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

Award #1931339

University of Delaware project team and collaborators

C. Cheung[1], P. Barakhshan[2], A. Marrs[1], 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,
[4]Petersburg Nuclear Physics Institute, Gatchina 188300, Russia
[5]St. Petersburg Electrotechnical University "LETI", St. Petersburg, Russia

Extraordinary progress in the control of atoms and ions

1997 Nobel Prize
Laser cooling and trapping

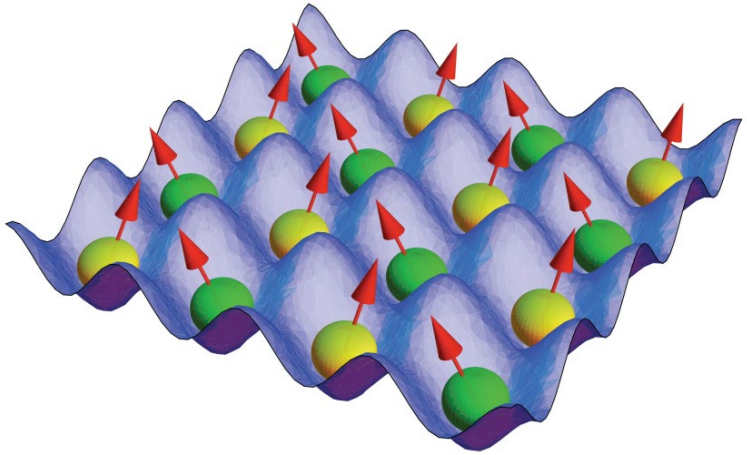
2001 Nobel Prize
Bose-Einstein Condensation

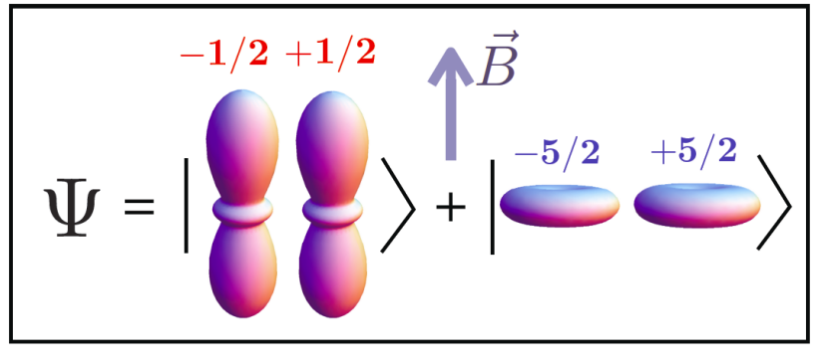
2005 Nobel Prize
Frequency combs

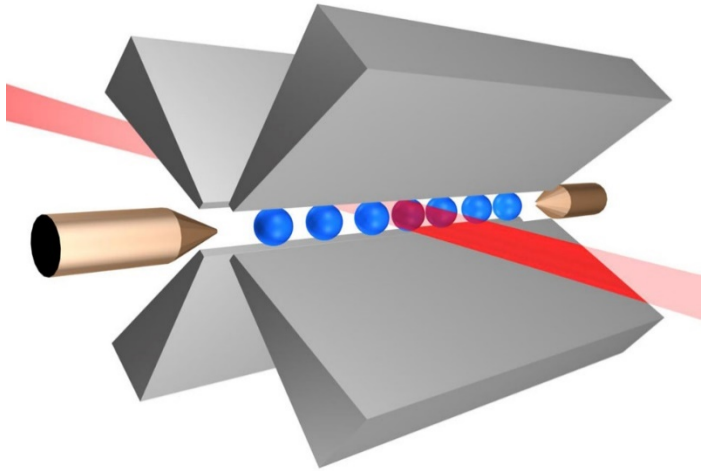
2012 Nobel prize
Quantum control

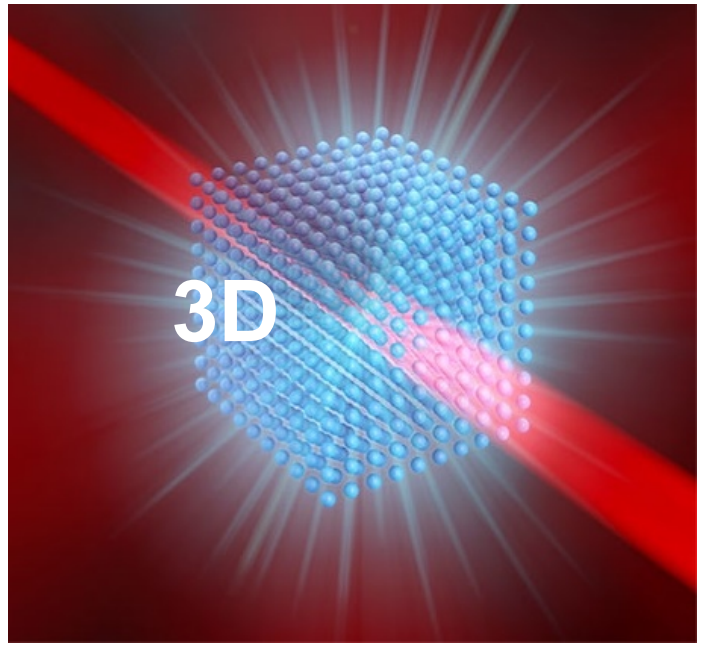
300K

pK



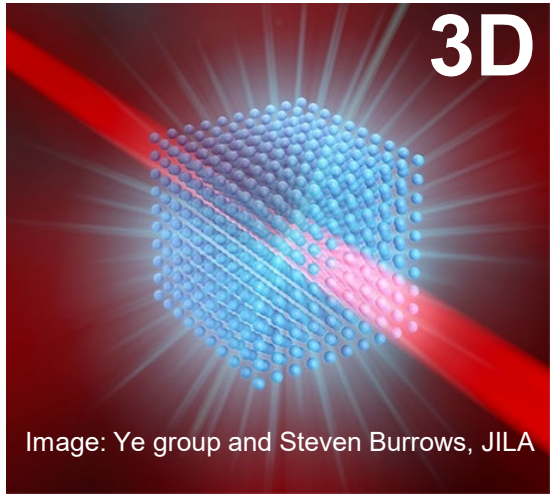




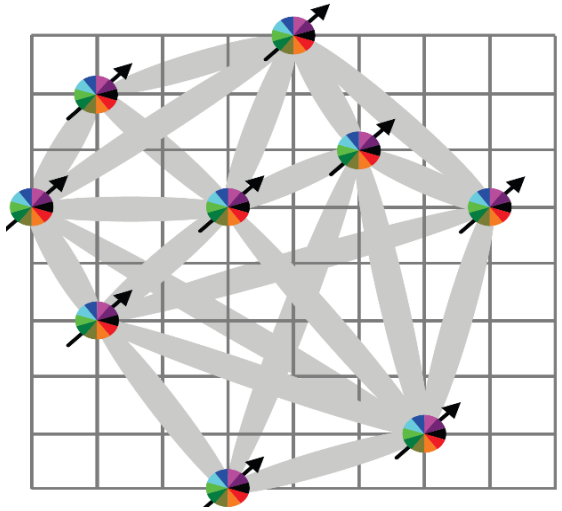


Atoms are now: **Ultracold** **Trapped** **Precisely controlled**

Numerous applications that need precise atomic data

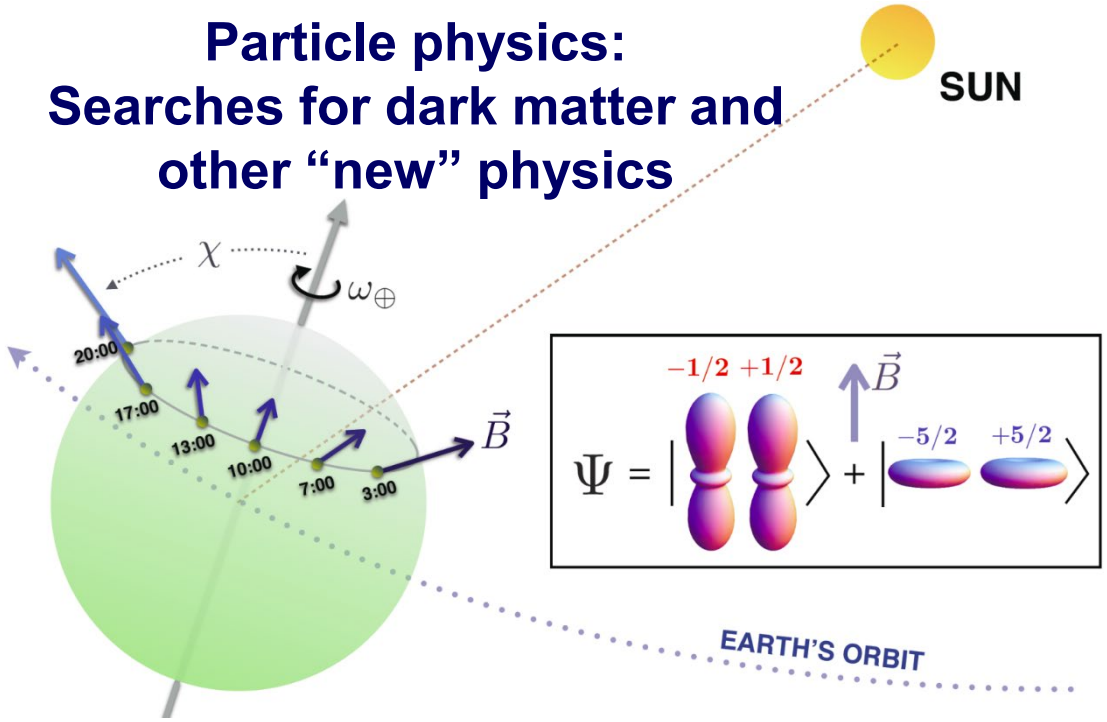


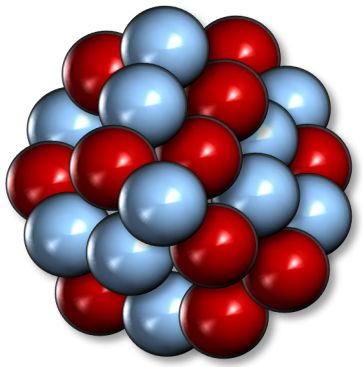
Atomic clocks



Ultracold atoms
Quantum computing and simulation

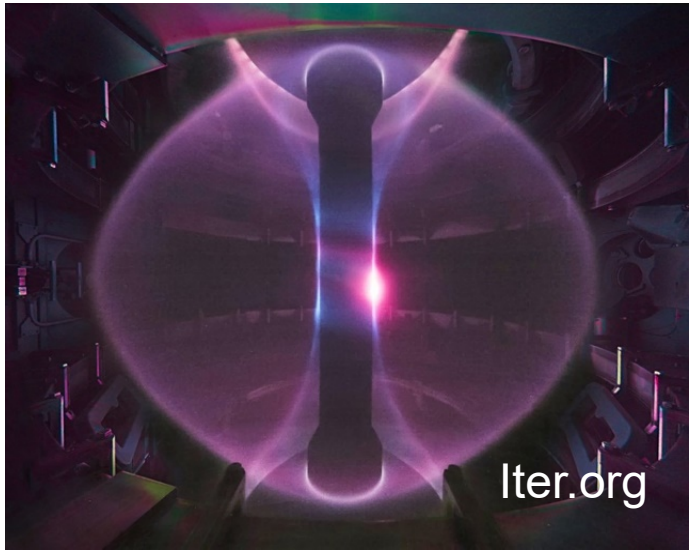
Particle physics:
Searches for dark matter and other "new" physics





Nuclear and hadronic physics - extracting nuclear properties

Astrophysics



Plasma physics

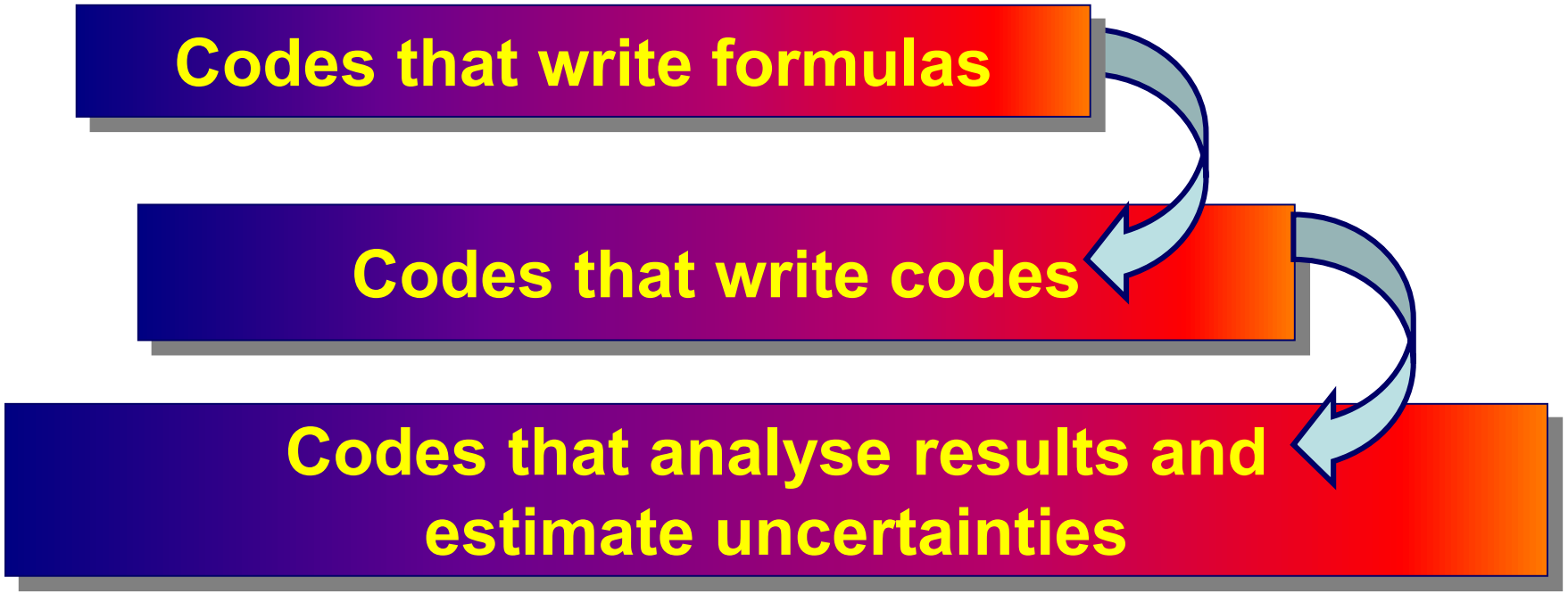
Problems with currently available atomic community codes

- 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?

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☆

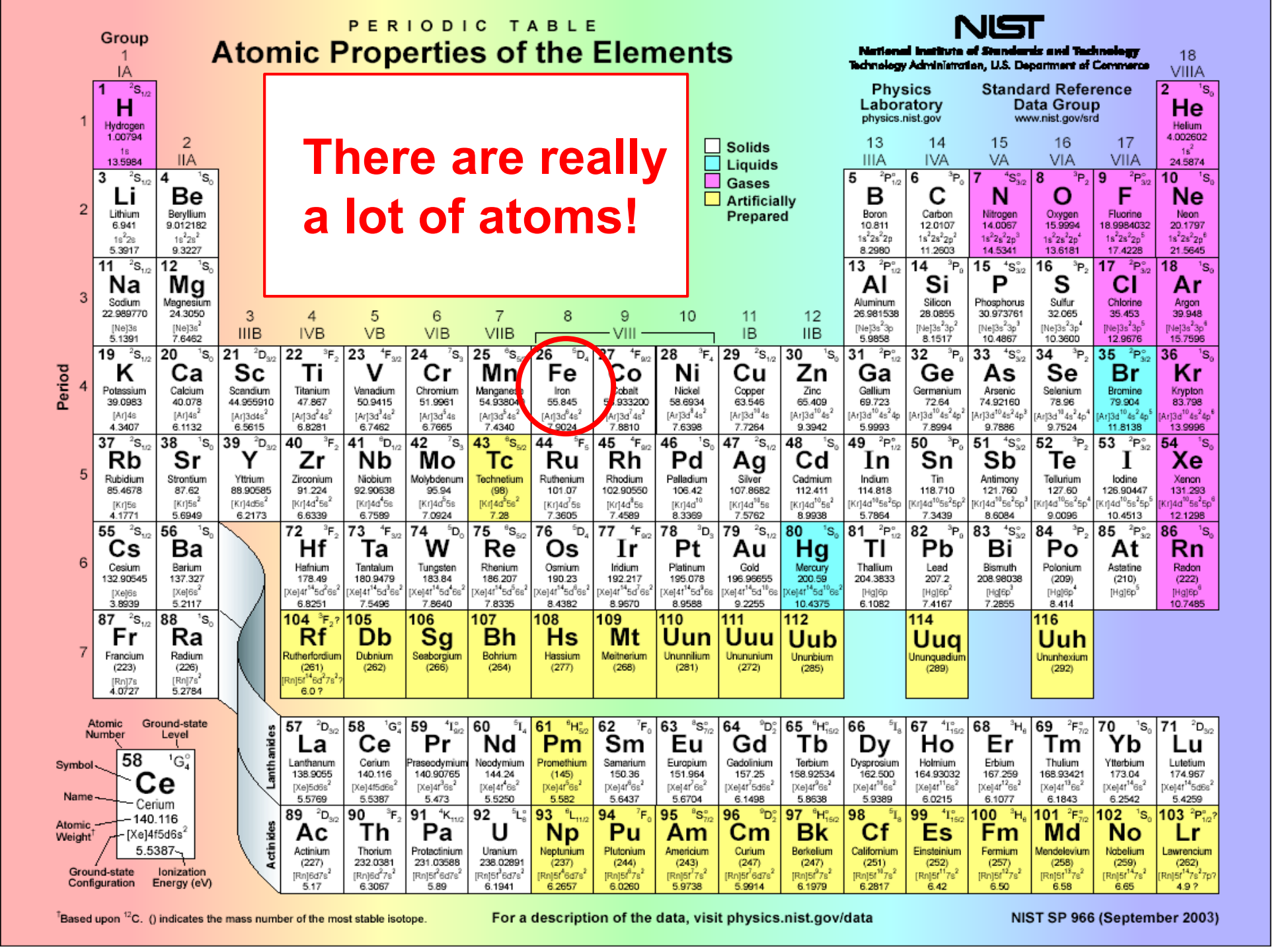
M.G. Kozlov[a,b,*], S.G. Porsev[a,c,**], M.S. Safronova[c,d], I.I. Tupitsyn[e]

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!



Neutral atom: Fe

Ions: keep removing electrons

Fe^{+} Fe^{14+}

Fe^{2+} Fe^{15+}

Fe^{3+} Fe^{16+}

Fe^{4+} Fe^{17+}

Fe^{5+} Fe^{18+}

Fe^{6+} Fe^{19+}

Fe^{7+} Fe^{20+}

Fe^{8+} Fe^{21+}

Fe^{9+} Fe^{22+}

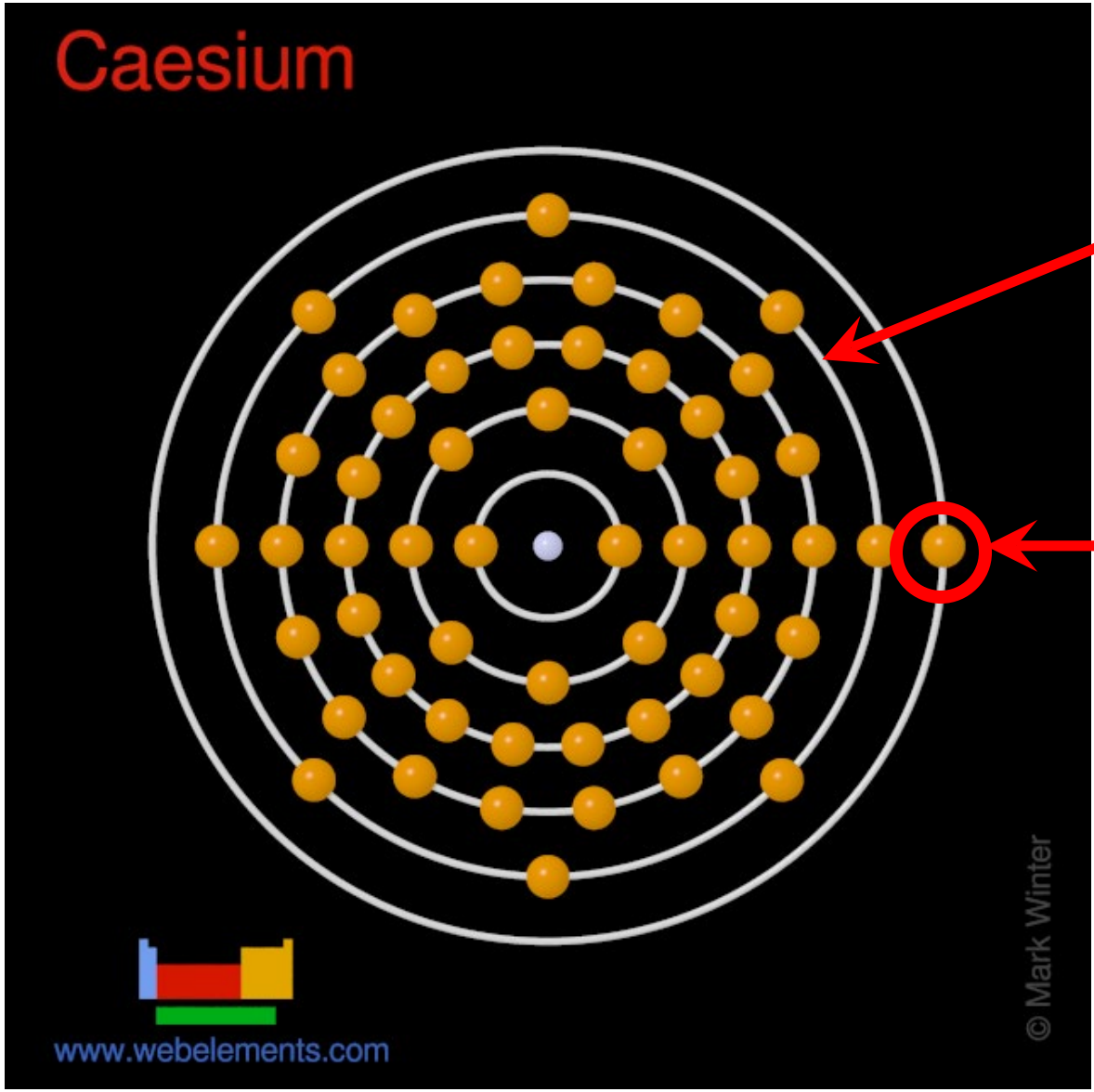
Fe^{10+} Fe^{23+}

Fe^{11+} Fe^{24+}

Fe^{12+} Fe^{25+}

Fe^{13+}

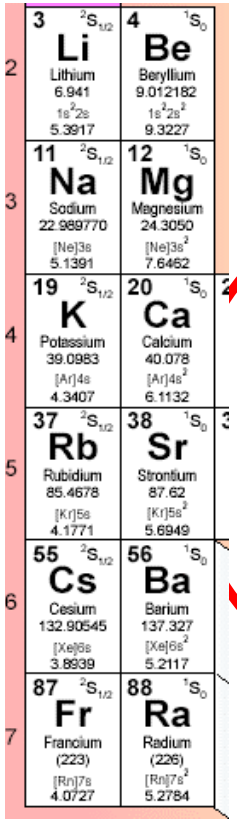
Classify atomic calculations by difficulty level



Closed shells
Can be approximated by a mean field

Single valence electron

Classify atomic calculations by difficulty level



Group 1
Calculations we can do "routinely", with default parameters

1 – 2(3) valence electrons

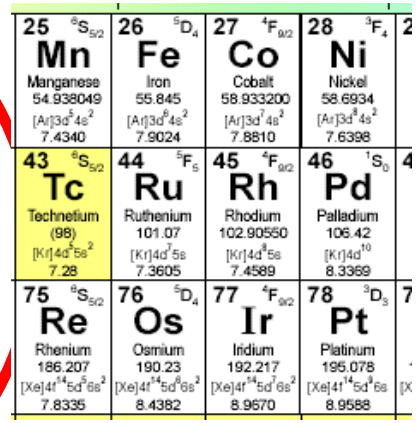
Can automate

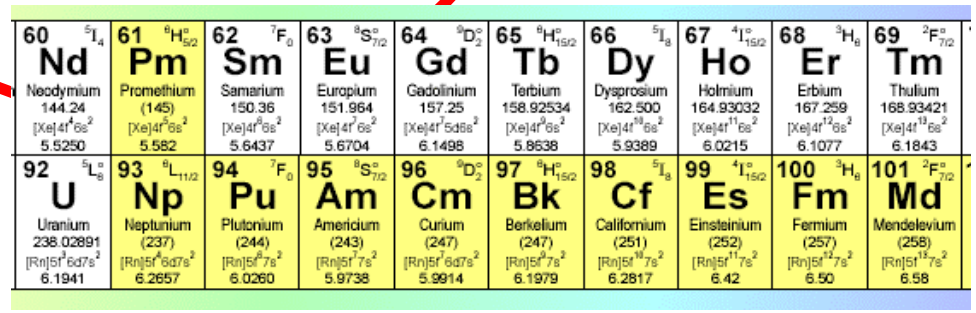
Group 2
Calculations that require expert knowledge

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

Only calculations of wave functions requires expert knowledge

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





Half-filled shells and holes in shells

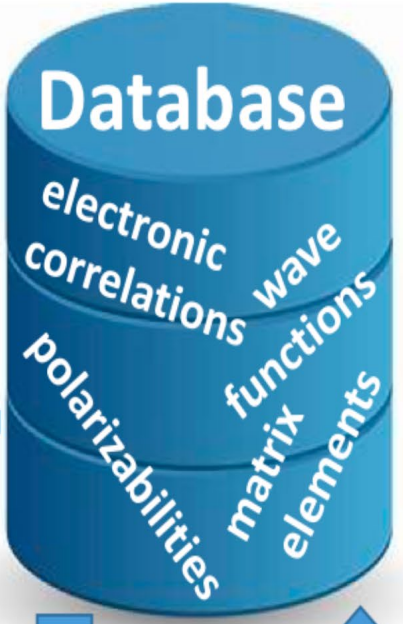
Method development in progress, need new ideas – machine learning

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

High-Precision Atomic Physics Portal



on-demand execution

automatic ingest

Atomic Physics computational codes

Difficulty Groups 1 and 2

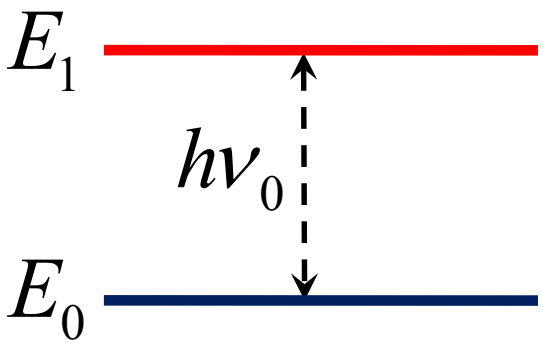
Building on:

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

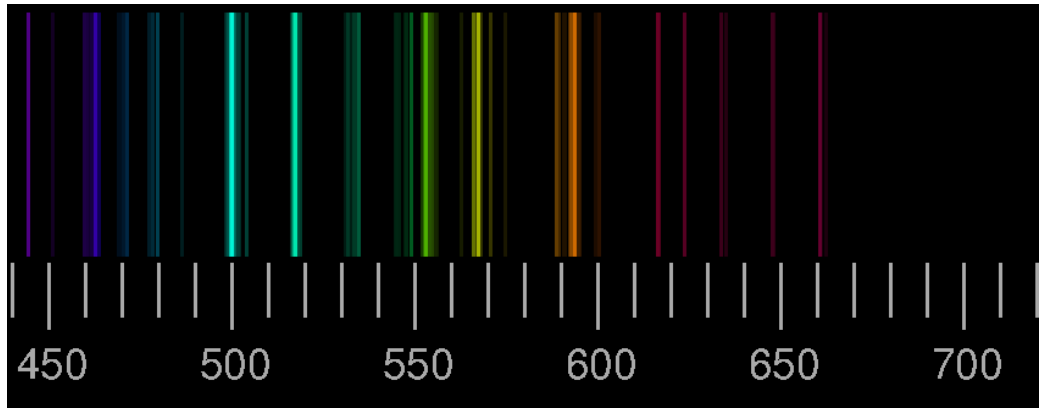
COMPUTER, CALCULATE!

How to serve the most diverse group of users?

Most requested data:
transition matrix elements and polarizabilities

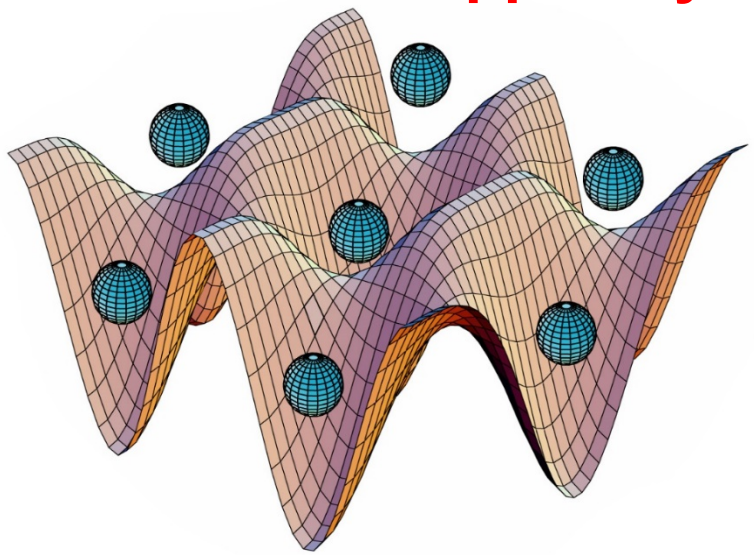


What is transition probability?



What is transition energy?

Atoms are now **trapped by light**



Need electric-dipole polarizability

α to determine how deep the trap will be for specified laser wavelength

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

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.

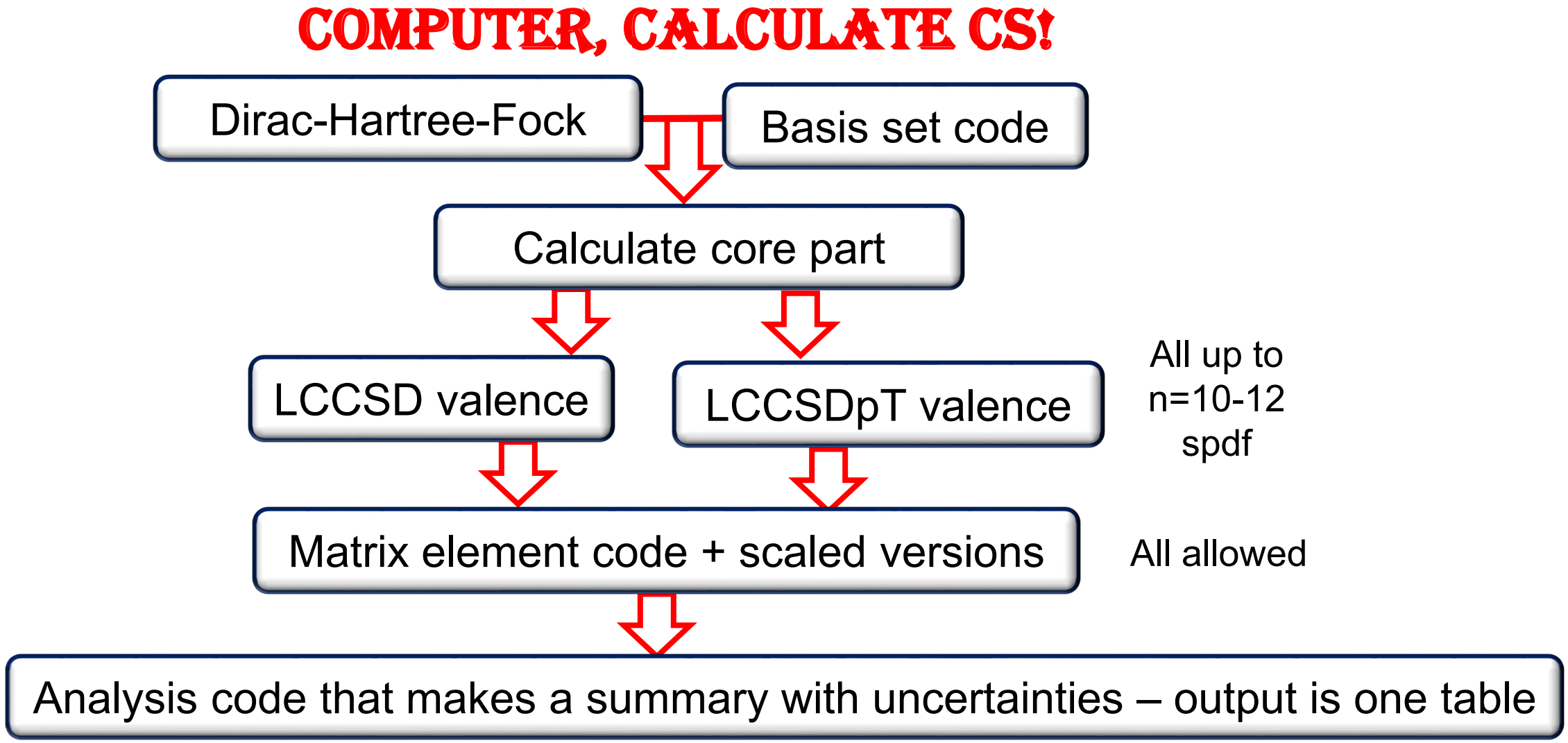
This will require vast computations so the code packages are being completely automated for such data production for Group 1 atoms/ions.

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



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^+	Th^{3+}
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^+	Th^{3+}
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 **$5s^2\ {}^1S_0$**

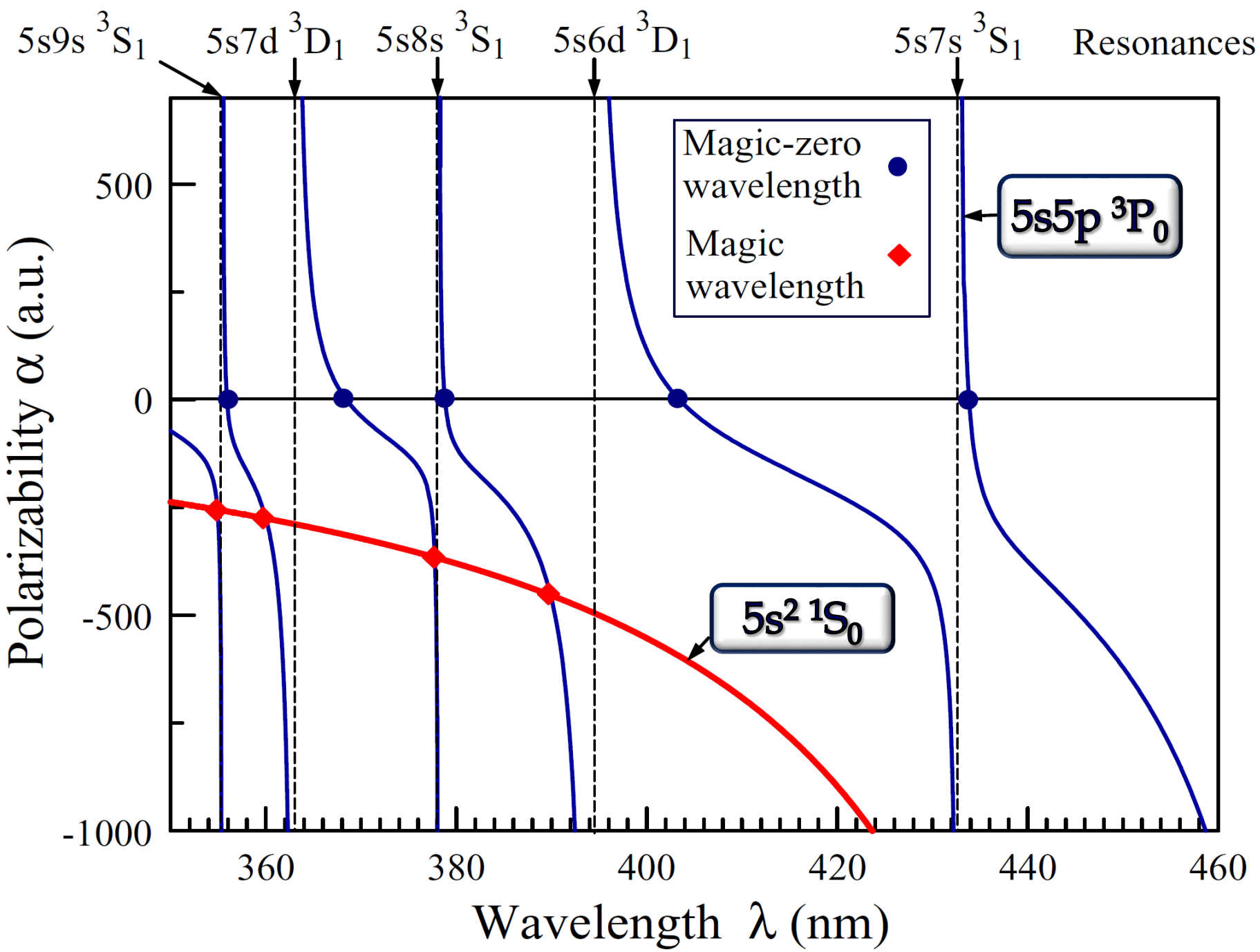
Could also select another state to get a magic wavelength (where two curves cross)

$5s5p\ {}^3P_0$

User will enter wavelength range or select a static option

Static **350 - 460 nm**

Sr


5s9s $^3S_1$
5s7d $^3D_1$
5s8s $^3S_1$
5s6d $^3D_1$
5s7s $^3S_1$
Resonances
Magic-zero wavelength
Magic wavelength
5s5p $^3P_0$
5s^2 $^1S_0$
Polarizability α (a.u.)
500
0
-500
-1000
360
380
400
420
440
460
Wavelength λ (nm)

Summary

Online portal 3-year project started in October 2019

Marianna Safronova Rudolf Eigenmann
Parinaz Barakhshan 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