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

Elements: Community Portal for High-Precision Atomic Physics Data and Computation

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University of Delaware project team and collaborators

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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

Atoms are now: Ultracold
Trapped
Precisely controlled

$\Psi = \left| \begin{array}{c} -1/2 \\ +1/2 \end{array} \right\rangle + \left| \begin{array}{c} -5/2 \\ +5/2 \end{array} \right\rangle$
Numerous applications that need precise atomic data

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

Atomic clocks

Ultracold atoms
Quantum computing and simulation

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

**Codes that write formulas**

**Codes that write codes**

**Codes that analyse results and estimate uncertainties**
We are building atomic clock
degenerate quantum gas microscope
tweezer arrays
quantum simulator with atoms
precision measurement experiment
for new physics searches
...

We need \([transition \ rates, \ branching \ ratios, \ lifetimes, \ polarizabilities, \ \ldots]\)
We found some data in your papers – will it be possible to provide \ldots\?

Would you collaborate with us on the interpretation of our measurements?
We have measured \ldots\ but the values differ strongly from the existing literature values.
Will it be possible for you to calculate these?
\textit{Variations: atoms are missing from the trap, no expected signal observed, \ldots}

We plan to measure \[\ldots\]. Will these quantities be useful in testing your new codes?
What else will be useful to measure?
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\textsuperscript{a,b,*}, S.G. Porsev\textsuperscript{a,c,**}, M.S. Safronova\textsuperscript{c,d}, I.I. Tupitsyn\textsuperscript{e}

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!
There are really a lot of atoms!

<table>
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<th>Group 2</th>
<th>Group 3</th>
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<td>Br</td>
<td>At</td>
<td>Rn</td>
<td>Fr</td>
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</tbody>
</table>

**Neutral atom:** Fe

**Ions:** keep removing electrons

- Fe⁺
- Fe₂⁺
- Fe³⁺
- Fe⁴⁺
- Fe⁵⁺
- Fe⁶⁺
- Fe⁷⁺
- Fe⁸⁺
- Fe⁹⁺
- Fe¹⁰⁺
- Fe¹¹⁺
- Fe¹²⁺
- Fe¹³⁺
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
- Can automate

**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

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

Difficulty Groups 1 and 2
To boldly go where no one has gone before …
How to serve the most diverse group of users?

Most requested data:
transition matrix elements and polarizabilities

Atoms are now trapped by light

Need electric-dipole polarizability $\alpha$ 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

**COMPUTER, CALCULATE CS!**

- Dirac-Hartree-Fock
- Basis set code

Calculate core part

- LCCSD valence
- LCCSDpT valence

Matrix element code + scaled versions

All up to $n=10-12$ spdf

All allowed

Analysis code that makes a summary with uncertainties – output is one table
## Final code output: transition E1 matrix elements in atomic units

<table>
<thead>
<tr>
<th>Transition</th>
<th>DHF</th>
<th>SD</th>
<th>SDsc</th>
<th>SDpT</th>
<th>SDpTsc</th>
<th>Final</th>
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<tr>
<td>$3d_{3/2} - 4f_{5/2}$</td>
<td>2.6059</td>
<td>1.8660</td>
<td>1.9265</td>
<td>1.9265</td>
<td>1.9051</td>
<td>1.93(2)</td>
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<td>$3d_{3/2} - 4p_{1/2}$</td>
<td>3.0825</td>
<td>2.4173</td>
<td>2.4636</td>
<td>2.4677</td>
<td>2.4503</td>
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<tr>
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<td>1.3764</td>
<td>1.0788</td>
<td>1.0996</td>
<td>1.1014</td>
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<td>1.100(6)</td>
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<td>1.5216</td>
<td>1.1655</td>
<td>1.1917</td>
<td>1.1937</td>
<td>1.1846</td>
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<td>$3d_{3/2} - 5p_{1/2}$</td>
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<td>0.1055</td>
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<td>0.1154</td>
<td>0.11(2)</td>
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<td>0.0607</td>
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<td>0.0285</td>
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<td>0.6303</td>
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<td>0.410(6)</td>
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<td>10f\textsubscript{7/2}</td>
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</table>
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.

<table>
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<th>6.38(8)</th>
<th></th>
<th>5d3/2</th>
<th>3.19(7)</th>
<th></th>
<th>5d5/2</th>
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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

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</tr>
</tbody>
</table>

- 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
Summary
Online portal 3-year project started in October 2019

Marianna Safronova     Rudolf Eigenmann
Parinaz Barakhshan     Adam Mars

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

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