Q-EYES 2025

Dec 9, 2025

# Enabling new physics searches with atomic theory and open science

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Q-SEnSE
An NSF Quantum Leap Challenge Institute

thorium nuclear clock

NSF

Office of Naval Research Science & Technology

European Research Council

# Problems with the Standard Model

## New physics is required to explain observations

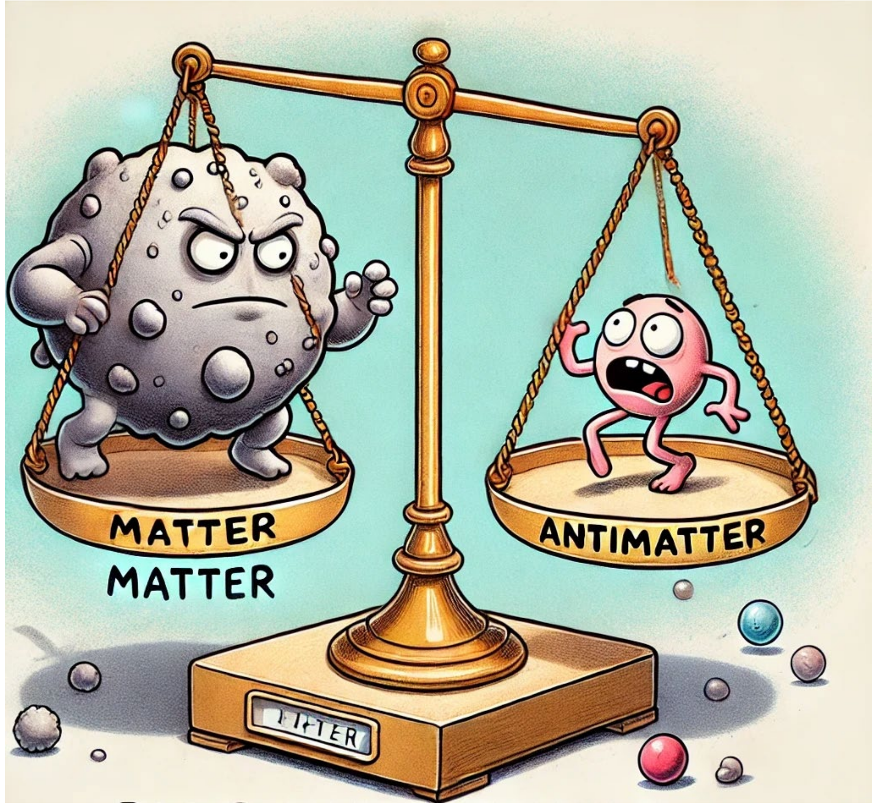
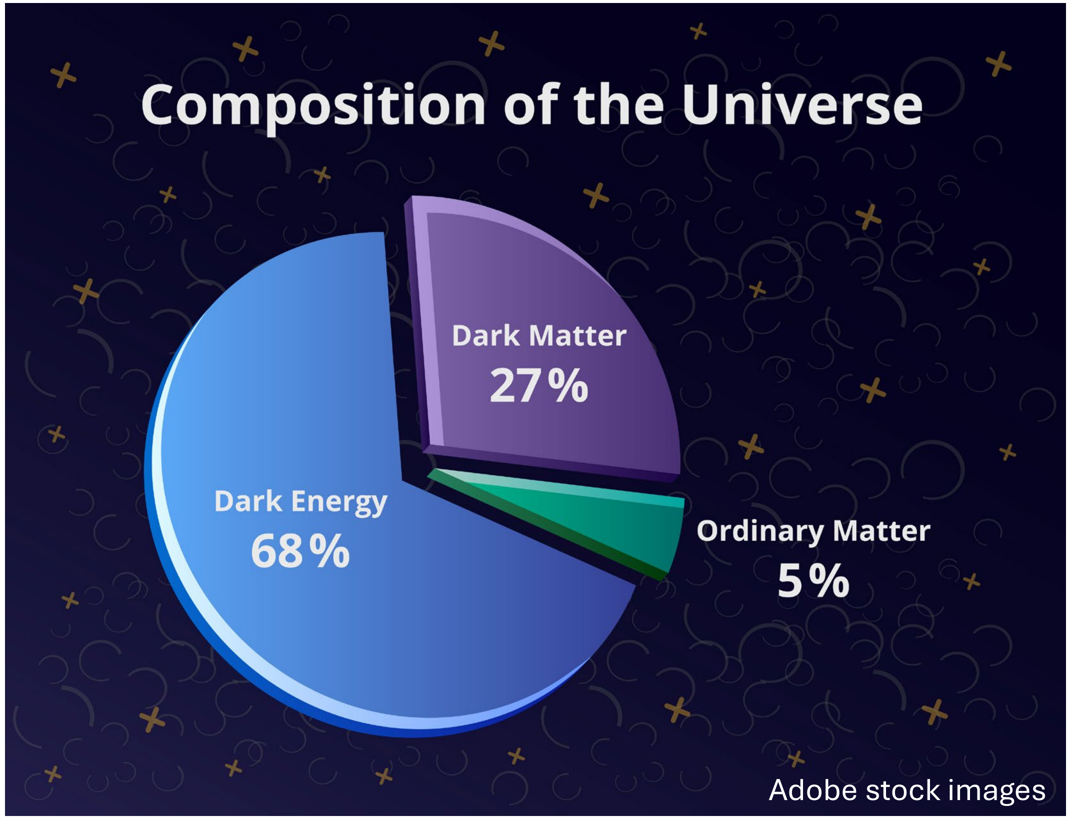


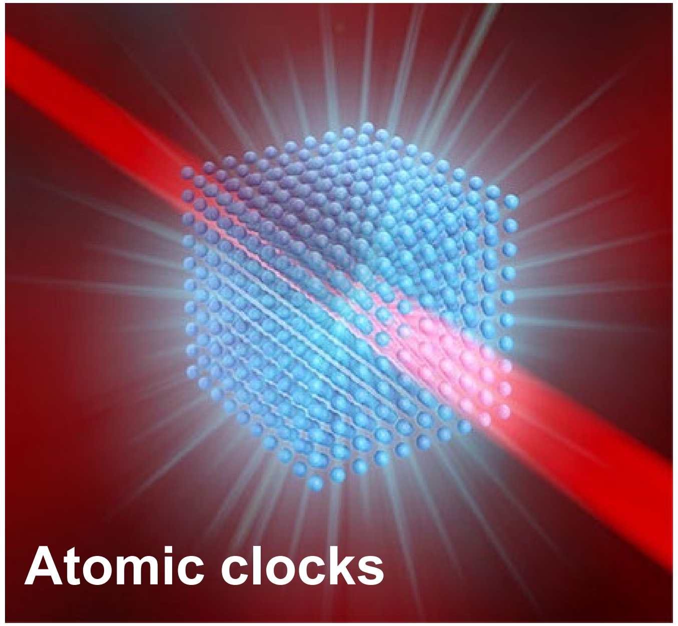

Image generated using OpenAI's DALL·E model

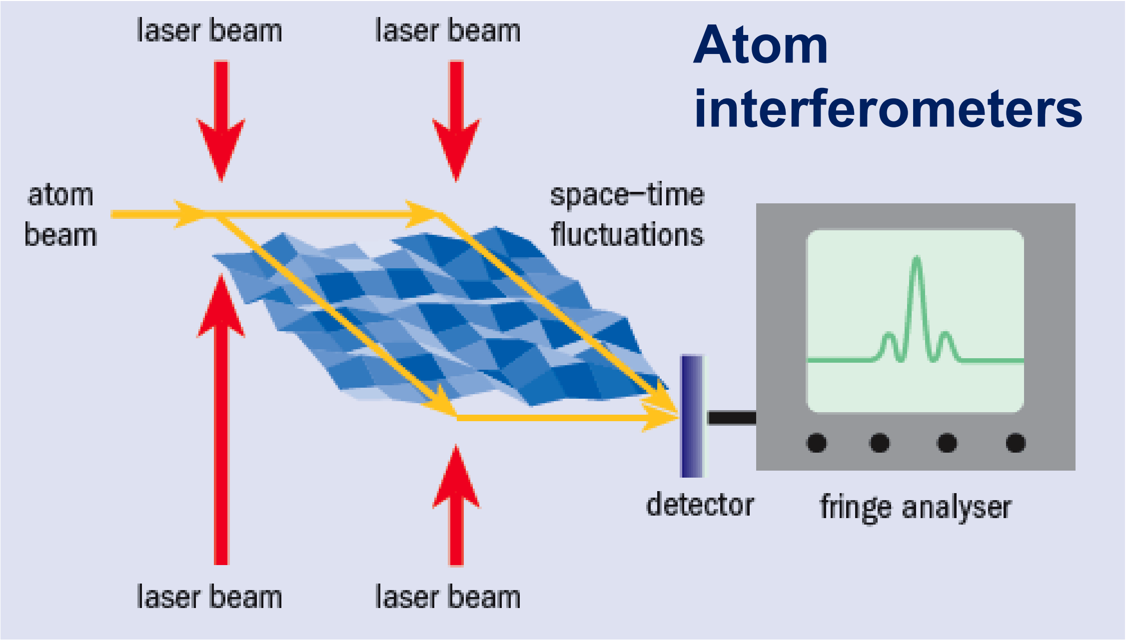


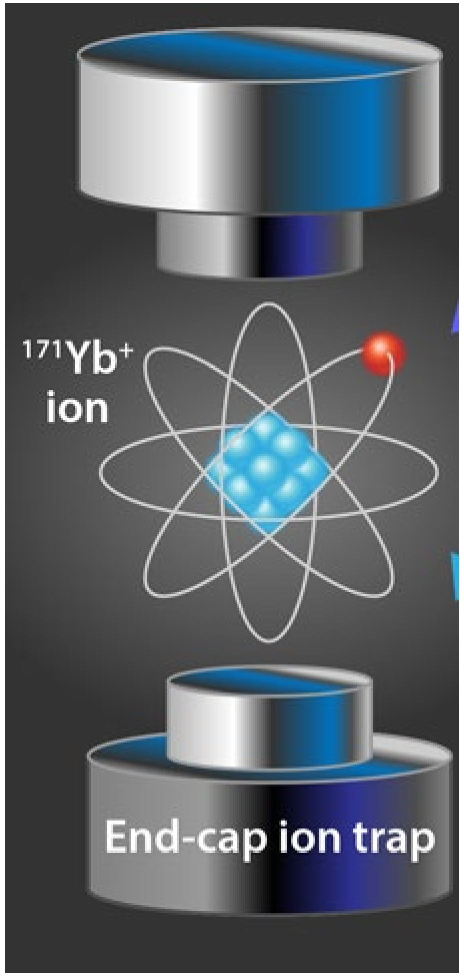

**We do not know what the universe is made of**

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

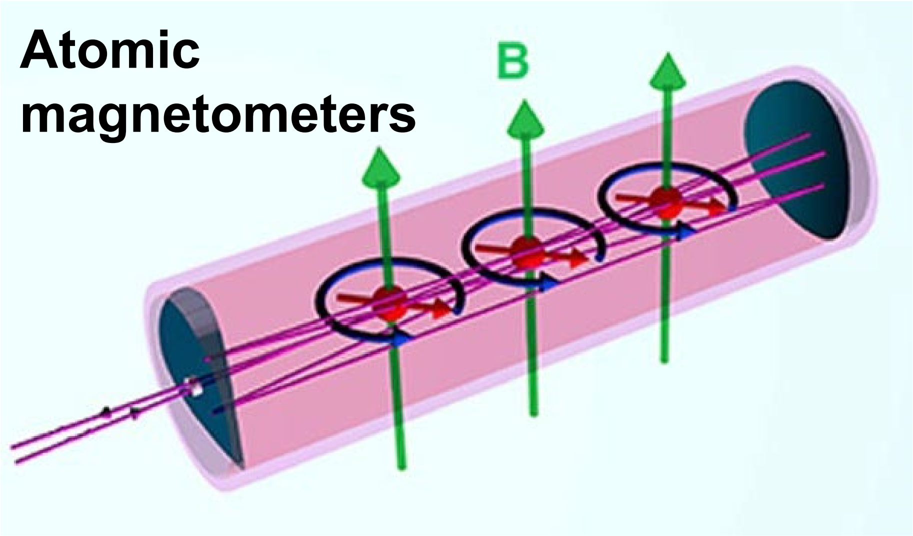
# Atomic Quantum Sensors




Trapped ions



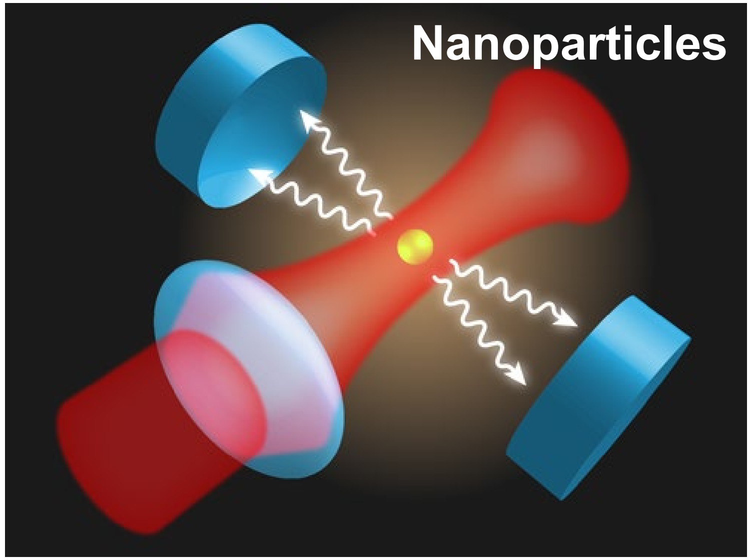
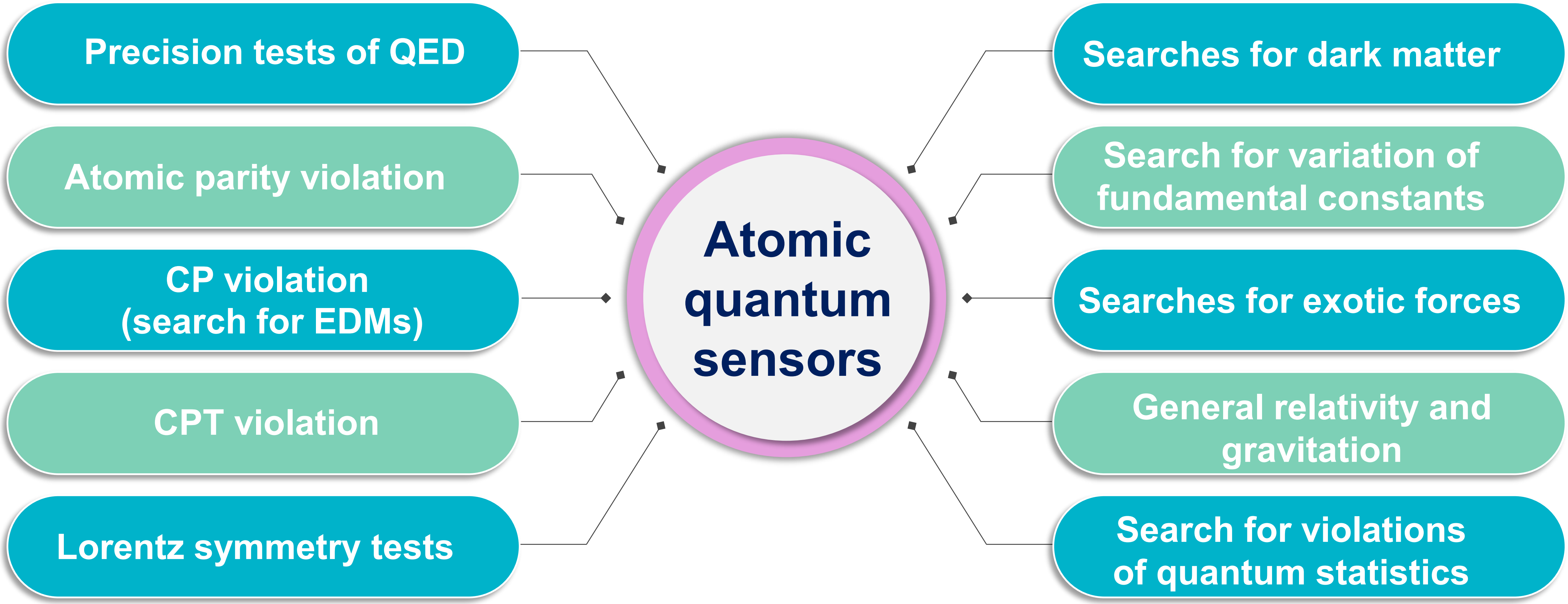




Image credit: JILA, APS/Alan Stonebraker, https://cerncourier.com/a/can-experiment-access-planck-scale-physics/, http://physicsworld.com/cws/article/news/2013/apr/24

# Very wide scope of AMO new physics searches

**AMO: atomic, molecular and optical**

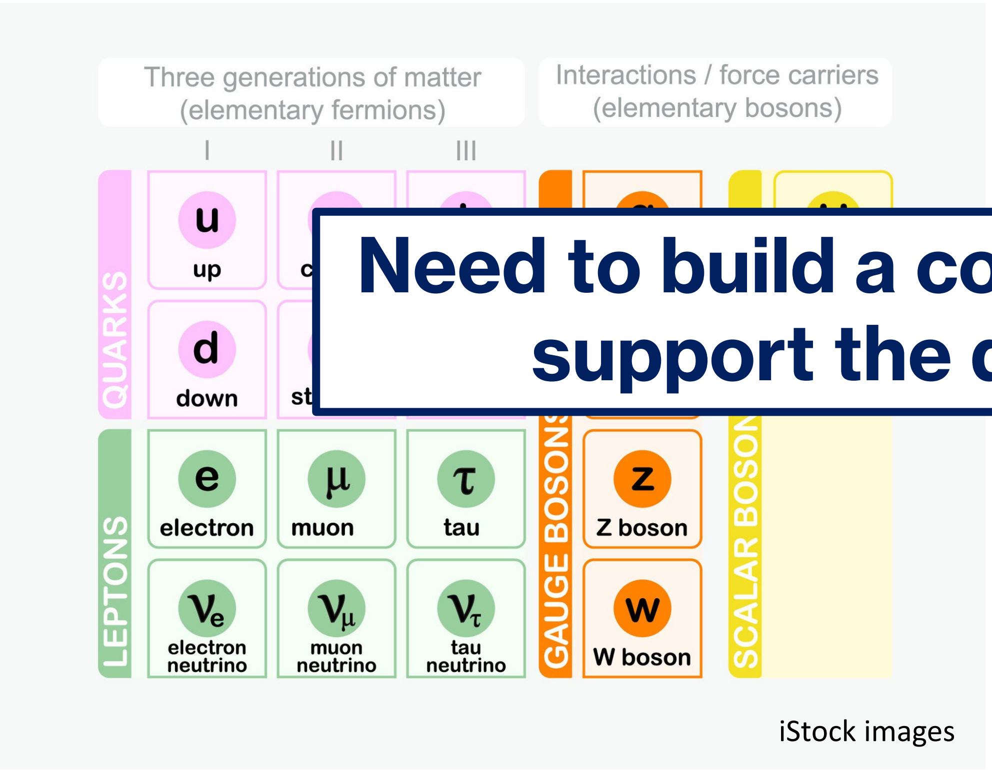



Search for new physics with atoms and molecules, M. S. Safronova, D. Budker, D. DeMille, Derek F. Jackson-Kimball, A. Derevianko, and Charles W. Clark, Rev. Mod. Phys. 90, 025008 (2018).

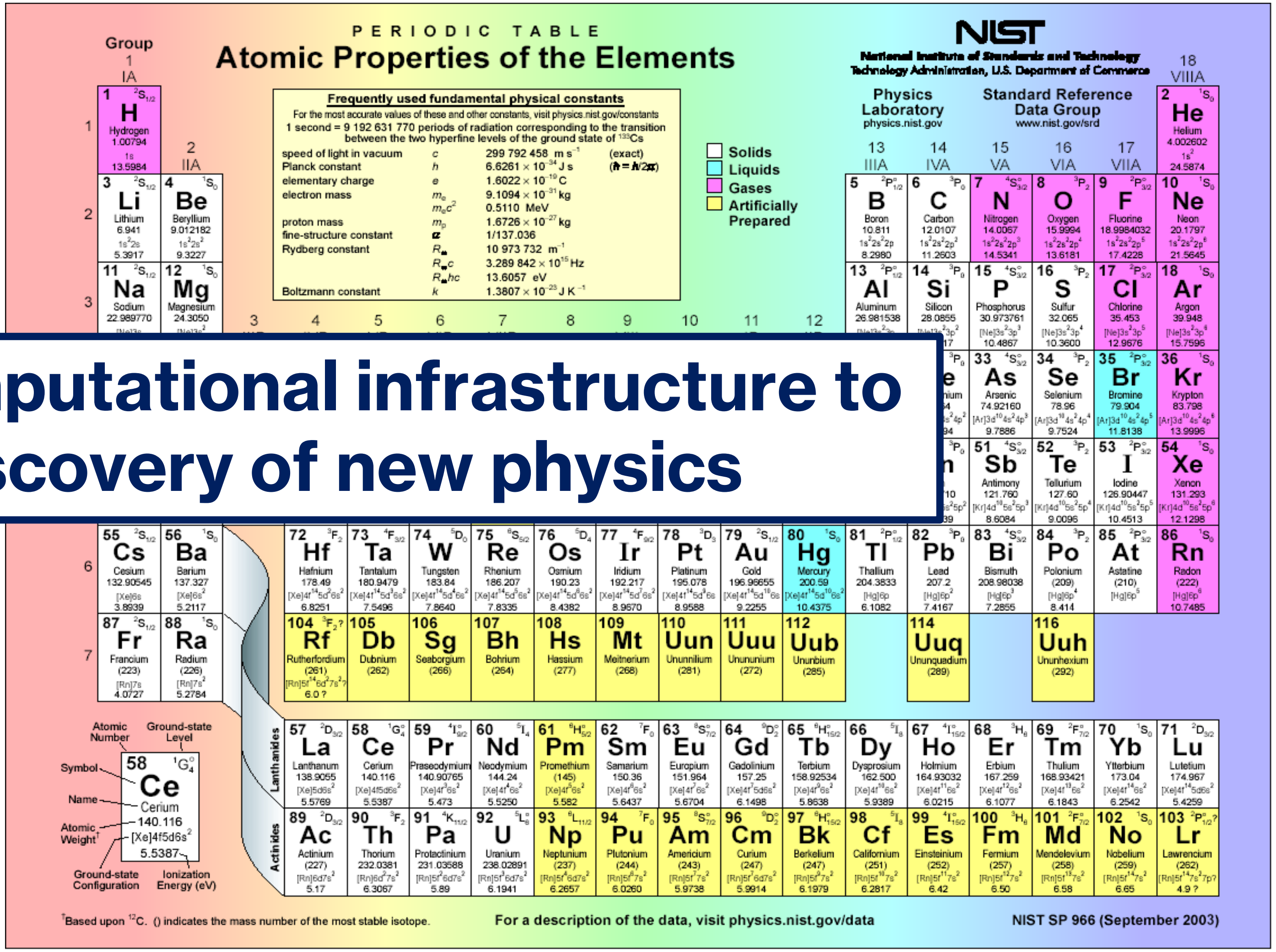
# Big Picture Questions in Atomic Theory

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




iStock images




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

# 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, $Yb^+$, $Ti^+$, $Th^+$, $Th^{3+}$, Ag, $Lu^+$, Ti, Cr, Y+, $La^-$, Fr, $Ra^+$, $Pr^{10+}$, $Ni^{12+}$

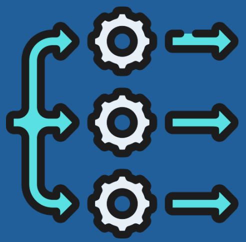
*Z*: energy levels, transition rates, branching ratios, lifetimes, polarizabilities

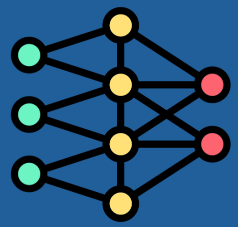
* Missing data in databases, conflicting literature values, data not accurate enough

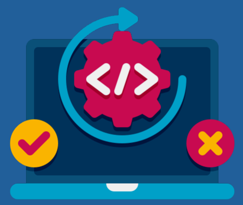
## Paradigm Shift

*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**

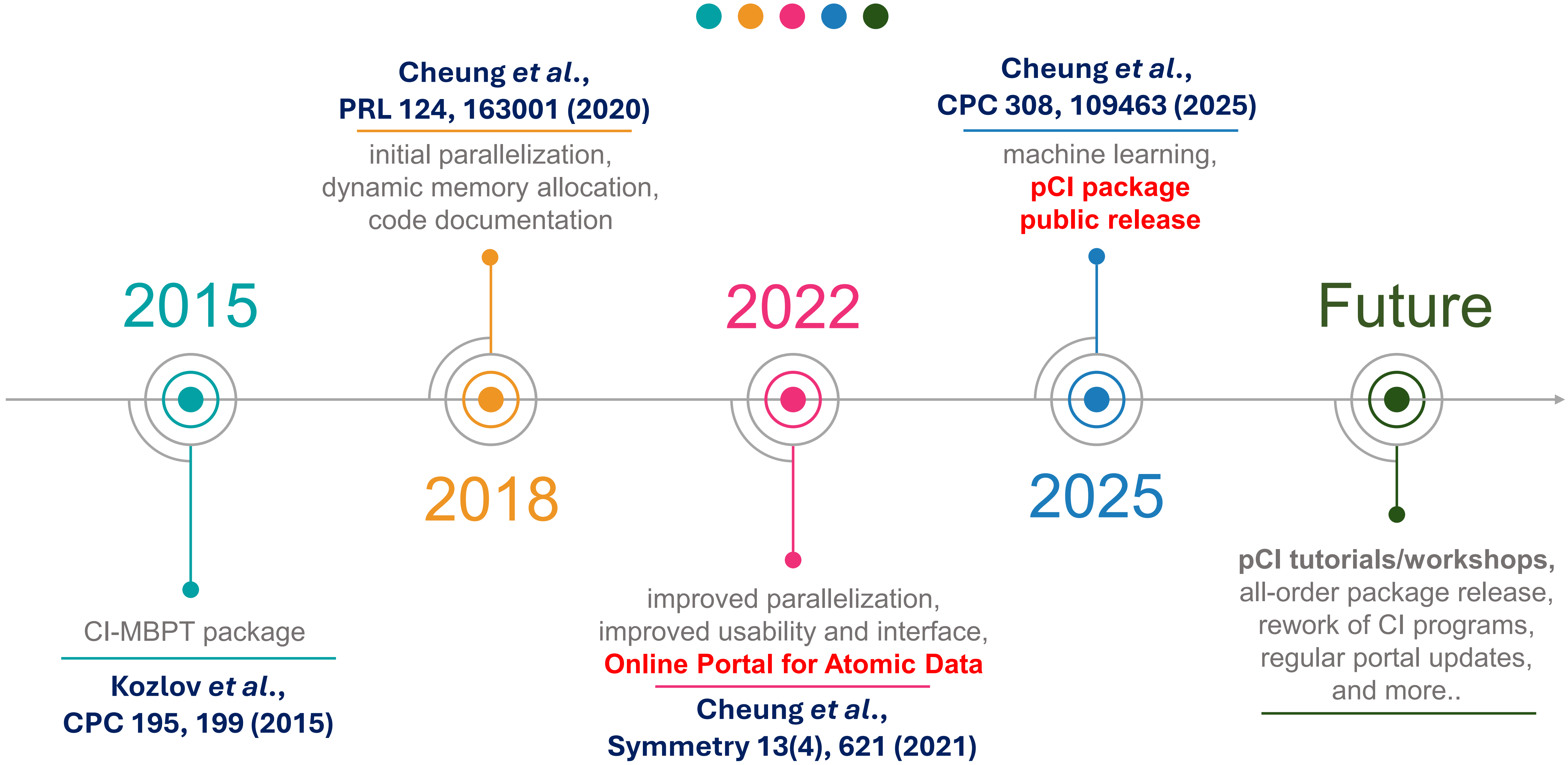
- Ability to compute properties of very complex atomic systems required for future experimental designs

**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

flaticon.com

# Code Package Development Timeline

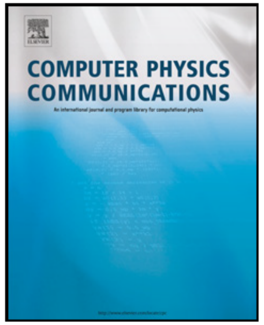


Computer Physics Communications 308 (2025) 109463

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

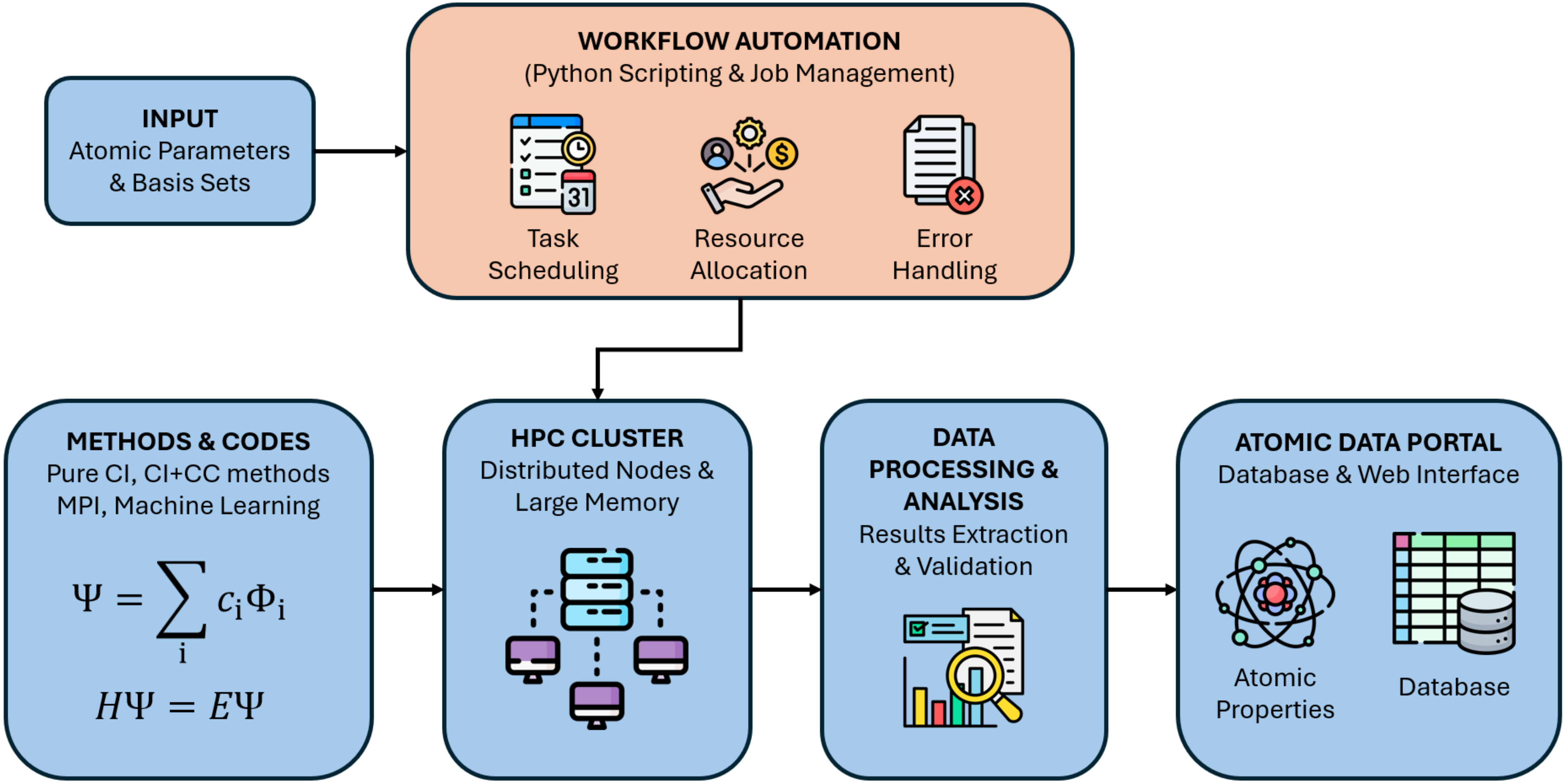
**Methods:** Pure CI, CI+MBPT, CI+all-order, CI+PT, +RPA, +QED, +ML

**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

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University of Delaware

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# 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 | $Ra^{+}$ |

| | | |
|---|---|---|
| $Cs^{6+}$ | $Ba^{7+}$ | $Ce^{9+}$ |
| $Pr^{10+}$ | $Nd^{11+}$ | $Nd^{12+}$ |
| $Nd^{13+}$ | $Sm^{13+}$ | $Sm^{14+}$ |
| $Sm^{15+}$ | $Eu^{14+}$ | $Cf^{15+}$ |
| $Cf^{17+}$ | | |

**udel.edu/atom**

**Portal provides recommended data:**

high-precision **experimental** values with reference > **theory** values with uncertainties

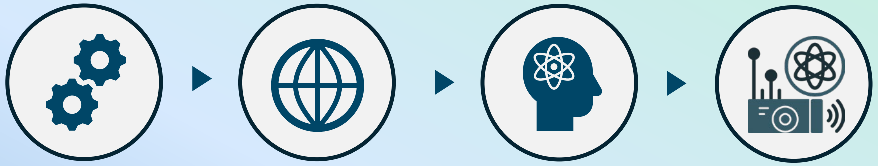
This project was supported by NSF Awards No. OAC-1931339 and OAC-2209639

**Portal:** Comput. Phys. Commun. **319**, 109951 (2026)

# Portal for High-Precision Atomic Data and Computation

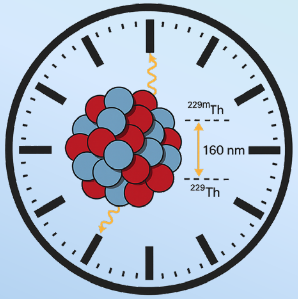
## From Data to Quantum Sensors

### FROM DATA TO QUANTUM SENSORS

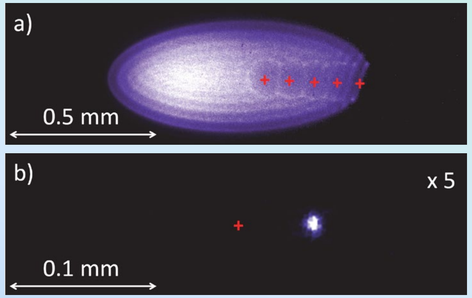


Automated Pipeline → Portal Data → Experimental Groups → Quantum Sensor

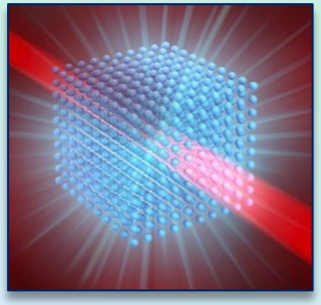
### BSM SEARCHES WITH CLOCKS




Nuclear clocks

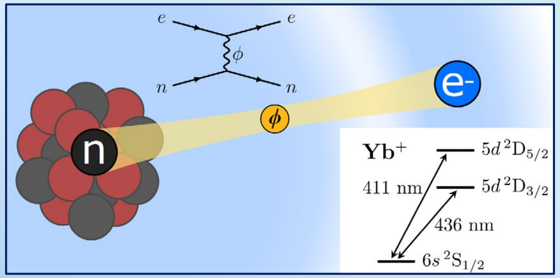



Highly charged ion clocks

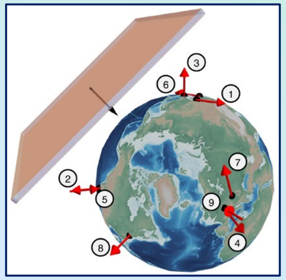


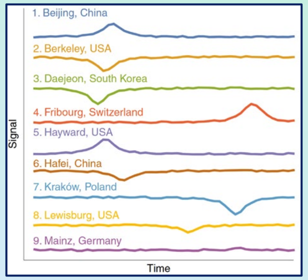
3D lattice clocks

### 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

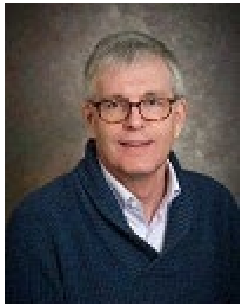
**100K+** page views

**7000+** users from 95 countries

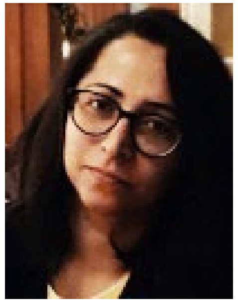
Data from Google Analytics

# UD team and collaborators

**Online portal team**



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



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**Sergey Porsev**
Research Associate III

**Dmytro Filin**
Research Associate III

**Charles Cheung**
Scientist

**Jason Arakawa**
Postdoc

## Collaborators:

**Code development: Mikhail Kozlov (PNPI, LETI), Ilya Tupitsyn (St. Petersburg University), Andrey Bondarev (Helmholtz Institute Jena, Germany)**

ERC Synergy: Thorsten Schumm, TU Wein Ekkehard Peik, PTB, Peter Thirolf, 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!