

Electric Dipole Moments 2026, Les Houches, March 2

Ultracold molecules: Fundamental Physics, Machine Learning, and the Need for Data



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<https://thoriumclock.eu/>

<https://www.colorado.edu/research/qsense/>



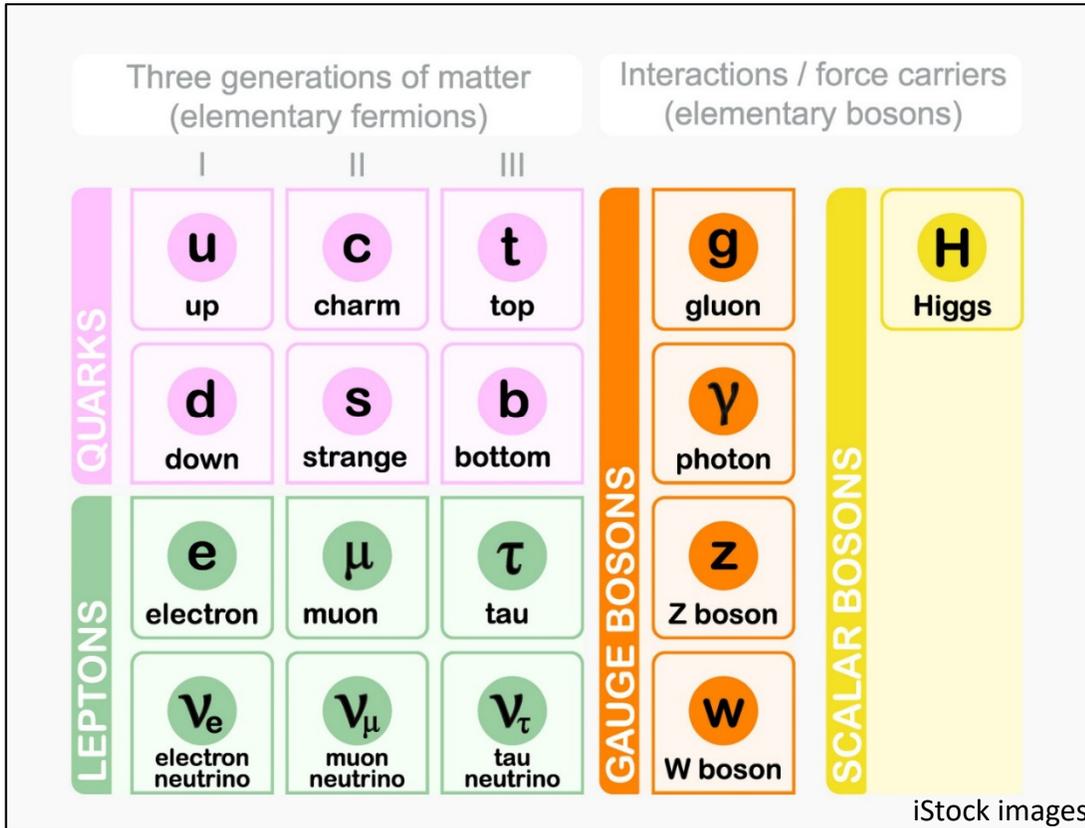
European Research Council

Asking big - picture questions in atomic theory

How to maximize the potential of atomic quantum technologies to discover new physics?

How to accurately compute any atomic properties and make them easily available?

Beyond the Standard Model



PERIODIC TABLE
Atomic Properties of the Elements

NIST National Institute of Standards and Technology
U.S. Department of Commerce
Physical Measurement Laboratory www.nist.gov/pml
Standard Reference Data www.nist.gov/srd

FREQUENTLY USED FUNDAMENTAL PHYSICAL CONSTANTS¹

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 c 299 792 458 m s⁻¹ (exact)

Planck constant h 6.626 070 15 × 10⁻³⁴ J Hz⁻¹ (exact)

elementary charge e 1.602 176 634 × 10⁻¹⁹ C (exact)

Avogadro constant N_A 6.022 140 76 × 10²³ mol⁻¹ (exact)

Boltzmann constant k_B 1.380 649 × 10⁻²³ J K⁻¹ (exact)

electron volt eV 1.602 176 634 × 10⁻¹⁹ J (exact)

electron mass m_e 9.109 383 70 × 10⁻³¹ kg (exact)

energy equivalent $m_e c^2$ 0.510 998 950 MeV² (exact)

proton mass m_p 1.672 621 924 × 10⁻²⁷ kg (exact)

energy equivalent $m_p c^2$ 938.272 088 MeV (exact)

fine-structure constant α 1/137.035 999 (exact)

Rydberg energy R_∞ 13.605 693 1230 eV (exact)

Newtonian constant of gravitation G 6.674 × 10⁻¹¹ m³ kg⁻¹ s⁻²

¹For the most accurate values of these and other constants, visit pml.nist.gov/constants.

Legend: Solids (white), Liquids (light blue), Gases (light green), Artificially Prepared (light purple)

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36
37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54
55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72
73	74	75	76	77	78	79	80	81	82	83	84	85	86	87	88	89	90
91	92	93	94	95	96	97	98	99	100	101	102	103	104	105	106	107	108
109	110	111	112	113	114	115	116	117	118	119	120	121	122	123	124	125	126
127	128	129	130	131	132	133	134	135	136	137	138	139	140	141	142	143	144

¹Based upon ¹²C. (C) indicates the mass number of the longest-lived isotope.

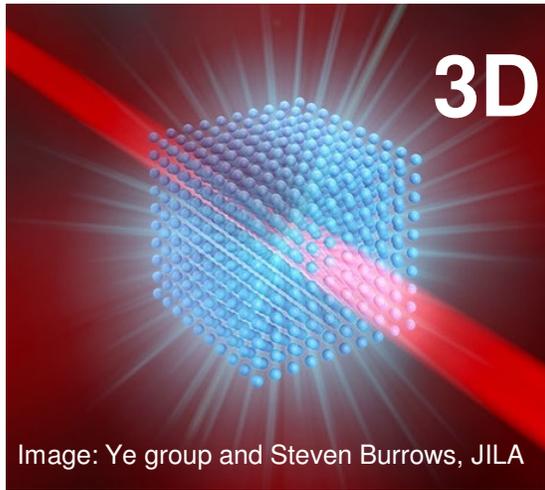
For the most precise values and uncertainties visit ciaw.org and pml.nist.gov/data.

NIST SP 966 (July 2019)

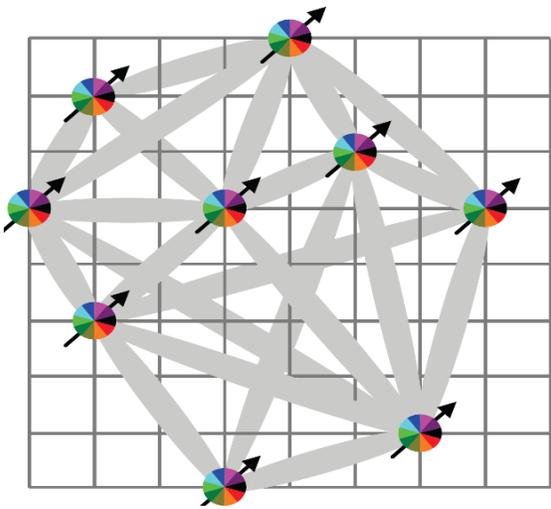
iStock images

Image credit: NIST

Numerous applications that need precise atomic data

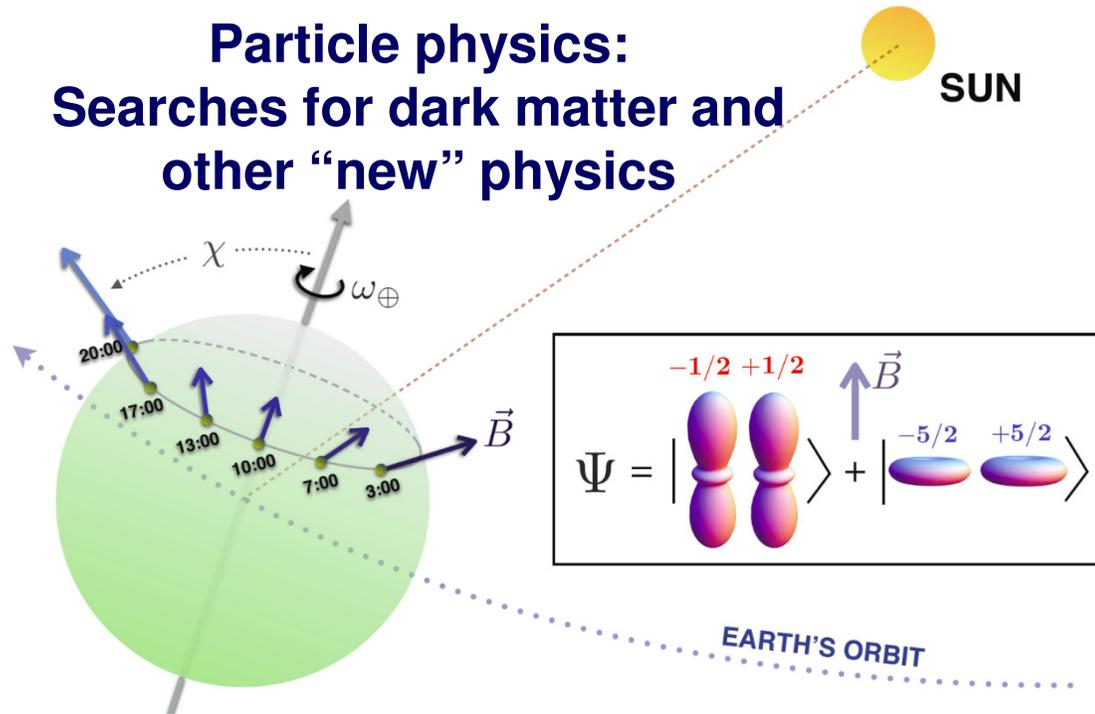


Atomic clocks



Ultracold atoms

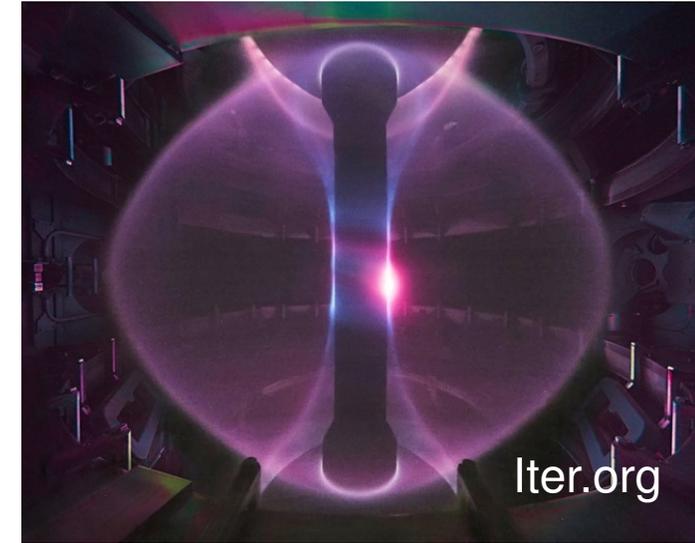
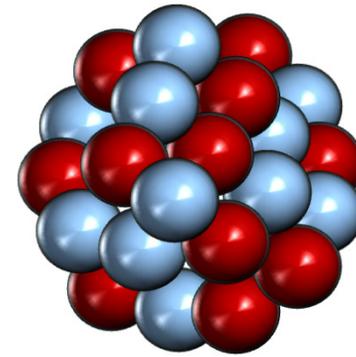
Quantum computing and simulation



Astrophysics



Nuclear and hadronic physics - extracting nuclear properties



Plasma physics

Development of new methods for high-precision atomic calculations

Method and code developers:

Charles Cheung (University of Delaware, USA)
Sergey Porsev (University of Delaware, USA)
Mikhail Kozlov (PNPI, Russia)
Ilya Tupitsyn (University of St. Petersburg, Russia)
Bindiya Arora (Perimeter Institute, Canada)
Andrey Bondarev, (University of Delaware, USA)
Marianna Safronova (University of Delaware, USA)

Methods:

Coupled-cluster (all-order) LCCSD, CCSDvT, **CCSDT (new)**, **new OpenMP codes**
Configuration interaction CI (**new MPI CI code**)
Configuration interaction + valence PT (MPI CI+PT code)
Hybrid configuration interaction and coupled-cluster approaches:
CI+MBPT and CI+all-order (CI+LCCSD and **new CI+CCSDT**)

Capabilities:

- (1) accurate calculations of a very wide range of atomic properties for atoms and positive and negative ions with a few valence electrons (currently tested up to 6 valence electrons)
 - (2) new capabilities to calculate more complicated systems with MPI CI
- Intrinsically relativistic, QED (can choose among 4 potentials) and full Breit interaction is included

Codes that write formulas

Codes that write codes

Codes that analyse results and estimate uncertainties

Codes that put our data into and online database

Why treating many valence electrons is hard?

Use **configuration interaction** (CI) method to treat valence correlations

$$\Psi = \sum_i c_i \Phi_i$$

$$\Phi_n = \frac{1}{\sqrt{N!}} \det \{ \phi_{n_1} \cdots \phi_{n_N} \}$$

One-electron basis functions
 $n = 1, \dots, m$

N = number of valence e^-

$$150^2 = 22\,500 \quad 2 \text{ valence } e^-$$

$$150^4 = 506\,250\,000 \quad 4 \text{ valence } e^-$$

$$150^6 = 11\,390\,625\,000\,000 \quad 6 \text{ valence } e^-$$

The Problem (Bad News)



Number of configurations
goes as $\sim m^N$ 

Good news:

Only a “small” subset of these configurations need to be included, but which ones?

How can we trust theory?

How to estimate **what we do not know?**

1. Calculate properties of similar “reference” systems where experimental data exist. Compare all computed quantities with all available experiments.
2. Use several different methods of increasing precision and compare results.
3. Calculate all major corrections separately, check for possible cancelations – use to estimate uncertainty.
4. Test the methods of evaluating uncertainties on “reference” systems.

We can provide theory values with error bars!

Example 1: Astrophysics: solving 3C/3D puzzle



José R. Crespo López-Urrutia
Heidelberg, MPIK

Summer school: Search for new physics with low-energy precision tests
June 2019, Ameland Island, Netherlands

3C/3D puzzle in Fe XVII



NASA's Chandra X-ray Observatory, and other space telescopes, detects radiation emitted by the hot astrophysical plasmas that lie in supernovae or galaxy clusters.

Some of the strongest x-ray emission lines originate from a highly ionized iron species called Fe XVII

Its two strongest x-ray lines 3C and 3D are used in astrophysics to determine the plasma's temperature, density, and other conditions.

$$3C \quad (2p^5)_{1/2}(3d)_{3/2} (J = 1) \rightarrow 2p^6 (J = 0)$$

$$3D \quad (2p^5)_{3/2}(3d)_{5/2} (J = 1) \rightarrow 2p^6$$

For decades, the measured intensity ratio of these lines has disagreed with theoretical models.

Phys. Rev. Lett. 124, 225001 (2020)

New measurement: 3.09(8)(6)

New theory: 3.55(5)

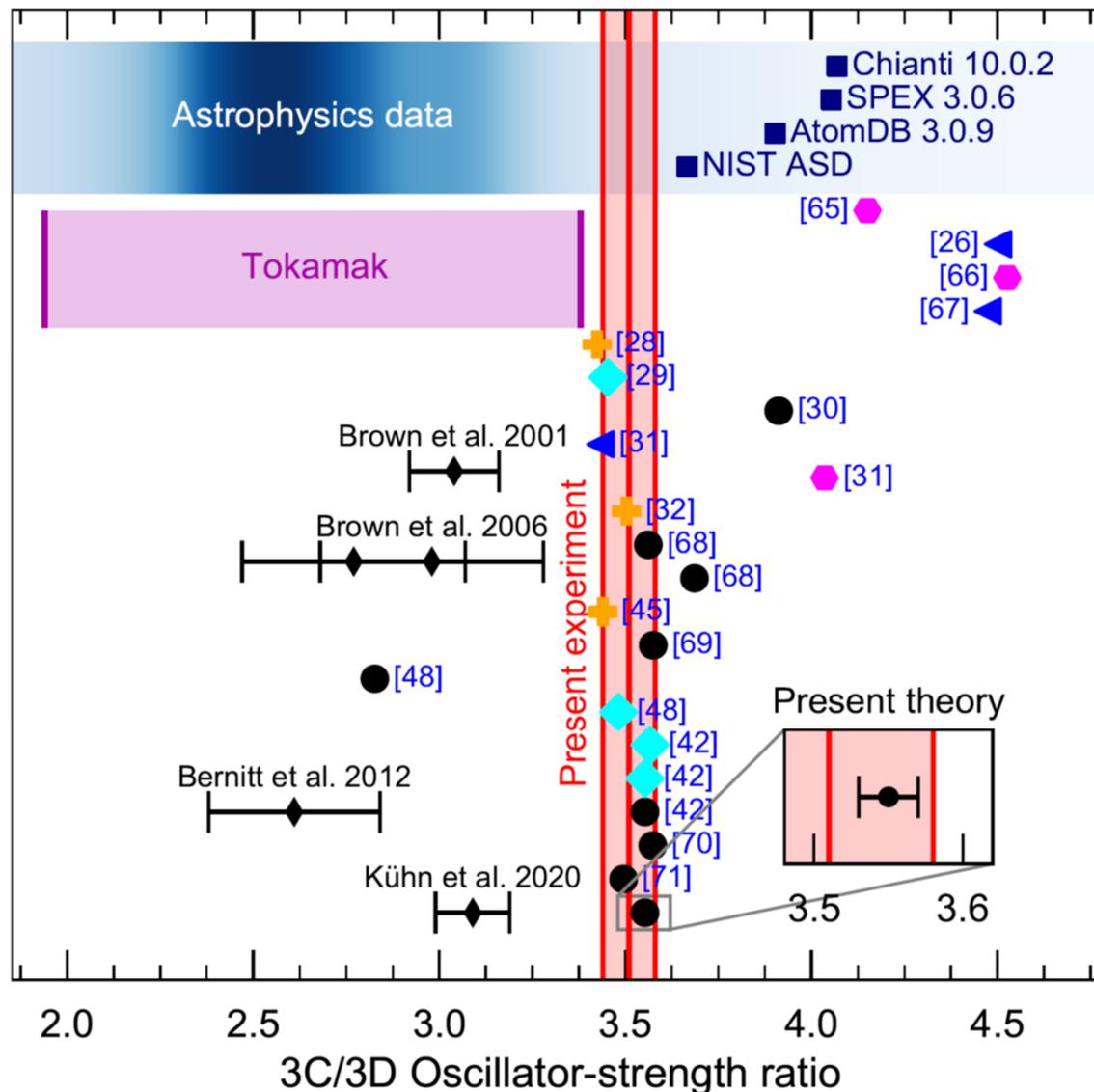
3C/3D puzzle in Fe XVII 10 electrons

3C $(2p^5)_{1/2}(3d)_{3/2} (J = 1) \rightarrow 2p^6 (J = 0)$

3D $(2p^5)_{3/2}(3d)_{5/2} (J = 1) \rightarrow 2p^6$

New measurement agrees perfectly with theory predictions!

Experiment $R=3.51(2)_{\text{stat}}(7)_{\text{sys}}$
Theory $R=3.55(2)$

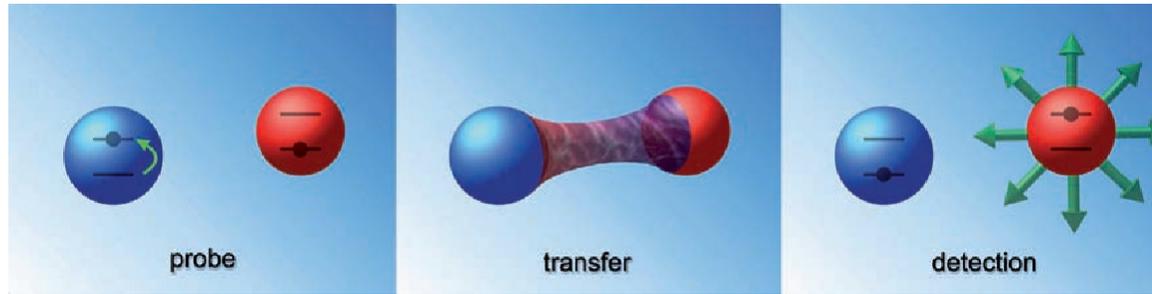


New Measurement Resolves Key Astrophysical Fe XVII Oscillator Strength Problem, Steffen Kühn et al., Phys. Rev. Lett. 129, 245001 (2022)

Example 2: Predicting clock transitions in highly charged ions

First optical atomic clock based on a highly charged ion

Steven King et al, Nature 611, 43–47 (2022)



Piet Schmidt

Shift	$\Delta\nu/\nu$ (10^{-17})		σ/ν (10^{-17})	
	$^{40}\text{Ar}^{13+}$	$^{36}\text{Ar}^{13+}$	$^{40}\text{Ar}^{13+}$	$^{36}\text{Ar}^{13+}$
Excess micromotion	-44.3	-55.0	2.2	2.1
Laser-induced a.c. Zeeman		0		0.2
Secular motion		-0.1		< 0.1
Quadrupole shift		0		< 0.1
Quadratic Zeeman		< 0.1		\ll 0.1
TOTAL	-44.4	-55.1	2.2	2.1

**Uncertainty:
 2.2×10^{-17}**

Example 2: Ni¹²⁺ clock transition

16 electrons



Piet Schmidt



98860 cm⁻¹



47346 cm⁻¹



19542 cm⁻¹



498(3) nm
G=0.008 Hz

Can we predict clock transition energy to 10 cm⁻¹?

We need to be sure we included everything at that level!

Expt: 20060(100) cm⁻¹

**Our prediction:
20081(10) cm⁻¹**

**New experiment:
20078.984(10) cm⁻¹**

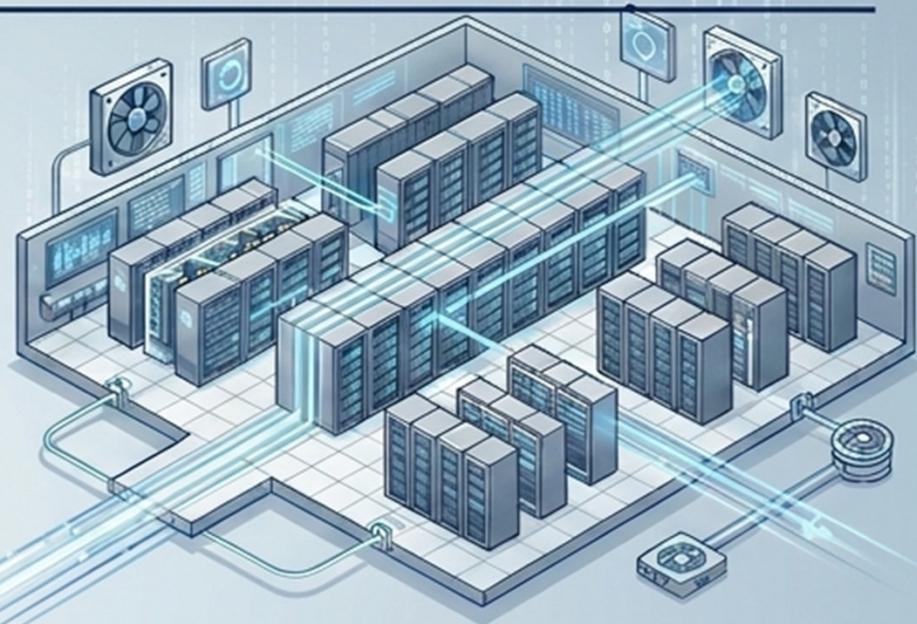
Finding the ultra-narrow ³P₂ → ³P₀ electric quadrupole transition in Ni¹²⁺ ion for an optical clock,
Charles Cheung, Sergey G. Porsev, Dmytro Filin, Marianna S. Safronova, Malte Wehrheim, Lukas J. Spieß, Shuying Chen, Alexander Wilzewski, José R. Crespo López-Urrutia, Piet O. Schmidt, Phys. Rev. Lett. 135, 093002 (2025).



COMPUTATIONAL RESOURCES LAW



No matter how many computers or computer memory you have now it is always less than you need by at least a factor of 10.



 31 TB MAX MEMORY LIMIT



5 MILLION DETERMINANTS



3 WEEKS

2019



250 MILLION DETERMINANTS



2-3 DAYS

2024

THE NEXT CHALLENGE

How can we do 5 billion determinants?



Need for Yb+, Yb open *f* shell states.



Numerous fantastic collaborations with 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⁺, Ti⁺, Th⁺,
Th³⁺, Ag, Lu⁺, Ti,
Cr, Y⁺, La⁻, Fr,
Ra⁺, Pr¹⁰⁺, Ni¹²⁺,
....

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?

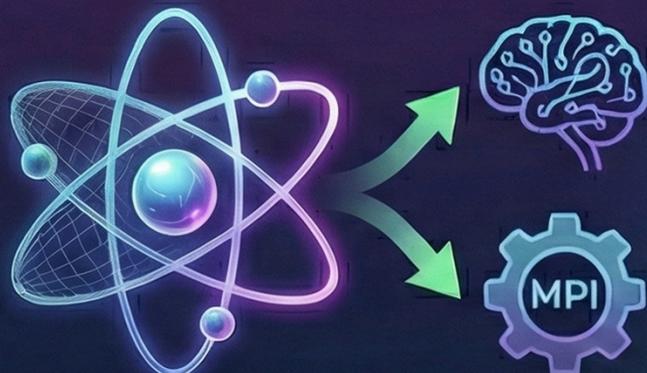
Atoms are missing from the trap, no expected signal observed, ...

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

What else will be useful to measure?

HOW TO ACCURATELY COMPUTE ANY ATOMIC PROPERTIES AND MAKE THEM EASILY AVAILABLE?

DEVELOP & INNOVATE (CODE & RELEASE)



TREAT COMPLICATED SYSTEMS & IMPROVE PRECISION

IMPROVE MPI EFFICIENCY & USE NEURAL NETWORKS

OPEN SOURCE



2015, 2025
PUBLIC RELEASE



PUBLICATIONS

SCALE & AUTOMATE (SOFTWARE TRANSITION)



RE-DESIGN FOR LARGE SCALE DATA GENERATION



TURN CODES INTO "SOFTWARE"
(PYTHON INTERFACES)



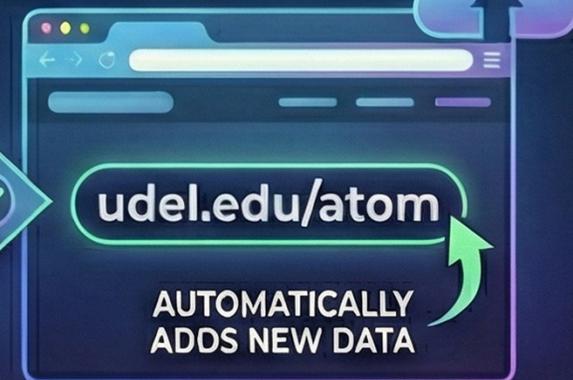
AUTOMATED UNCERTAINTY ESTIMATES



AUTOMATED DATA CHECKS

AUTOMATED DATA PORTAL (PORTAL & INTERFACE)

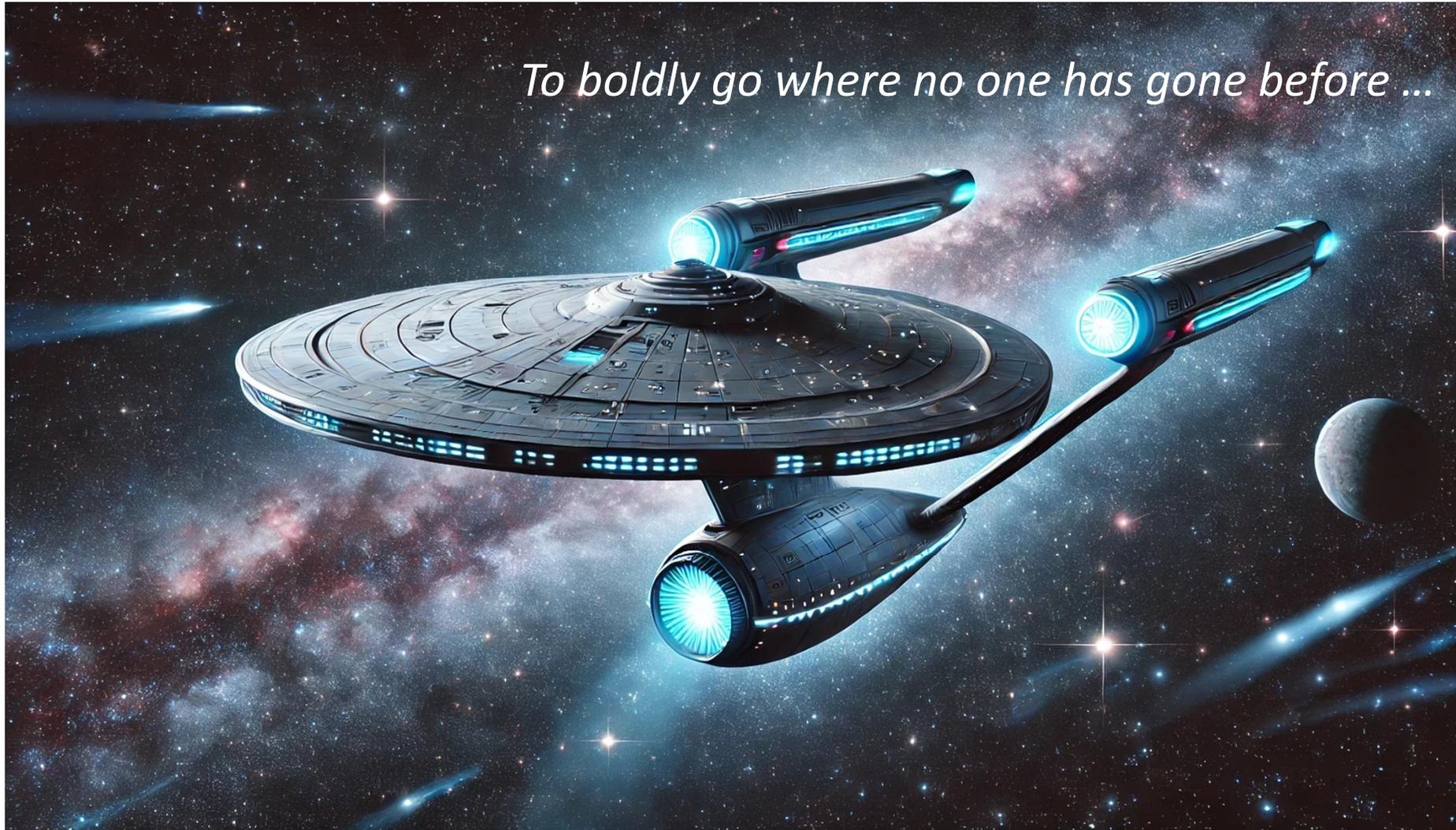
DEVELOP SUSTAINABLE
EASY TO USE FREE PORTAL



"FIND BEST ATOM FOR
MY EXPERIMENT"

HUMAN LANGUAGE INTERFACE

COMPUTER, CALCULATE!



Automating all codes for massive data generation

Turn research codes into software!

Classify atomic calculations by difficulty level

3 Li Lithium 6.941 $1s^2 2s^1$ 5.3917	4 Be Beryllium 9.012182 $1s^2 2s^2$ 9.3227
11 Na Sodium 22.989770 [Ne]3s ¹ 5.1391	12 Mg Magnesium 24.3050 [Ne]3s ² 7.6462
19 K Potassium 39.0983 [Ar]4s ¹ 4.3407	20 Ca Calcium 40.078 [Ar]4s ² 6.1132
37 Rb Rubidium 85.4678 [Kr]5s ¹ 4.1771	38 Sr Strontium 87.62 [Kr]5s ² 5.6949
55 Cs Cesium 132.90545 [Xe]6s ¹ 3.8939	56 Ba Barium 137.327 [Xe]6s ² 5.2117
87 Fr Francium (223) [Rn]7s ¹ 4.0727	88 Ra Radium (226) [Rn]7s ² 5.2784

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

1 – 3 valence electrons

Automated

Group 2
Calculations that require expert knowledge

4 - 6 valence electrons, special hole cases, up to 10 - 16 electrons in highly charged ions

Only calculations of wave functions requires expert knowledge, could automate some

Group 3
Exponential scaling with the number of valence electrons
New MPI code
Machine learning

61 Pm Promethium (145) [Xe]4f ⁶ 6s ² 5.582	62 Sm Samarium 150.36 [Xe]4f ⁶ 6s ² 5.6437	63 Eu Europium 151.964 [Xe]4f ⁷ 6s ² 5.6704	64 Gd Gadolinium 157.25 [Xe]4f ⁷ 5d ¹ 6s ² 6.1498	65 Tb Terbium 158.92534 [Xe]4f ⁷ 6s ² 5.8538	66 Dy Dysprosium 162.500 [Xe]4f ⁹ 6s ² 5.9389	67 Ho Holmium 164.93032 [Xe]4f ¹¹ 6s ² 6.0215	68 Er Erbium 167.259 [Xe]4f ¹² 6s ² 6.1077	69 Tm Thulium 168.93421 [Xe]4f ¹³ 6s ² 6.1843
93 Np Neptunium (237) [Rn]5f ⁶ 6d ¹ 7s ² 6.2657	94 Pu Plutonium (244) [Rn]5f ⁷ 7s ² 6.0260	95 Am Americium (243) [Rn]5f ⁷ 7s ² 5.9738	96 Cm Curium (247) [Rn]5f ⁷ 6d ¹ 7s ² 5.9914	97 Bk Berkelium (247) [Rn]5f ⁹ 7s ² 6.1979	98 Cf Californium (251) [Rn]5f ¹⁰ 7s ² 6.2917	99 Es Einsteinium (252) [Rn]5f ¹¹ 7s ² 6.42	100 Fm Fermium (257) [Rn]5f ¹² 7s ² 6.50	101 Md Mendelevium (258) [Rn]5f ¹³ 7s ² 6.58

Half-filled shells and holes in shells

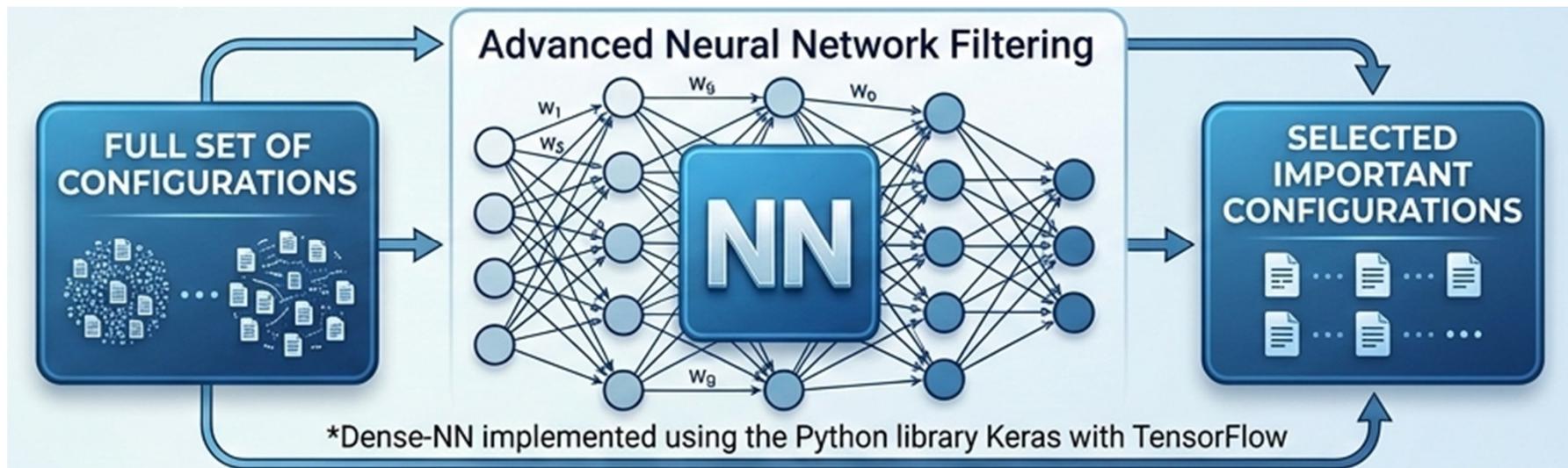
Method development in progress, need new ideas – machine learning
Efficient memory distribution in MPI code

25 Mn Manganese 54.938049 [Ar]3d ⁵ 4s ² 7.4340	26 Fe Iron 55.845 [Ar]3d ⁶ 4s ² 7.9024	27 Co Cobalt 58.933200 [Ar]3d ⁷ 4s ² 7.8810	28 Ni Nickel 58.6934 [Ar]3d ⁸ 4s ² 7.6398
43 Tc Technetium (98) [Kr]4d ⁵ 5s ² 7.28	44 Ru Ruthenium 101.07 [Kr]4d ⁷ 5s ¹ 7.3605	45 Rh Rhodium 102.90550 [Kr]4d ⁸ 5s ¹ 7.4589	46 Pd Palladium 106.42 [Kr]4d ¹⁰ 8.3389
75 Re Rhenium 186.207 [Xe]4f ¹⁴ 5d ⁵ 6s ² 7.8335	76 Os Osmium 190.23 [Xe]4f ¹⁴ 5d ⁶ 6s ² 8.4382	77 Ir Iridium 192.217 [Xe]4f ¹⁴ 5d ⁷ 6s ² 8.9570	78 Pt Platinum 195.078 [Xe]4f ¹⁴ 5d ⁹ 6s ¹ 8.9588

Selecting the important configurations

$$\Psi = \sum_i c_i \Phi_i$$

Problem: too many configurations!



APPLICATIONS

1.



For users who do not have access to large computer clusters

2.



For problems beyond current computational capabilities

Machine learning for configuration interaction (MLCI)

Example: Ni¹²⁺ clock transition Basis set upscaling

NN-supported CI			
Iteration	num_procs	mem_per_core	time (hr)
Start	640	21.7	2.5
-10	640	21.1	2.2
-10.5	640	22.4	5.3
-11	640	24.7	11.1
-11.5	640	27.8	19.7
-12	640	31.5	30.5
Total	—	—	71.2

$$\Psi = \sum_i c_i \Phi_i$$

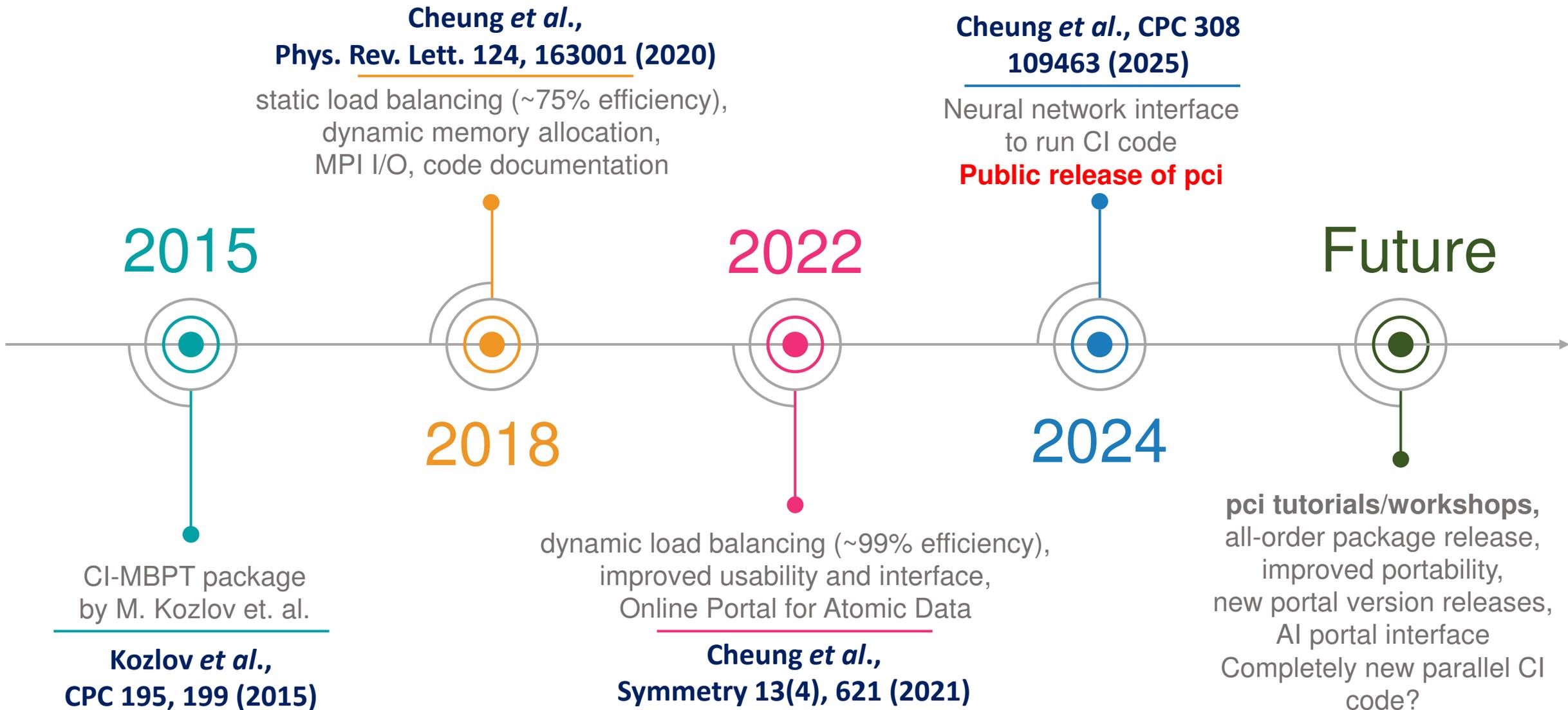
MLCI vs Exact CI

0.02% difference
~3X LESS CONFIG-S
~3X LESS MEMORY
~4X LESS RUNTIME
~4X LESS TOTAL RUNS

**A MLCI user just make a configuration list.
The neural network handles the rest!**

Direct CI			
Basis	num_procs	mem_per_core	time (hr)
17g	1124	8.3	4
22g	1124	17.7	13
17h	1124	15.1	9.5
20h	704	14.4	10.5
22h	850	13.1	10
17i	840	29.4	27
20i	704	25.2	25
17k	840	17.8	19
20k	810	28.3	34
17l	640	29.7	47
18l	1350	15.4	10.5
19l	1056	20.4	15.5
20l	1000	25.3	24
17h ^a	800	3.7	2.5
20h ^a	640	5.9	2
17i ^a	900	5.9	4
20i ^a	950	9.3	4.5
20i ^b	900	7	2
17k ^a	950	8.8	6.5
17l ^b	1350	8	2
18l ^b	576	11.5	5.5
19l ^b	660	13.9	5.5
Total	—	—	283.5

From research codes to data for all



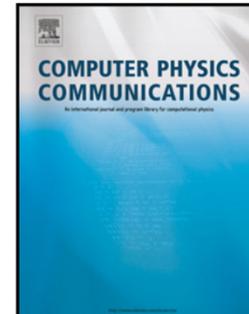


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Contents lists available at ScienceDirect

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, +RPA, +QED

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

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

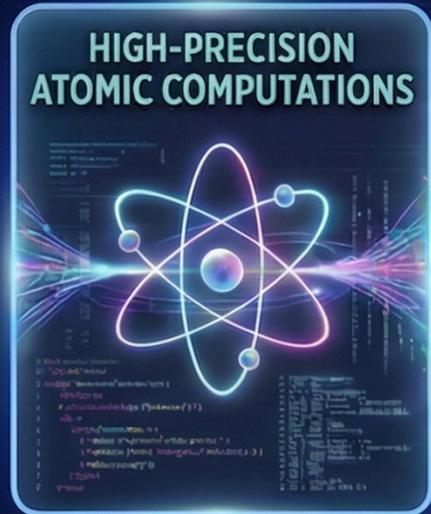
Available on GitHub: <https://github.com/ud-pci/pCI>

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



ATOMIC DATA PORTAL

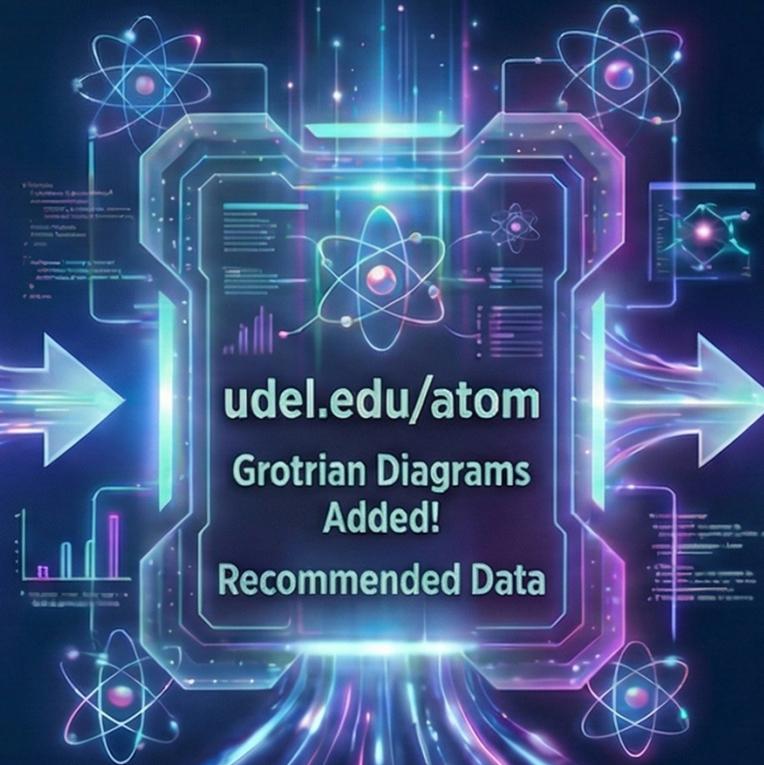
Computer Physics Communications 319, 109951 (2026)



ATOMIC COMPUTATIONS
& EXPERIMENTAL DATA



DATABASE OF
ATOMIC PROPERTIES

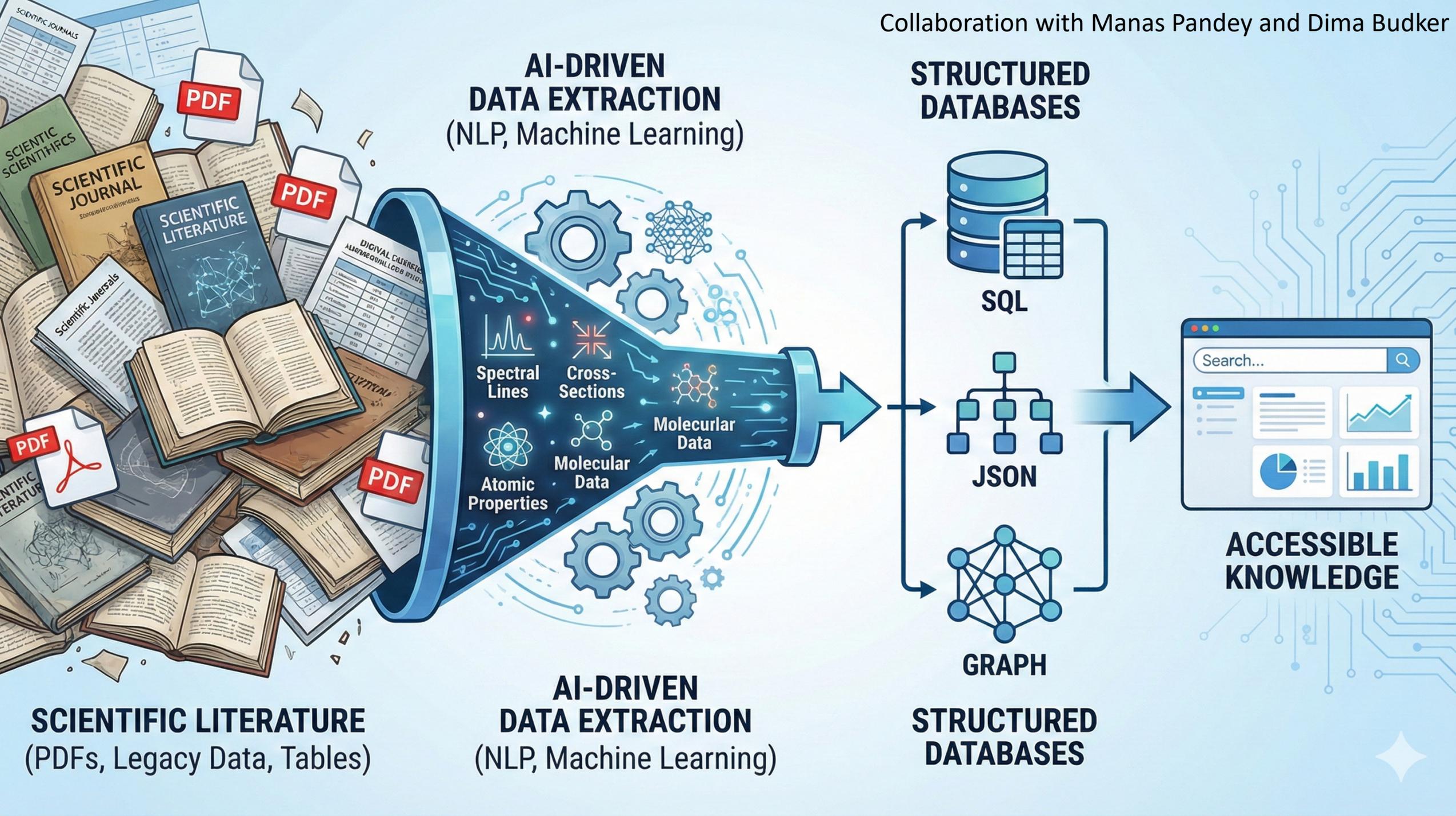


ONLINE HIGH-PRECISION
ATOMIC DATA PORTAL



FREE USER
ACCESS





**AI-DRIVEN
DATA EXTRACTION**
(NLP, Machine Learning)

**STRUCTURED
DATABASES**

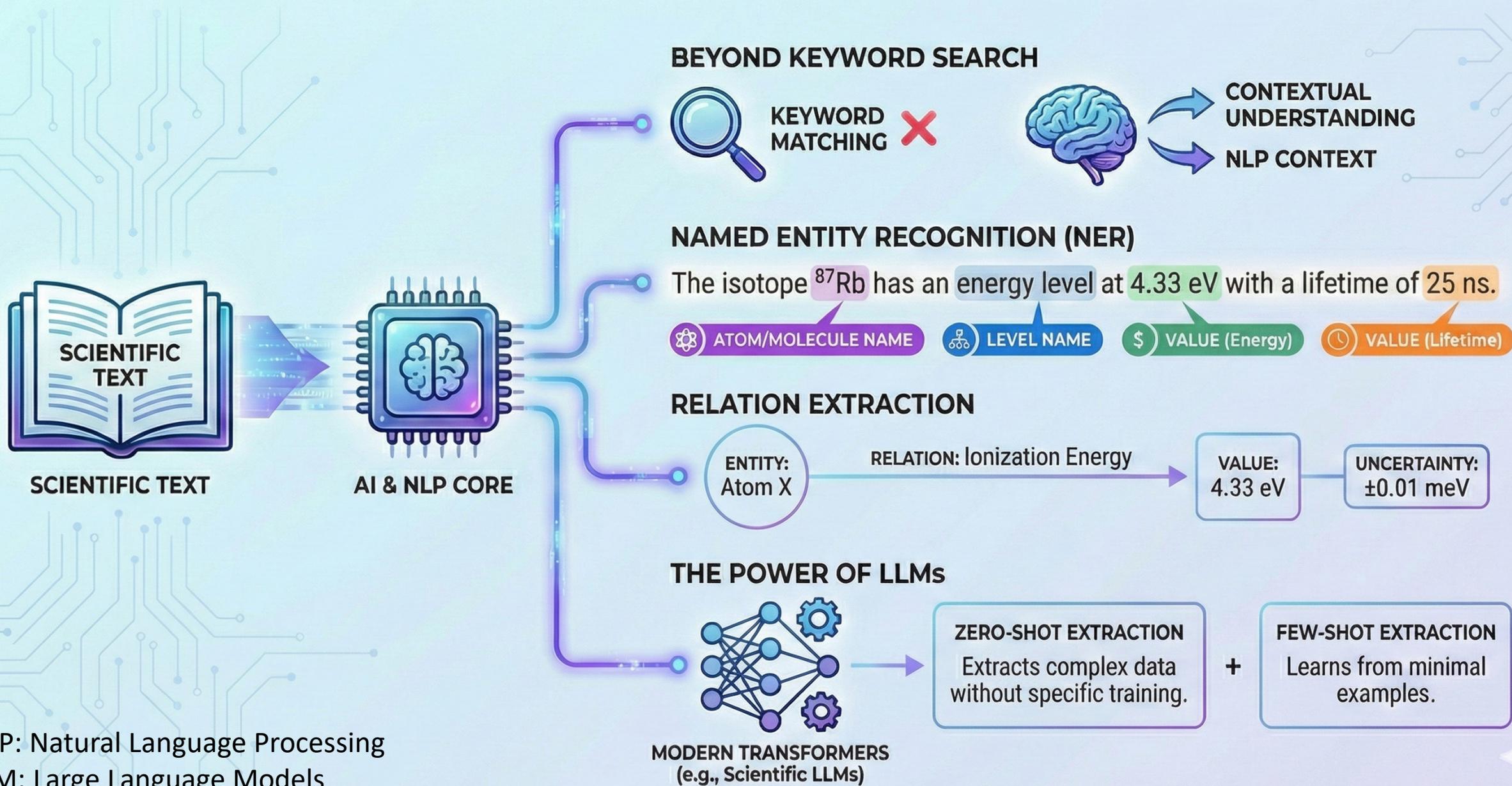
SCIENTIFIC LITERATURE
(PDFs, Legacy Data, Tables)

**AI-DRIVEN
DATA EXTRACTION**
(NLP, Machine Learning)

**STRUCTURED
DATABASES**

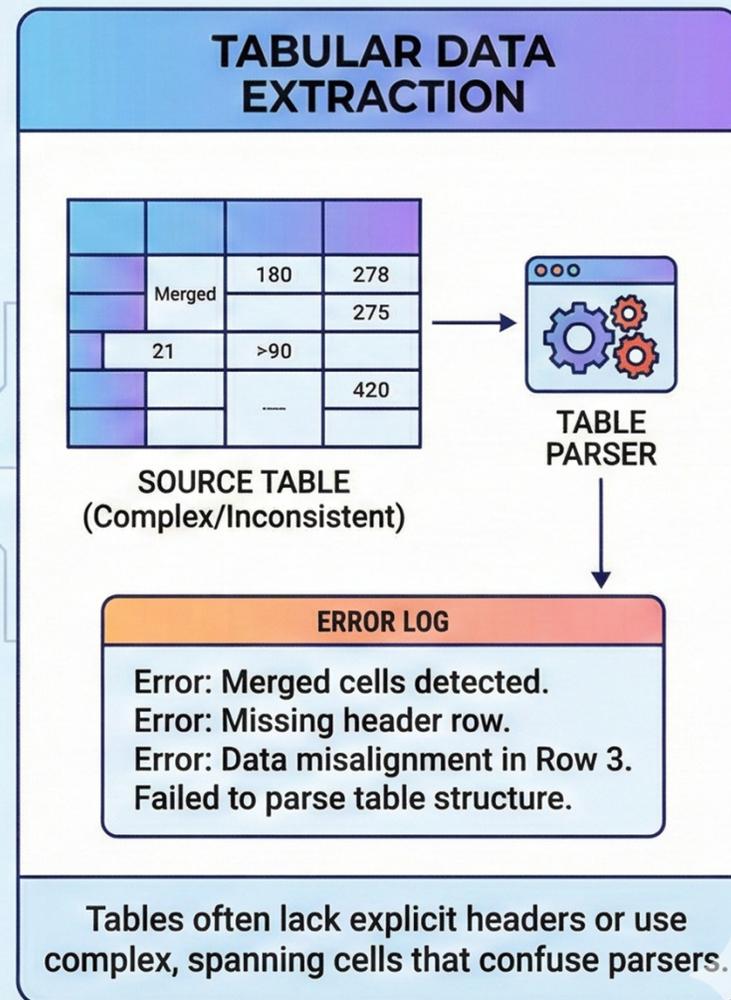
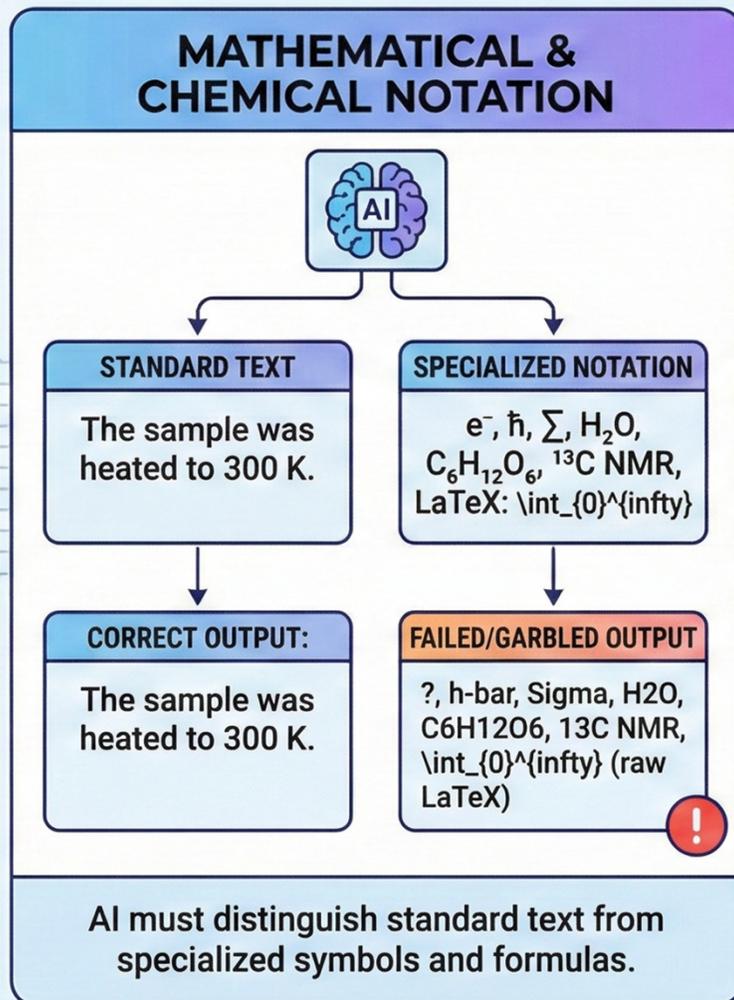
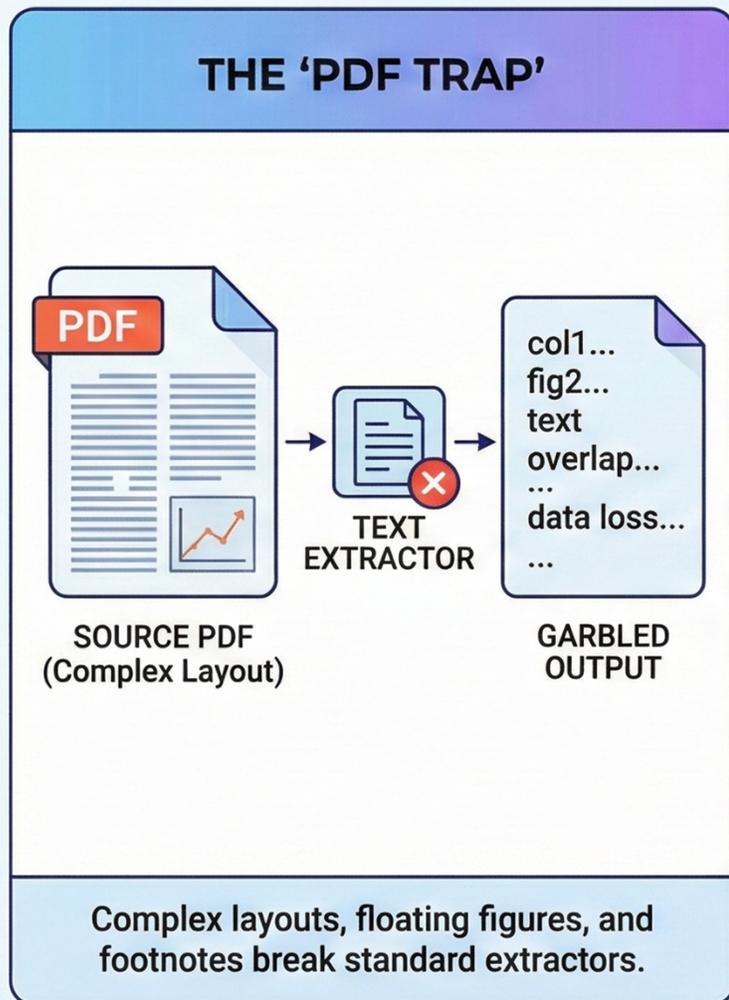
**ACCESSIBLE
KNOWLEDGE**

THE MECHANISM: HOW AI 'READS' SCIENTIFIC LITERATURE

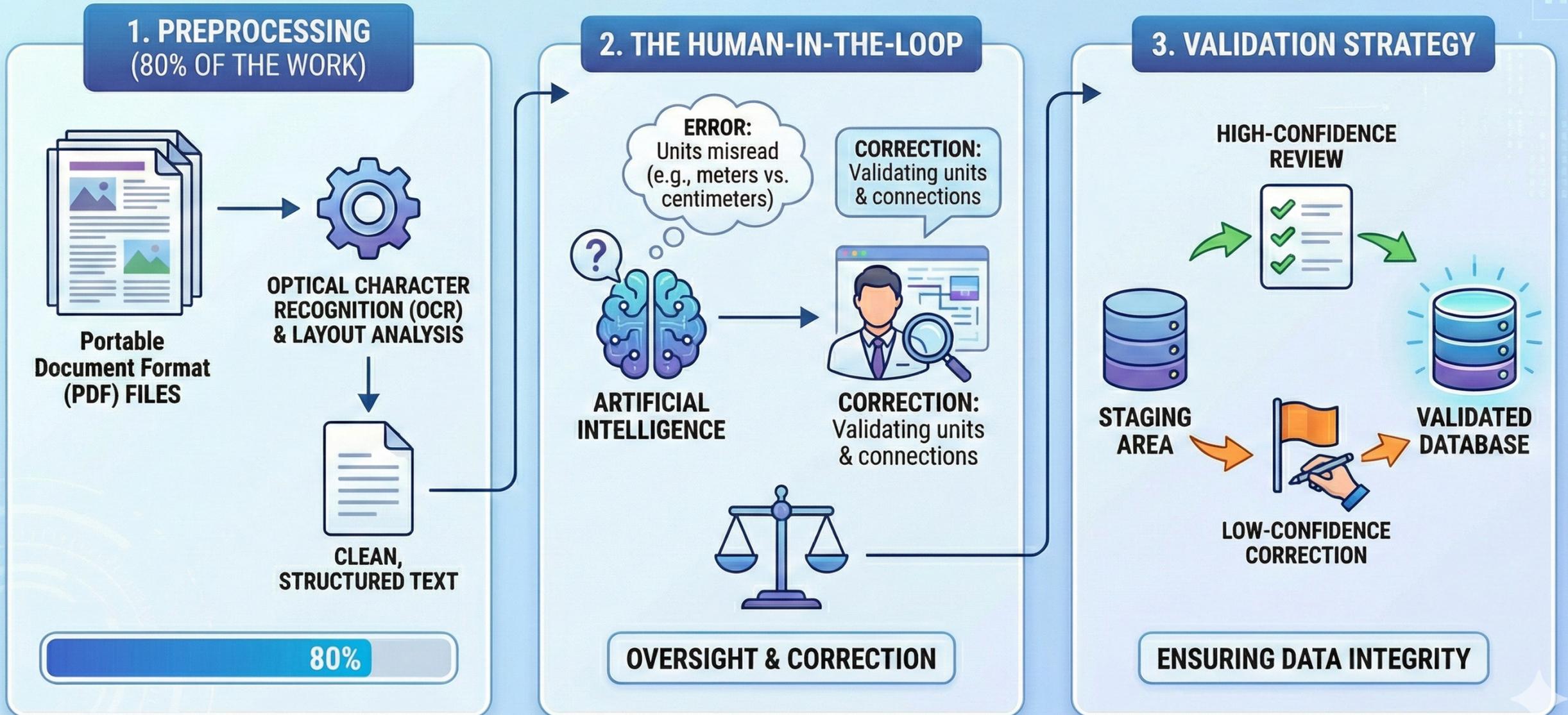


NLP: Natural Language Processing
LLM: Large Language Models

SPECIFIC CHALLENGES IN ATOMIC & MOLECULAR PHYSICS DATA EXTRACTION



ARTIFICIAL INTELLIGENCE-ASSISTED, HUMAN-VALIDATED WORKFLOW



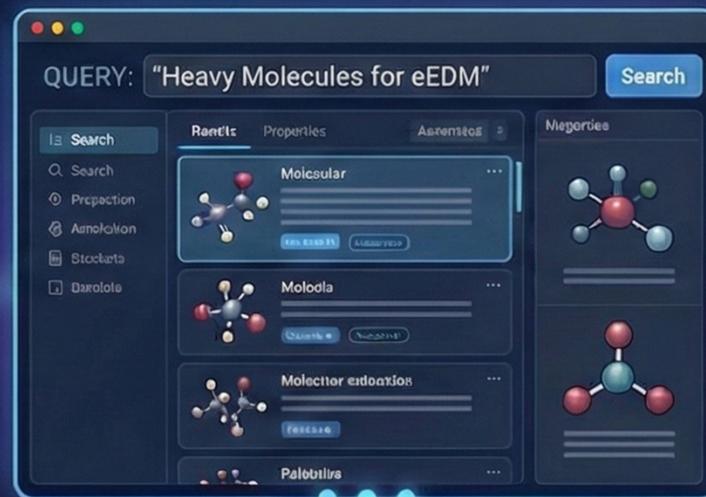
FUTURE: MOLECULAR AI DATA PROJECT

THE PROBLEM:
DATA FRAGMENTATION
& COMPLEXITY



THE SOLUTION:
CENTRALIZED,
INTELLIGENT DISCOVERY

**AI-POWERED
DATA EXTRACTION &
KNOWLEDGE**



**ULTRACOLD
MOLECULES**

**FUNDAMENTAL
PHYSICS**

**QUANTUM
SENSORS**

What data do you need?



UD team and collaborators

Online portal team



Prof. Rudolf Eigenmann
UD (EECS)



Prof. Bindiya Arora
Guru Nanak Dev U., India



Parinaz Barakhshan
UD (CE)
Graduated 2025



Miguel Torres Sanchez
UD (CE) Grad. student



Akshay Bhosale
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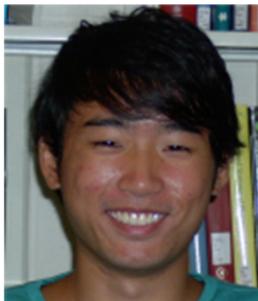
Amani Kiruga
UD (CE)
2025



Dr. Sergey Porsev
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Dr. Dmytro Filin
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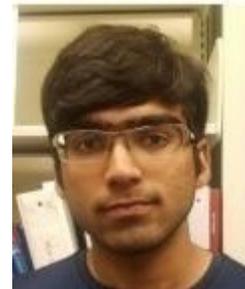
Dr. Charles Cheung
Scientist

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