

Enabling new physics searches with atomic theory and open science



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Problems with the Standard Model

New physics is required to explain observations

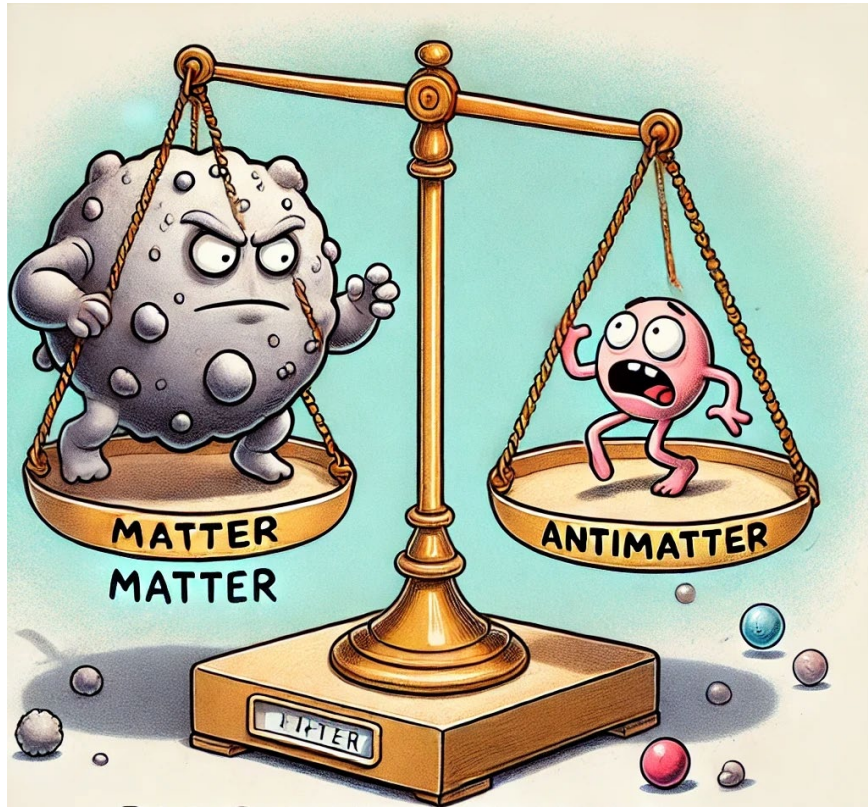
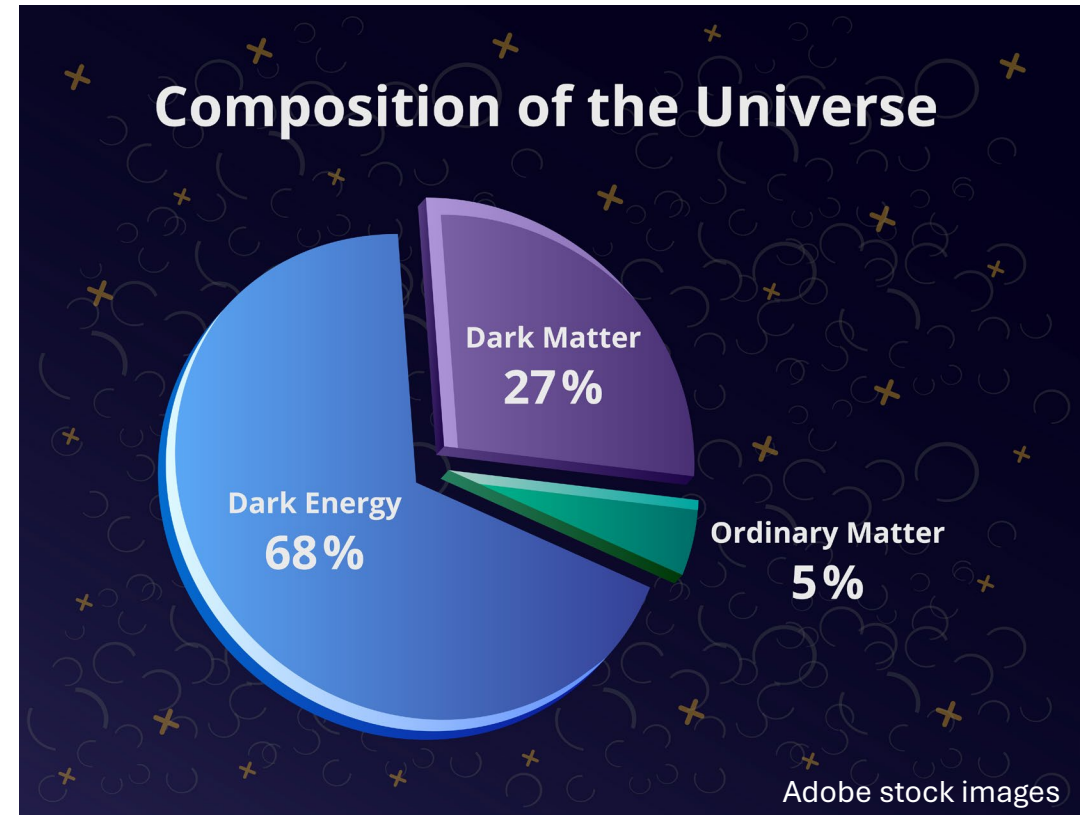


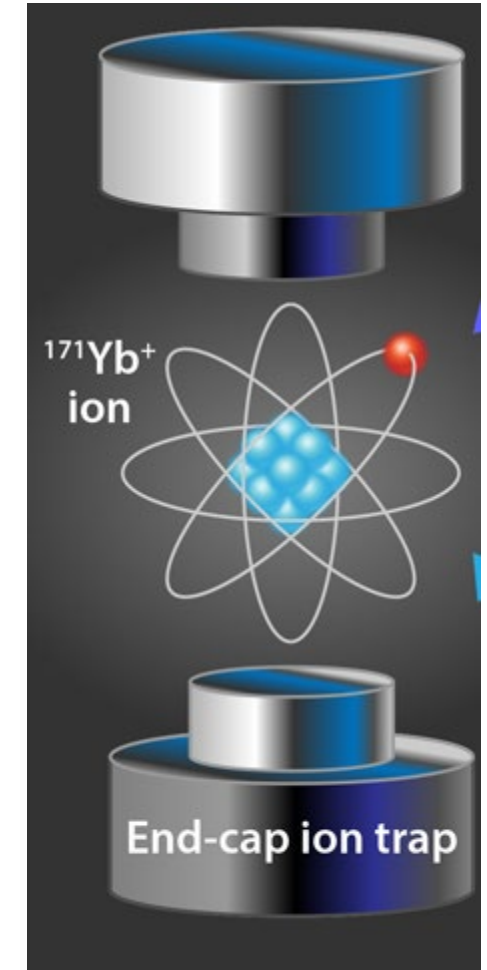
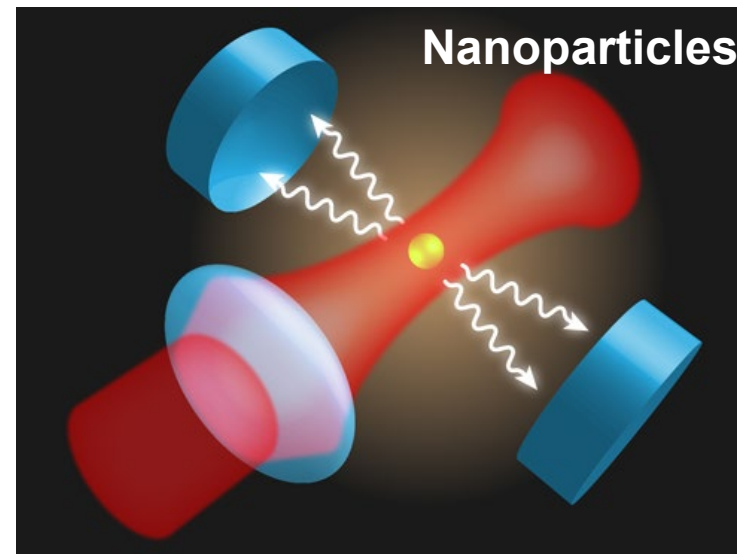
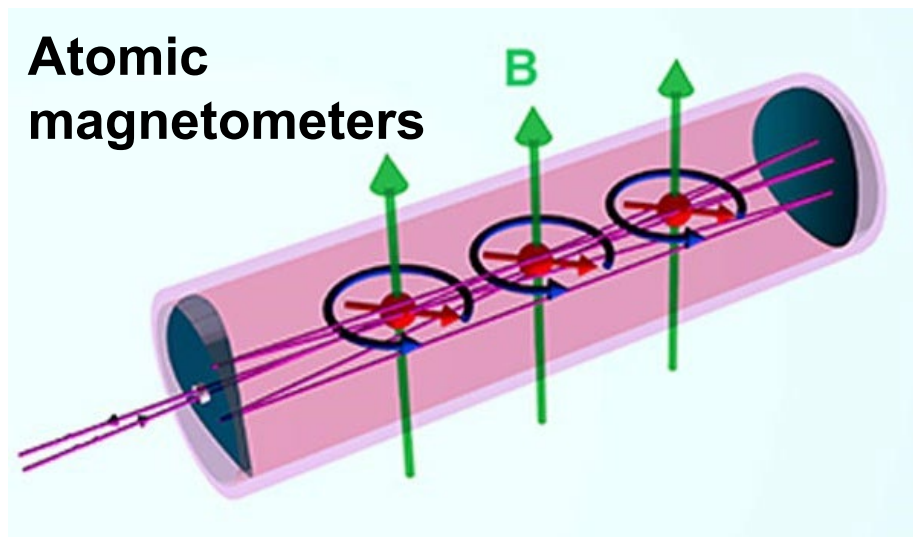
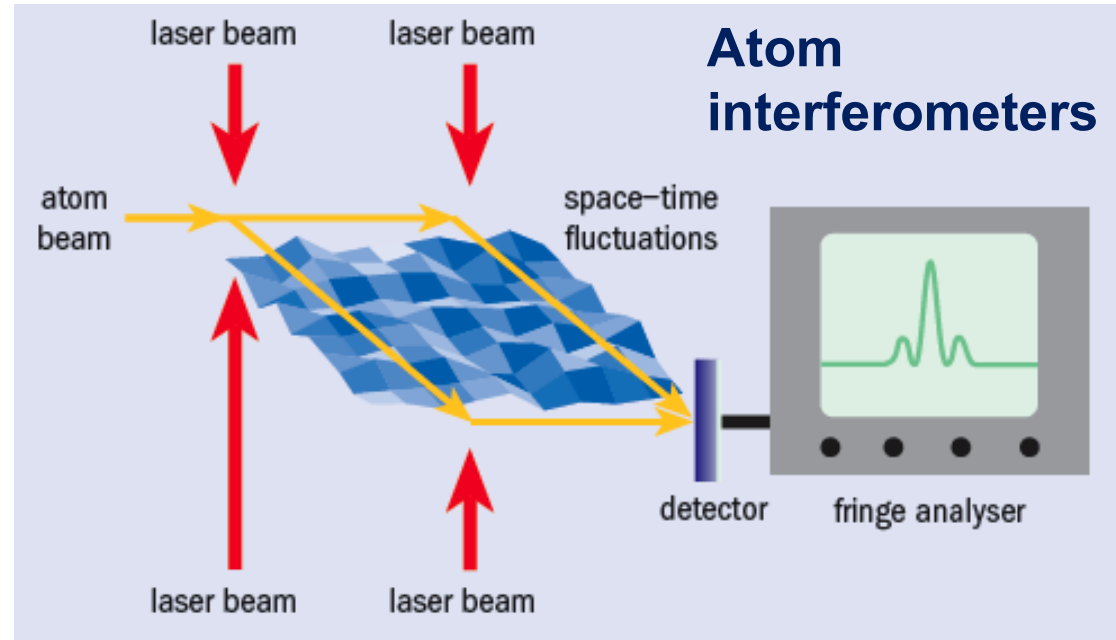
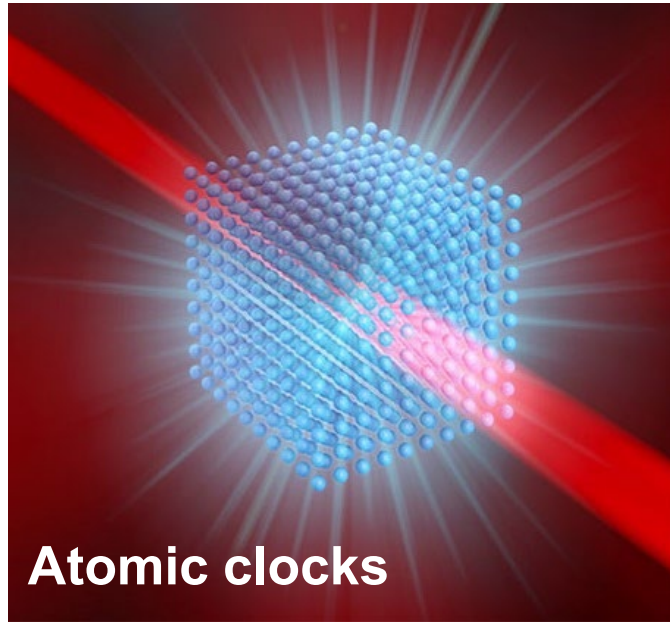
Image generated using OpenAI's DALL-E model

- Dark matter
- Matter-antimatter asymmetry
- Neutrino masses
- Accelerating expansion of the Universe (dark energy/cosmological constant?)



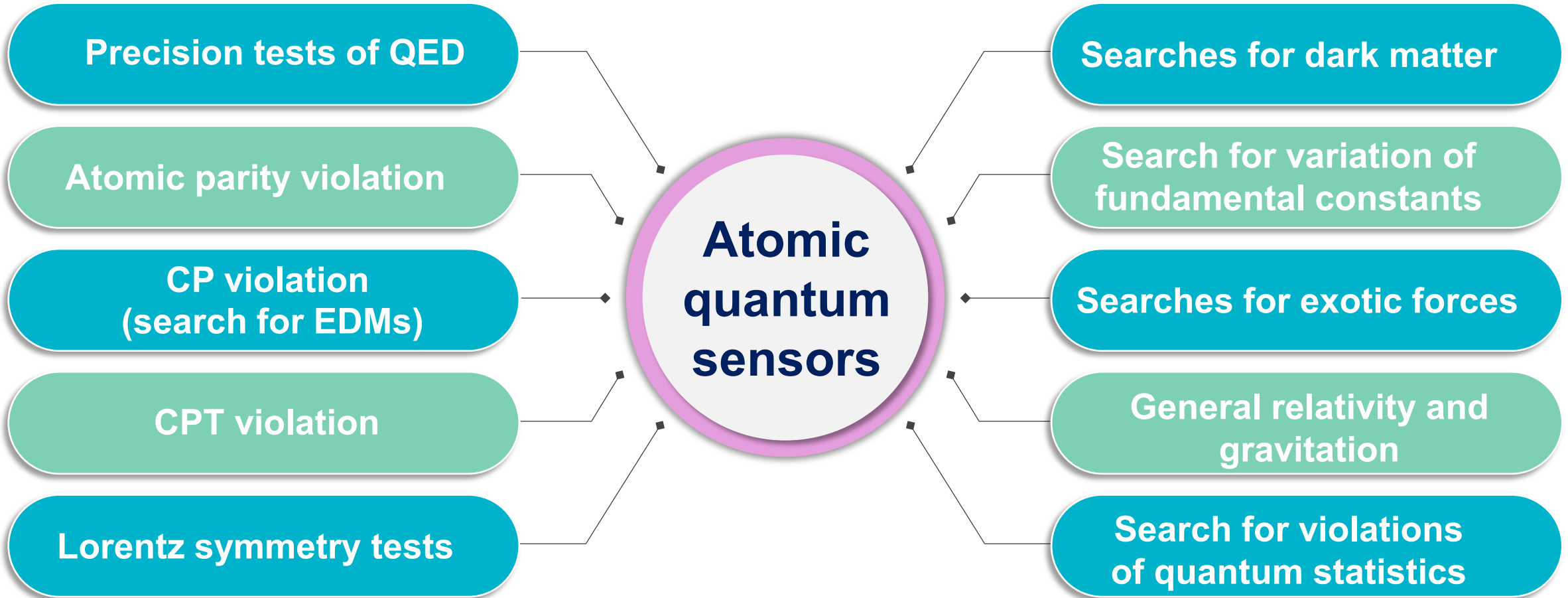
We do not know what the universe is made of

Atomic Quantum Sensors



Very wide scope of AMO new physics searches

AMO: atomic, molecular and optical



Search for new physics with atoms and molecules, M. S. Safronova, D. Budker, D. DeMille, Derek F. Jackson-Kimball, A. Derevianko, and Charles W. Clark, Rev. Mod. Phys. 90, 025008 (2018).

Big Picture Questions in Atomic Theory

1. How to maximize the potential of AMO quantum technologies to discover new physics?
2. How to accurately compute any atomic properties and make them easily available?

Beyond the Standard Model

Three generations of matter
(elementary fermions)

Interactions / force carriers
(elementary bosons)

QUARKS	I	II	III
	u up	d down	s strange
LEPTONS	e electron	μ muon	τ tau
	ν_e electron neutrino	ν_μ muon neutrino	ν_τ tau neutrino
GAUGE BOSONS	Z Z boson	SCALAR BOSON	
	W W boson		

Need to build a computational infrastructure to support the discovery of new physics

PERIODIC TABLE

Atomic Properties of the Elements

NIST
National Institute of Standards and Technology
Technology Administration, U.S. Department of Commerce

18
VIIIA

Group
1

IA

1
¹H_{1.00794}

Hydrogen

1s
13.5984

2
IIA

4
⁴Be_{9.012182}

Beryllium

1s²2s²
9.3227

3
IIIA

3
³Li_{6.941}

Lithium

1s²2s¹
5.3917

4
IIA

12
¹²Mg_{24.3050}

Magnesium

1s²2s²2p⁶
24.3050

11
IIA

11
¹¹Na_{22.989770}

Sodium

1s²2s²2p⁶
24.3050

10
IIA

10
¹⁰Ne_{20.1797}

Neon

1s²2s²2p⁶
21.5645

9
VIIA

9
⁹F_{18.9984032}

Fluorine

1s²2s²2p⁵
17.4228

8
VIA

8
⁸O_{15.9994}

Oxygen

1s²2s²2p⁴
13.6181

7
VA

7
⁷N_{14.0067}

Nitrogen

1s²2s²2p³
14.5341

6
IVA

6
⁶C_{12.0107}

Carbon

1s²2s²2p²
11.2603

5
IIIA

5
⁵B_{10.811}

Boron

1s²2s²2p¹
8.2960

4
IIA

4
⁴Be_{9.012182}

Beryllium

1s²2s²
9.3227

Frequently used fundamental physical constants

For the most accurate values of these and other constants, visit physics.nist.gov/constants
1 second = 9 192 631 770 periods of radiation corresponding to the transition between the two hyperfine levels of the ground state of ¹³³Cs

speed of light in vacuum	<i>c</i>	299 792 458 m s ⁻¹ (exact)
Planck constant	<i>h</i>	6.6261 × 10 ⁻³⁴ J s
elementary charge	<i>e</i>	1.6022 × 10 ⁻¹⁹ C
electron mass	<i>m_e</i>	9.1094 × 10 ⁻³¹ kg
proton mass	<i>m_p</i>	0.5110 MeV
fine-structure constant	<i>α</i>	1/137.036
Rydberg constant	<i>R_∞</i>	10 973 732 m ⁻¹
<i>R_∞c</i>		3.289 842 × 10 ¹⁵ Hz
<i>R_∞hc</i>		13.6057 eV
Boltzmann constant	<i>k</i>	1.3807 × 10 ⁻²³ J K ⁻¹

□ Solids
□ Liquids
□ Gases
□ Artificially Prepared

Physics
Laboratory
physics.nist.gov

Standard Reference
Data Group
www.nist.gov/srd

13 IIIA	14 IVA	15 VA	16 VIA	17 VIIA	18 VIIIA
5 ⁵ B _{10.811} Boron 1s ² 2s ² 2p ¹ 8.2960	6 ⁶ C _{12.0107} Carbon 1s ² 2s ² 2p ² 11.2603	7 ⁷ N _{14.0067} Nitrogen 1s ² 2s ² 2p ³ 14.5341	8 ⁸ O _{15.9994} Oxygen 1s ² 2s ² 2p ⁴ 13.6181	9 ⁹ F _{18.9984032} Fluorine 1s ² 2s ² 2p ⁵ 17.4228	10 ¹⁰ Ne _{20.1797} Neon 1s ² 2s ² 2p ⁶ 21.5645
13 ¹³ Al _{26.981538} Aluminum 1s ² 2s ² 2p ¹ 10.4867	14 ¹⁴ Si _{28.0855} Silicon 1s ² 2s ² 2p ² 10.3600	15 ¹⁵ P _{30.973761} Phosphorus 1s ² 2s ² 2p ³ 12.9676	16 ¹⁶ S _{32.065} Sulfur 1s ² 2s ² 2p ⁴ 12.9676	17 ¹⁷ Cl _{35.453} Chlorine 1s ² 2s ² 2p ⁵ 12.9676	18 ¹⁸ Ar _{39.948} Argon 1s ² 2s ² 2p ⁶ 12.9676
33 ³³ As _{74.9216} Arsenic 1s ² 2s ² 2p ³ 12.9676	34 ³⁴ Se _{78.96} Selenium 1s ² 2s ² 2p ⁴ 12.9676	35 ³⁵ Br _{79.904} Bromine 1s ² 2s ² 2p ⁵ 12.9676	36 ³⁶ Kr _{83.798} Krypton 1s ² 2s ² 2p ⁶ 12.9676	51 ⁵¹ Sb _{121.757} Antimony 1s ² 2s ² 2p ³ 12.9676	52 ⁵² Te _{127.60} Tellurium 1s ² 2s ² 2p ⁴ 12.9676
81 ⁸¹ Tl _{204.3833} Thallium 1s ² 2s ² 2p ¹ 10.4513	82 ⁸² Pb _{207.2} Lead 1s ² 2s ² 2p ² 10.4513	83 ⁸³ Bi _{208.98038} Bismuth 1s ² 2s ² 2p ³ 10.4513	84 ⁸⁴ Po ₍₂₀₉₎ Polonium 1s ² 2s ² 2p ⁴ 10.4513	85 ⁸⁵ At ₍₂₁₀₎ Astatine 1s ² 2s ² 2p ⁵ 10.4513	86 ⁸⁶ Rn ₍₂₂₂₎ Radon 1s ² 2s ² 2p ⁶ 10.4513
114 ¹¹⁴ Uuq Ununquadium (289)	115 ¹¹⁵ Uup Ununpentium (288)	116 ¹¹⁶ Uuh Ununhexium (292)	117 ¹¹⁷ Uus Ununseptium (294)	118 ¹¹⁸ Uuo Ununoctium (294)	119 ¹¹⁹ Uus Ununseptium (294)

Computational infrastructure to discover of new physics

6
⁶Cs_{132.90545}

Cesium

1s²2s²2p⁶
3.8939

56
⁵⁶Ba_{137.327}

Barium

1s²2s²2p⁶
5.2117

87
⁸⁷Fr₍₂₂₃₎

Francium

1s²2s²2p⁶
4.0727

88
⁸⁸Ra₍₂₂₆₎

Radium

1s²2s²2p⁶
5.2784

72
⁷²Hf_{178.49}

Hafnium

1s²2s²2p⁶
6.8251

73
⁷³Ta_{180.9479}

Tantalum

1s²2s²2p⁶
7.5496

74
⁷⁴W_{183.84}

Tungsten

1s²2s²2p⁶
7.8335

75
⁷⁵Re_{186.207}

Rhenium

1s²2s²2p⁶
7.8335

76
⁷⁶Os_{190.23}

Osmium

1s²2s²2p⁶
8.4362

77
⁷⁷Ir_{192.222}

Iridium

1s²2s²2p⁶
8.9670

78
⁷⁸Pt_{195.078}

Platinum

1s²2s²2p⁶
9.2255

79
⁷⁹Au_{196.96655}

Gold

1s²2s²2p⁶
9.2255

80
⁸⁰Hg_{200.59}

Mercury

1s²2s²2p⁶
10.4375

81
⁸¹Tl_{204.3833}

Thallium

1s²2s²2p¹
10.4513

82
⁸²Pb_{207.2}

Lead

1s²2s²2p²
10.4513

83
⁸³Bi_{208.98038}

Bismuth

1s²2s²2p³
10.4513

84
⁸⁴Po₍₂₀₉₎

Polonium

1s²2s²2p⁴
10.4513

85
⁸⁵At₍₂₁₀₎

Astatine

1s²2s²2p⁵
10.4513

86
⁸⁶Rn₍₂₂₂₎

Radon

1s²2s²2p⁶
10.4513

104
¹⁰⁴Rf₍₂₆₁₎

Rutherfordium

1s²2s²2p⁶
6.07

105
¹⁰⁵Db₍₂₆₂₎

Dubnium

1s²2s²2p⁶
6.07

106
¹⁰⁶Sg₍₂₆₆₎

Seaborgium

1s²2s²2p⁶
6.07

107
¹⁰⁷Bh₍₂₆₄₎

Bohrium

1s²2s²2p⁶
6.07

108
¹⁰⁸Hs₍₂₇₇₎

Hassium

1s²2s²2p⁶
6.07

109
¹⁰⁹Mt₍₂₆₈₎

Meitnerium

1s²2s²2p⁶
6.07

110
¹¹⁰Uun₍₂₈₁₎

Ununnilium

1s²2s²2p⁶
6.07

111
¹¹¹Uuu₍₂₇₂₎

Ununtrium

1s²2s²2p⁶
6.07

112
¹¹²Uub₍₂₈₅₎

Ununbium

1s²2s²2p⁶
6.07

113
¹¹³Uut₍₂₈₄₎

Ununtrium

1s²2s²2p⁶
6.07

114
¹¹⁴Uuq₍₂₈₉₎

Ununquadium

1s²2s²2p⁶
6.07

115
¹¹⁵Uup₍₂₈₈₎

Ununpentium

1s²2s²2p⁶
6.07

116
¹¹⁶Uuh₍₂₉₂₎

Ununhexium

1s²2s²2p⁶
6.07

117
¹¹⁷Uus₍₂₉₄₎

Ununseptium

1s²2s²2p⁶
6.07

118
¹¹⁸Uuo₍₂₉₄₎

Ununoctium

1s²2s²2p⁶
6.07

119
¹¹⁹Uus₍₂₉₄₎

Ununseptium

1s²2s²2p⁶
6.07

120
¹²⁰Uuo₍₂₉₄₎

Ununoctium

Building a Computational Infrastructure

Demand

*"We are building X... with Y...
and need Z*..."*

X: atomic clock, quantum simulator,
precision measurement
experiment for new physics
searches

Y: Li, K, Rb, Cs, Ca, Al⁺, Ca⁺, Sr, Sr⁺, Yb,
Yb⁺, Ti⁺, Th⁺, Th³⁺, Ag, Lu⁺, Ti, Cr, Y⁺,
La⁻, Fr, Ra⁺, Pr¹⁰⁺, Ni¹²⁺

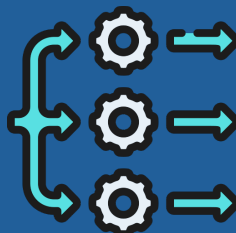
Z: energy levels, transition rates,
branching ratios, lifetimes,
polarizabilities

* Missing data in databases,
conflicting literature values,
data not accurate enough

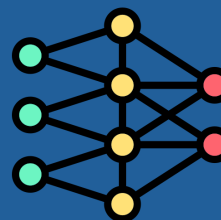
Paradigm Shift

*Moving from codes to automated,
on-demand data generation*

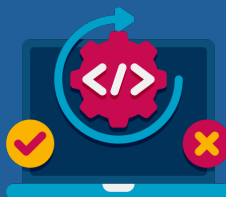
Leverage modern technologies:



parallelization



machine learning



automation



standardized
data formats

Deliverables

*Computational infrastructure to
support discovery*

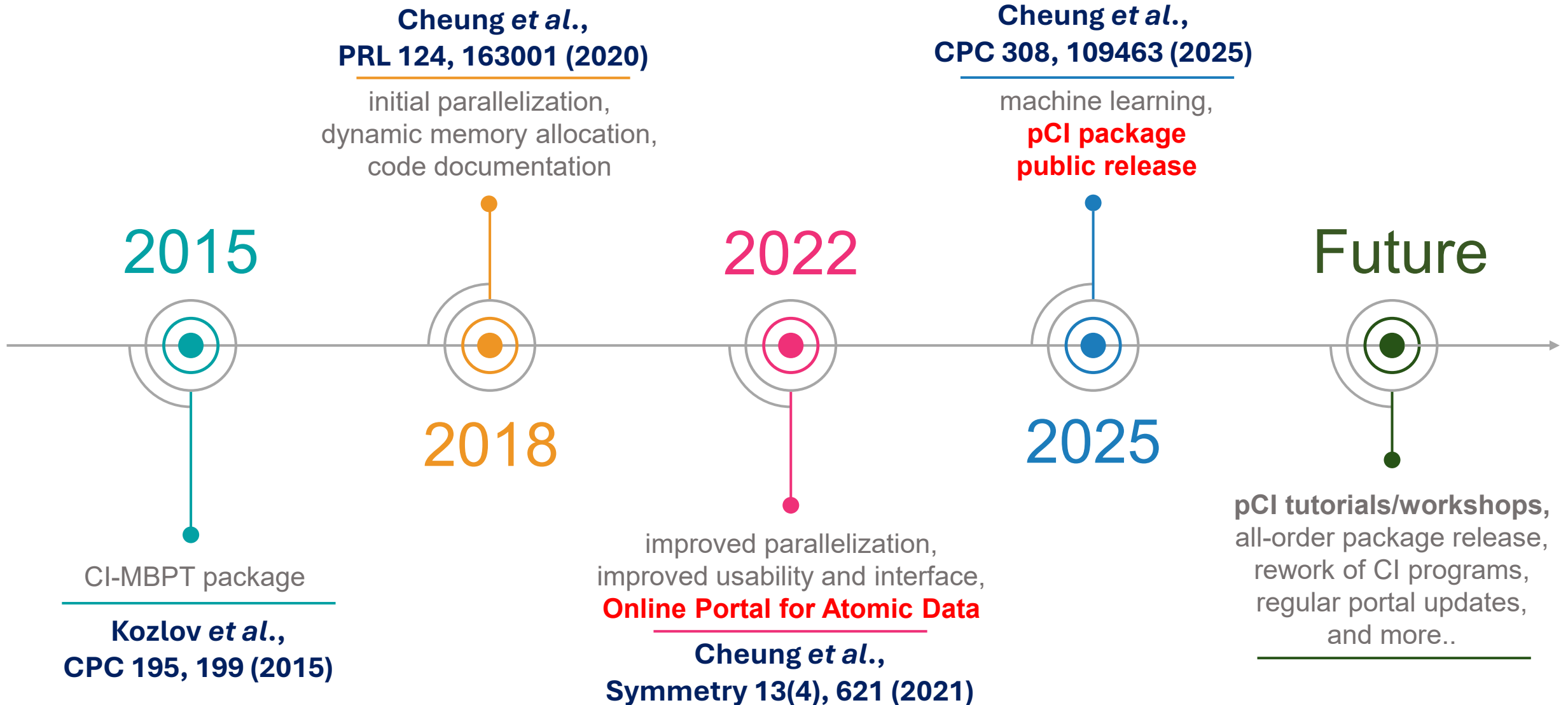
1. Modern high-precision atomic structure code package

- Ability to compute properties of very complex atomic systems required for future experimental designs

2. Portal for High-Precision Atomic Data and Computation

- Online, easy-access atomic data portal
- Focus on scalability and sustainability
- Automatic data generating workflow with accuracy assessments

Code Package Development Timeline

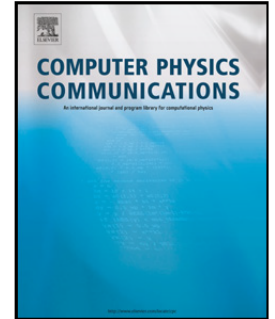




Contents lists available at [ScienceDirect](#)

Computer Physics Communications

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



Computer Programs in Physics

pCI: A parallel configuration interaction software package for high-precision atomic structure calculations ☆

Charles Cheung^{a,*}, Mikhail G. Kozlov^{b,c}, Sergey G. Porsev^a, Marianna S. Safronova^a, Ilya I. Tupitsyn^d, Andrey I. Bondarev^{e,f}

Features:

Designed for use on HPC platforms (scalable to many nodes/cores via MPI)

Python helper scripts to automate workflows

Methods: Pure CI, CI+MBPT, CI+all-order, CI+PT, +RPA, +QED, +ML

Observables: energies, g-factors, multipole transition data,

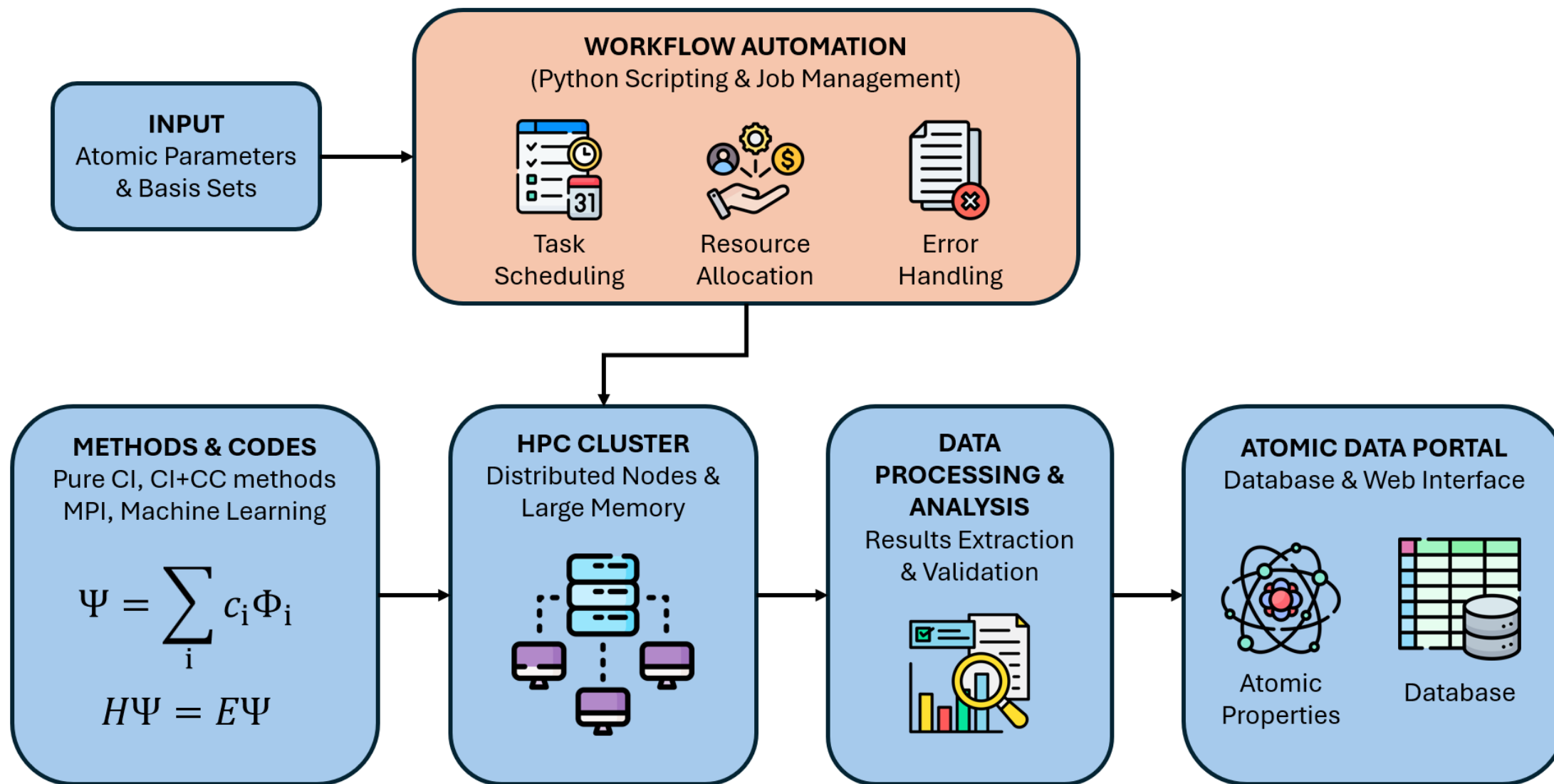
A and B hyperfine constants, polarizabilities, and more..!

Available on GitHub: <https://github.com/ud-pci/pCI>

Read the Docs: <https://pci.readthedocs.io/en/latest/>



Building a Computational Infrastructure





Portal for High-Precision Atomic Data and Computation

Sr

[Close](#)

Matrix elements

Transition rates

Polarizabilities

Energies

Hyperfine constants

Nuclear data

Click on an element to display its properties

Li

Be⁺

Na

Mg

Mg⁺

K

Ca

Ca⁺

Rb

Sr

Sr⁺

Cs

Ba⁺

Fr

Ra⁺

Cs⁶⁺

Ba⁷⁺

Ce⁹⁺

Pr¹⁰⁺

Nd¹¹⁺

Nd¹²⁺

Nd¹³⁺

Sm¹³⁺

Sm¹⁴⁺

Sm¹⁵⁺

Eu¹⁴⁺

Cf¹⁵⁺

Cf¹⁷⁺

udel.edu/atom

**Portal provides
recommended data:**

high-precision
experimental
values with
reference

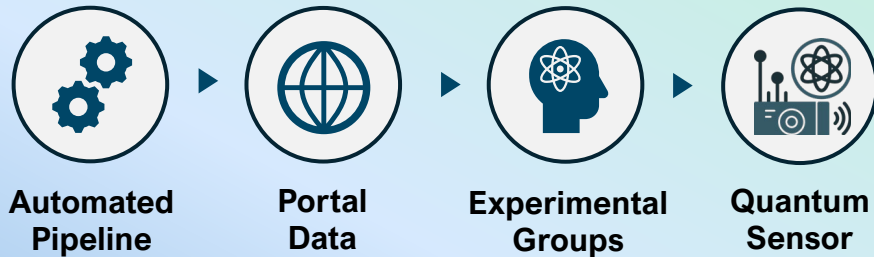
theory
> values with
uncertainties



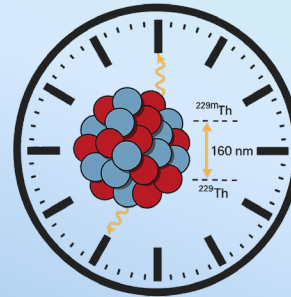
Portal for High-Precision Atomic Data and Computation

From Data to Quantum Sensors

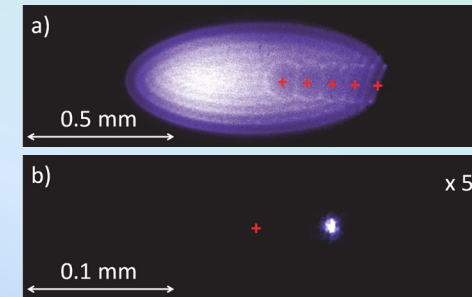
FROM DATA TO QUANTUM SENSORS



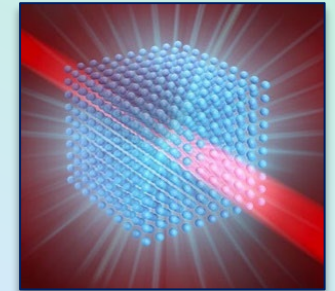
BSM SEARCHES WITH CLOCKS



Nuclear clocks

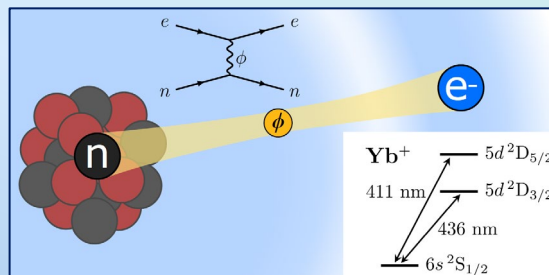


Highly charged ion clocks

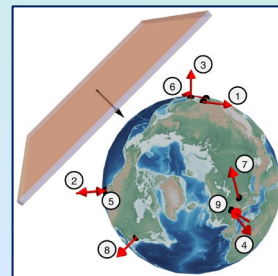


3D lattice clocks

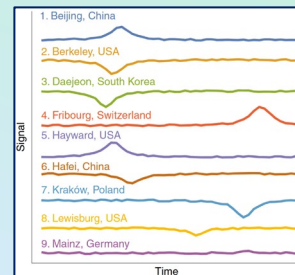
DARK MATTER SEARCHES



Fifth force searches with precision spectroscopy with atoms and ions



GNOME: global network of optical magnetometers for exotic physics searches



GLOBAL REACH & IMPACT



Data from Google Analytics

UD team and collaborators

Online portal team



**Prof. Rudolf
Eigenmann**
UD (EECS)



**Prof. Bindiya
Arora**
Guru Nanak Dev
U., India



**Miguel
Sanchez**
UD (ECE)



**Prof.
Marianna
Safronova**



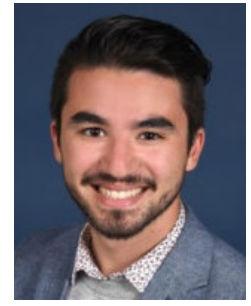
**Sergey
Porsev**
Research
Associate III



**Dmytro
Filin**
Research
Associate III



**Charles
Cheung**
Scientist



**Jason
Arakawa**
Postdoc

Collaborators:

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Andrey Bondarev (Helmholtz Institute Jena, Germany)

ERC Synergy: Thorsten Schumm, TU Wein Ekkehard Peik, PTB, Peter Thierolf, LMU,
Adriana Pálffy (FAU); Q-SEnSE: Jun Ye, Dave Leibrandt, Leo Hollberg, Nate Newbury, Vladan Vuletic

Particle physics: Josh Eby (IPMU, Tokyo), Volodymyr Takhistov (QUP, Tokyo), Gilad Perez' group
(Weizmann Institute of Science, Israel), Yu-Dai Tsai (UC Irvine)

Dmitry Budker, Mainz and UC Berkeley, Andrew Jayich, UCSB, Murray Barrett, CQT, Singapore,
José Crespo López-Urrutia, MPIK, Heidelberg, Piet Schmidt, PTB, University of Hannover,
Nan Yu (JPL), Charles Clark, JQI, and many others!