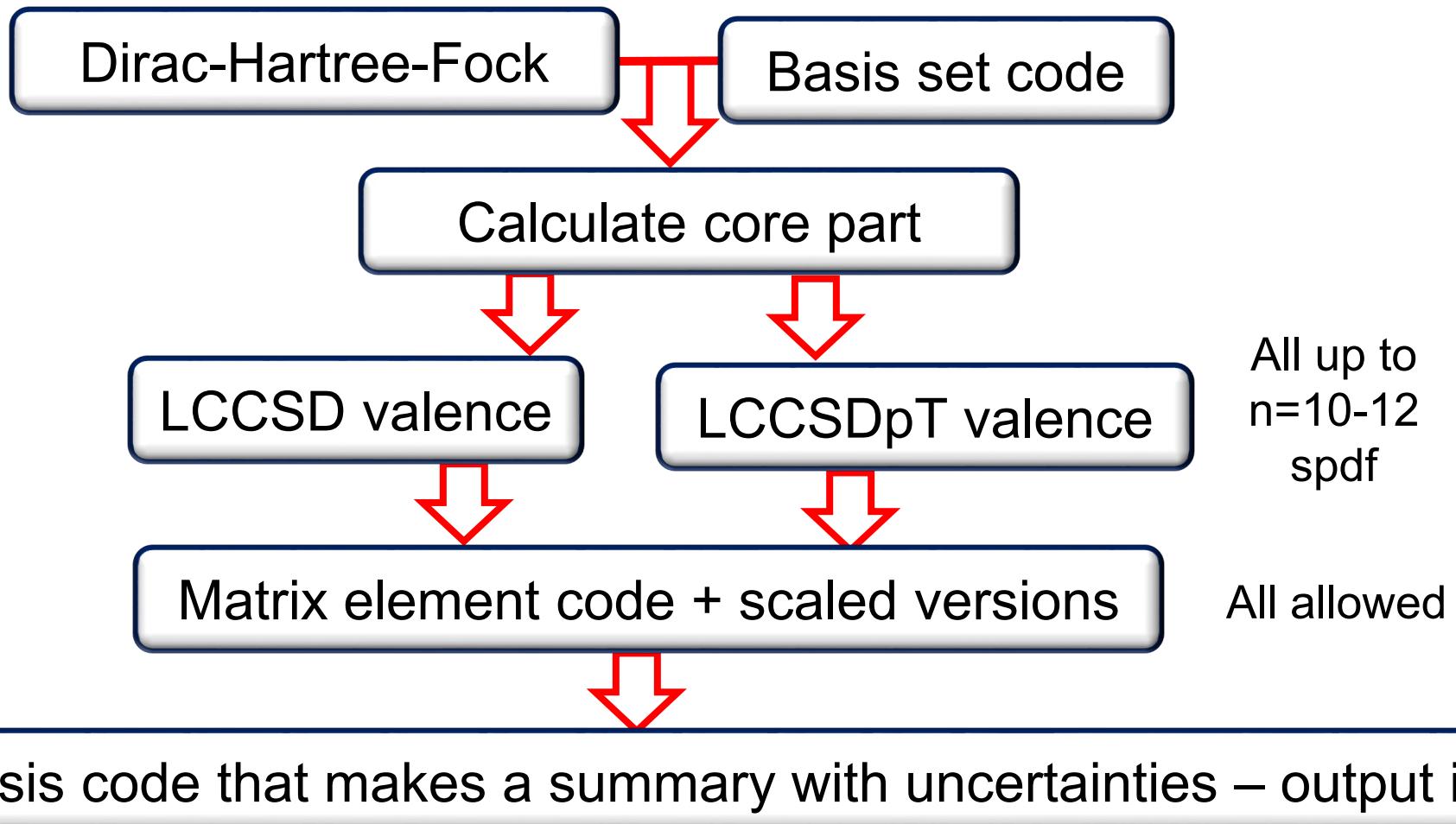
Other groups will send us representatives for several months to train as experts

Population of the database will be completely automated.

Example: monovalent systems

Present data are incomplete and scattered through the projects

COMPUTER, CALCULATE CS!



Final code output: transition E1 matrix elements in atomic units

Transition	DHF	SD	SDsc	SDpT	SDpTsc	Final
$3d_{3/2} - 4f_{5/2}$	2.6059	1.8660	1.9265	1.9265	1.9051	1.93(2)
$3d_{3/2} - 4p_{1/2}$	3.0825	2.4173	2.4636	2.4677	2.4503	2.46(1)
$3d_{3/2} - 4p_{3/2}$	1.3764	1.0788	1.0996	1.1014	1.0937	1.100(6)
$3d_{3/2} - 5f_{5/2}$	1.5216	1.1655	1.1917	1.1937	1.1846	1.192(7)
$3d_{3/2} - 5p_{1/2}$	0.0063	0.1254	0.1055	0.1097	0.1154	0.11(2)
$3d_{3/2} - 5p_{3/2}$	0.0008	0.0590	0.0501	0.0521	0.0545	0.050(9)
$3d_{3/2} - 6f_{5/2}$	1.0430	0.8195	0.8347	0.8366	0.8313	0.83(2)
$3d_{3/2} - 6p_{1/2}$	0.0276	0.0683	0.0607	0.0623	0.0640	0.061(8)
$3d_{3/2} - 6p_{3/2}$	0.0138	0.0319	0.0285	0.0293	0.0300	0.028(3)
$3d_{3/2} - 7f_{5/2}$	0.7794	0.6201	0.6303	0.6319	0.6283	0.63(1)
$3d_{3/2} - 7p_{1/2}$	0.0266	0.0464	0.0418	0.0429	0.0436	0.042(7)
$3d_{3/2} - 7p_{3/2}$	0.0128	0.0217	0.0196	0.0201	0.0204	0.020(3)
$3d_{3/2} - 8f_{5/2}$	0.6142	0.4921	0.4996	0.5009	0.4982	0.500(8)
$3d_{3/2} - 8p_{1/2}$	0.0227	0.0346		0.0322		0.032(3)
$3d_{3/2} - 8p_{3/2}$	0.0108	0.0161		0.0151		0.015(2)
$3d_{3/2} - 9f_{5/2}$	0.5017	0.4037	0.4096	0.4107	0.4086	0.410(6)
$3d_{3/2} - 9p_{1/2}$	0.0191	0.0272		0.0254		0.025(3)
$3d_{3/2} - 9p_{3/2}$	0.0090	0.0127		0.0119		0.012(1)
$3d_{5/2} - 10f_{5/2}$	0.1126	0.0910	0.0922	0.0925	0.0920	0.092(1)
$3d_{5/2} - 10f_{7/2}$	0.5035	0.4068	0.4124	0.4136	0.4115	0.412(6)

Li

Na

K

Rb

Cs

Fr

Be⁺

Mg⁺

Ca⁺

Sr⁺

Ba⁺

Ra⁺

Be

Mg

Ca

Sr

Ba

Ra

B⁺

Al⁺

In⁺

Lu⁺

Tl⁺

Th³⁺

Cd

In

Lu

Tl

Pb

Th

Li

Na

K

Rb

Cs

Fr

Be⁺

Mg⁺

Ca⁺

Sr⁺

Ba⁺

Ra⁺

Be

Mg

Ca

Sr

Ba

Ra

B⁺

Al⁺

In⁺

Lu⁺

Tl⁺

Th³⁺

Cd

In

Lu

Tl

Pb

Th

Cs**All data**

6s	6p _{1/2}	6p _{3/2}	5d _{3/2}	5d _{5/2}	4f _{5/2}	4f _{7/2}
7s	7p _{1/2}	7p _{3/2}	6d _{3/2}	6d _{5/2}	5f _{5/2}	5f _{7/2}
8s	8p _{1/2}	8p _{3/2}	7d _{3/2}	7d _{5/2}	6f _{5/2}	6f _{7/2}
9s	9p _{1/2}	9p _{3/2}	8d _{3/2}	8d _{5/2}	7f _{5/2}	7f _{7/2}
10s	10p _{1/2}	10p _{3/2}	9d _{3/2}	9d _{5/2}	8f _{5/2}	8f _{7/2}
11s	11p _{1/2}	11p _{3/2}	10d _{3/2}	10d _{5/2}	9f _{5/2}	9f _{7/2}
12s	12p _{1/2}	12p _{3/2}	11d _{3/2}	11d _{5/2}	10f _{5/2}	10f _{7/2}

Cs**All data**

6s	6p _{1/2}	6p_{3/2}	5d _{3/2}	5d _{5/2}	4f _{5/2}	4f _{7/2}
7s	7p _{1/2}	7p _{3/2}	6d _{3/2}	6d _{5/2}	5f _{5/2}	5f _{7/2}
8s	8p _{1/2}	8p _{3/2}	7d _{3/2}	7d _{5/2}	6f _{5/2}	6f _{7/2}
9s	9p _{1/2}	9p _{3/2}	8d _{3/2}	8d _{5/2}	7f _{5/2}	7f _{7/2}
10s	10p _{1/2}	10p _{3/2}	9d _{3/2}	9d _{5/2}	8f _{5/2}	8f _{7/2}
11s	11p _{1/2}	11p _{3/2}	10d _{3/2}	10d _{5/2}	9f _{5/2}	9f _{7/2}
12s	12p _{1/2}	12p _{3/2}	11d _{3/2}	11d _{5/2}	10f _{5/2}	10f _{7/2}

Output: table of electric-dipole matrix elements

Print or download in Excel format

Transition rates, branching ratios and lifetime options will be added as well.

6p3/2	6s1/2	6.38(8)	6p3/2	5d3/2	3.19(7)	6p3/2	5d5/2	9.7(2)
6p3/2	7s1/2	6.48(2)	6p3/2	6d3/2	2.09(3)	6p3/2	6d5/2	6.13(9)
6p3/2	8s1/2	1.46(2)	6p3/2	7d3/2	0.976(0)	6p3/2	7d5/2	2.89(3)
6p3/2	9s1/2	0.766(9)	6p3/2	8d3/2	0.607(8)	6p3/2	8d5/2	1.81(2)
6p3/2	10s1/2	0.505(6)	6p3/2	9d3/2	0.430(6)	6p3/2	9d5/2	1.28(2)
6p3/2	11s1/2	0.370(4)	6p3/2	10d3/2	0.328(5)	6p3/2	10d5/2	0.979(6)
6p3/2	12s1/2	0.289(3)	6p3/2	11d3/2	0.262(4)	6p3/2	11d5/2	0.782(5)
6p3/2	13s1/2	0.235(3)	6p3/2	12d3/2	0.2201	6p3/2	12d5/2	0.6585

Uncertainties are given in parenthesis.

High-precision experimental data will be provided where available with references.
The goal of the portal is to provide recommended data.

Cs

Other properties not in database

6s	6p _{1/2}	6p _{3/2}	5d _{3/2}	5d _{5/2}	4f _{5/2}	4f _{7/2}
7s	7p _{1/2}	7p _{3/2}	6d _{3/2}	6d _{5/2}	5f _{5/2}	5f _{7/2}
8s	8p _{1/2}	8p _{3/2}	7d _{3/2}	7d _{5/2}	6f _{5/2}	6f _{7/2}
9s	9p _{1/2}	9p _{3/2}	8d _{3/2}	8d _{5/2}	7f _{5/2}	7f _{7/2}
10s	10p _{1/2}	10p _{3/2}	9d _{3/2}	9d _{5/2}	8f _{5/2}	8f _{7/2}
11s	11p _{1/2}	11p _{3/2}	10d _{3/2}	10d _{5/2}	9f _{5/2}	9f _{7/2}
12s	12p _{1/2}	12p _{3/2}	11d _{3/2}	11d _{5/2}	10f _{5/2}	10f _{7/2}

- E2, E3, M1, M2, M3 transition matrix elements
- A and B hyperfine constants
- Parity-violating matrix element
- T-odd matrix element
- Lorentz violating matrix elements

- Click on 1 or 2 states (depends on a property)
- Select needed property from the pull-down menu – it will be computed automatically using pre-stored wave functions

Polarizability portal page

User will click on element

Sr

Then select a state from the list

$5s^2 \ 1S_0$

Could also select another state to get a magic wavelength (where two curves cross)

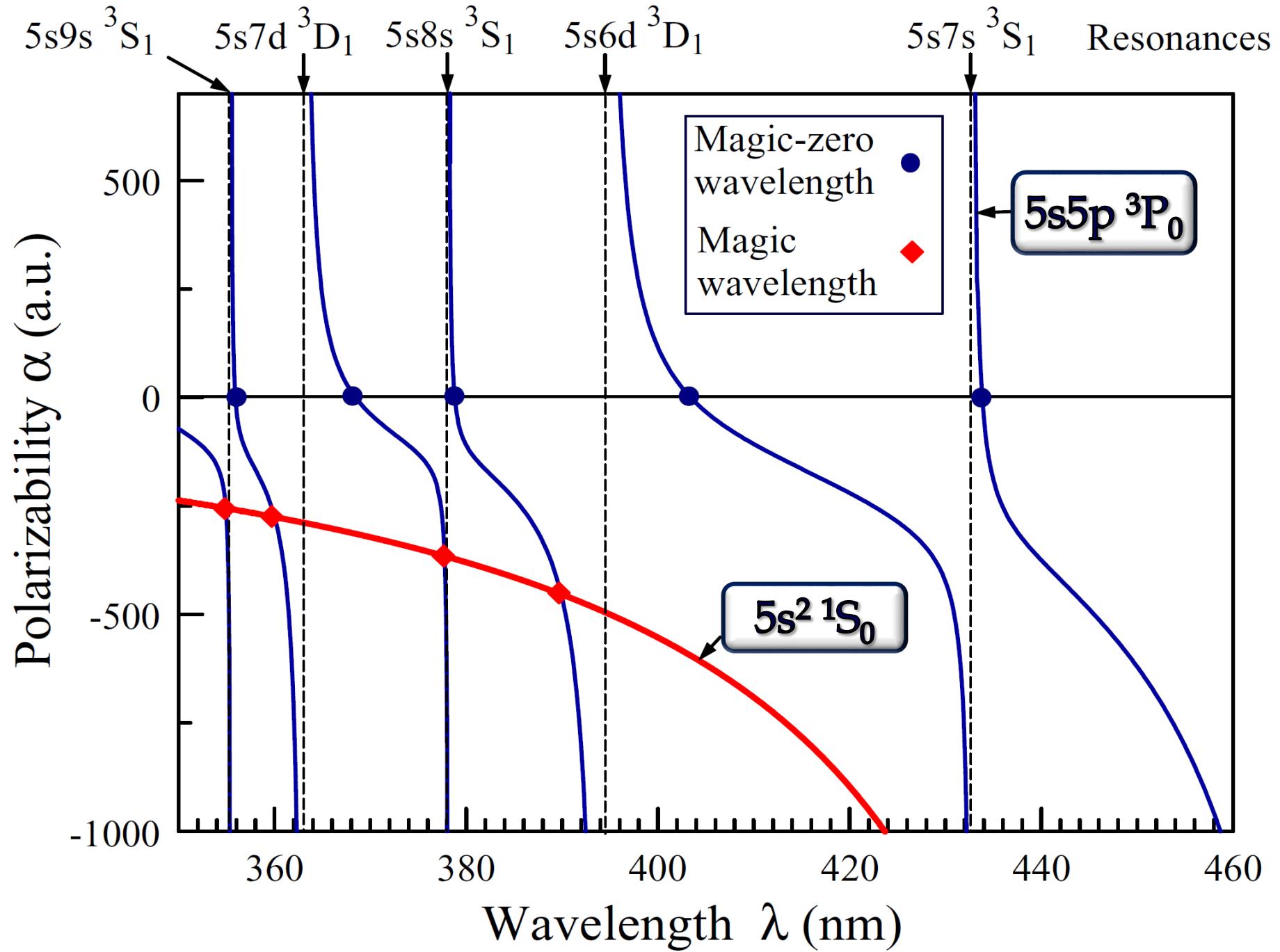
$5s5p \ ^3P_0$

User will enter wavelength range or select a static option

Static

350 - 460 nm

Sr



Summary

Online portal 3-year project started in October 2019



Marianna Safronova
Parinaz Barakhshan

Rudolf Eigenmann
Adam Mars

It is extremely useful for physicists to collaborate with computer scientists!

First version will be online for trial users by DAMOP meeting (June 1, 2020)

Continuing method and code development

Charles Cheung (University of Delaware, USA)

Sergey Porsev (University of Delaware, USA, PNPI, Russia)

Mikhail Kozlov (PNPI, Russia)

Ilya Tupitsyn (University of St. Petersburg, Russia)

International collaboration will be established to maintain the portal beyond the 3-year project

Our vision: data for the entire periodic table accessible through the portal