WHERE TO FIND, OR HOW TO GENERATE, ELECTRON COLLISION DATA FOR PLASMA APPLICATIONS

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OVERVIEW

- Types of atomic data
- Who uses electron collision data?
- Why is data provenance important?
- Where to find electron collision data:
  - Literature
  - Databases
- How to generate electron collision data:
  - Experiment } Collaboration
  - Theory
  - AMOS Gateway } On your own!

DISCLAIMER

This presentation is incomplete!

TYPES OF ATOMIC DATA

Atomic Structure

- Energy Levels
- Ionization energies
- Mean radii
- Oscillator Strengths
- Transition Rates
- Polarizabilities

Electron Collisions

- Excitation cross-sections
- Ionization cross-sections
- Momentum-transfer cross-sections
- Scattering lengths

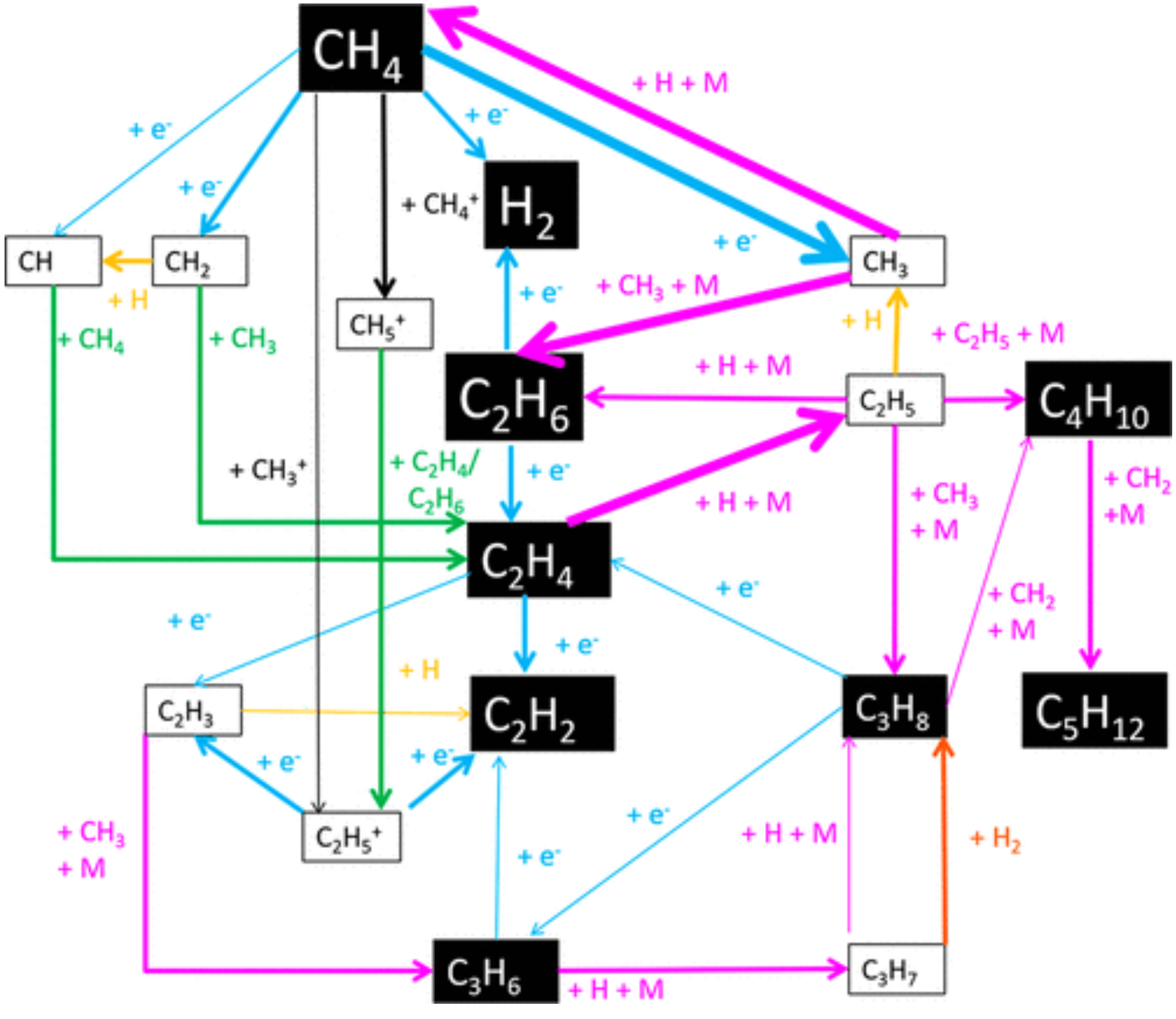
Photon Collisions

- Ionization cross-sections
- Dielectric Recombination

WHO USES ELECTRON COLLISION DATA?

- Other atomic physicists
  - Comparison with other methods / techniques
  - Time-dependent calculations
- Plasma Modellers
  - Laboratory Plasmas (DPALs, nano-fabrication)
  - Astrophysical Plasmas (stars, nebulae)
  - Fusion

WHAT DO THEY NEED?



J. Phys. Chem. C 2020, 124, 13, 7016–7030 (2020)

WHY IS DATA PROVENANCE IMPORTANT?

"Trash in = Trash out"

WHY IS DATA PROVENANCE IMPORTANT?

- Uncertainty Quantification
  - Typical in experimental data
  - "New" concept for theory
- Limitations due to how data was acquired / generated
  - Scope of experiment
  - Amount and type of data available
  - Theoretical approach used

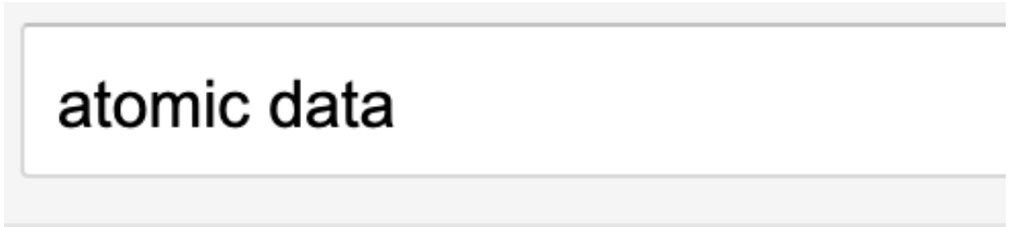
WHERE TO FIND ELECTRON COLLISION DATA?

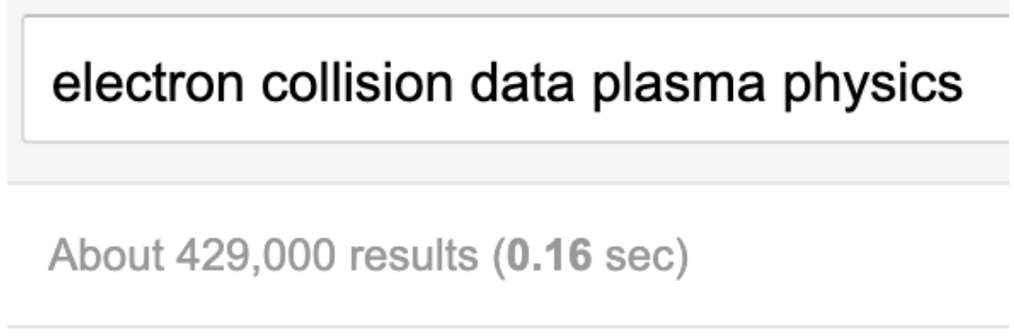
- In the literature

- Single-application or community databases

ELECTRON COLLISION LITERATURE

- Vast amount
- Difficult to search through
- Incomplete
- Age and data availability





DON MADISON'S CONTRIBUTION TO THE LITERATURE

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D. H. Madison

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DATABASES - NIST

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Atomic Spectra Database

NIST Standard Reference Database 78

Version 5.10

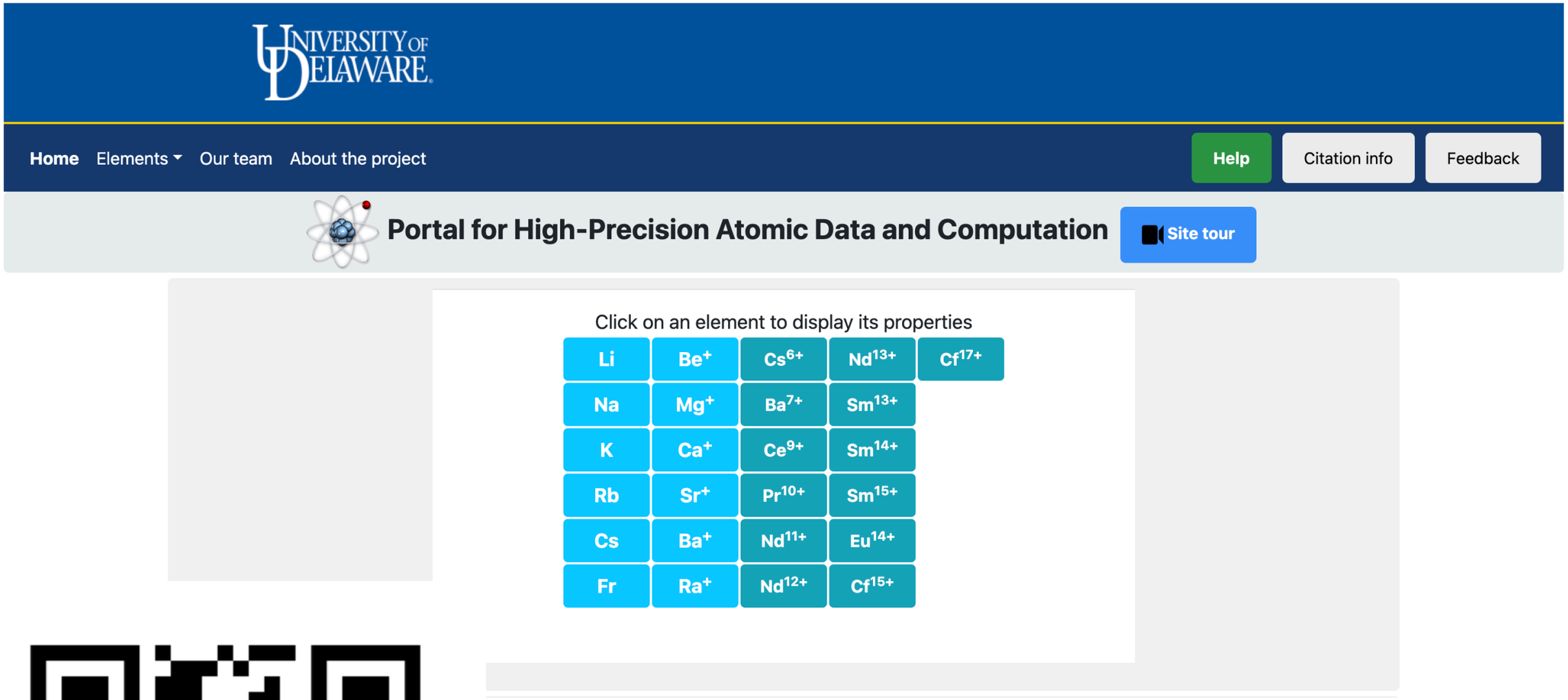
Last Update to Data Content: October 2022 | Version History & Citation Information | Disclaimer |
DOI: https://dx.doi.org/10.18434/T4W30F

Welcome to the NIST Atomic Spectra Database, NIST Standard Reference Database #78. The spectroscopic data may be selected and displayed according to wavelengths or energy levels by choosing one of the following options:

LINES	Spectral lines and associated energy levels displayed in wavelength order with all selected spectra intermixed or in multiplet order. Transition probabilities for the lines are also displayec where available.
LEVELS	Energy levels of a particular atom or ion displayed in order of energy above the ground state.
GROUND STATES & IONIZATION ENERGIES	Ground states and ionization energies of atoms and atomic ions.
LIBS	ASD Interface for Laser Induced Breakdown Spectroscopy (LIBS)

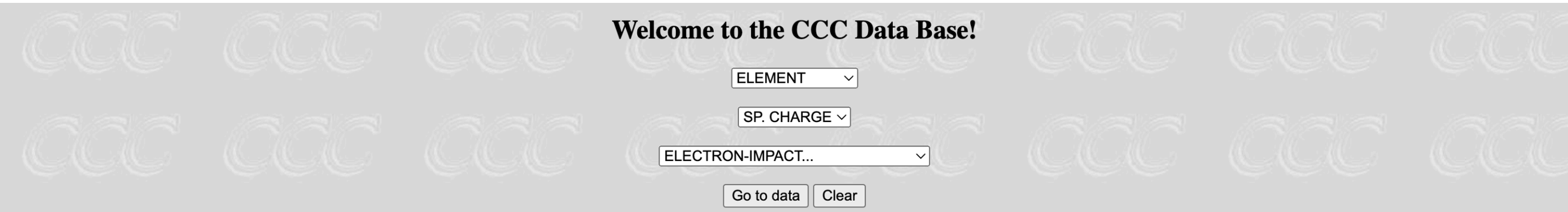
https://www.nist.gov/pml/atomic-spectra-database

DATABASES -PORTAL FOR HIGH-PRECISION ATOMIC DATA AND COMPUTATION



https://www1.udel.edu/atom/

DATABASES - CCC



https://atom.curtin.edu.au/CCC-WWW/

DATABASES - IRON + OPACITY PROJECTS

The Iron Project - The Opacity Project

IPOPv2

Home | The Opacity Project | The Iron Project | TOPbase | TIPbase | OPserver | OP tables | Contact

The Opacity Project - The Iron Project

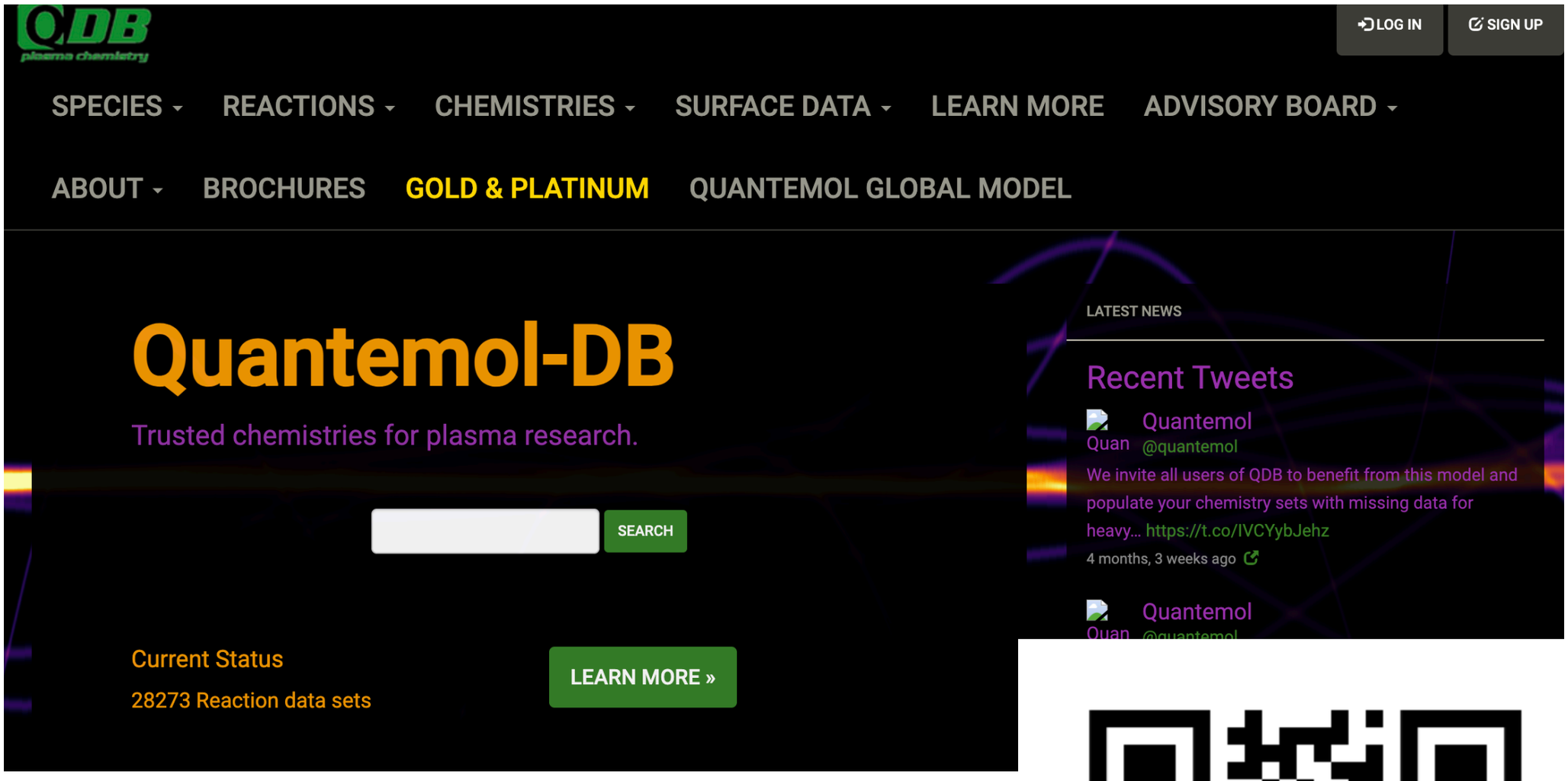
The names Opacity Project (OP) and Iron Project (OP) refer to an international collaboration that was formed in 1984 to calculate the extensive atomic data required to estimate stellar envelope opacities and to compute Rosseland mean opacities and other related quantities. It involved research groups from France, Germany, the United Kingdom, the United States and Venezuela. The approach adopted by the OP to calculate opacities is based on a new formalism of the equation of state and on the computation by ab initio methods of accurate atomic properties such as energy levels, f-values and photoionization cross sections. The OP final results are discussed by Seaton et al.

About us - List of members

Badnell Nigel, Ballance Connor, Bautista Manuel, Butler Keith, Delahaye Franck, Del Zanna Giulio, Eissner Werner, Fivet Vanessa, Hudson Claire, Liang Guiyun, Mason Helen, McLaughlin Brendan, Mendoza Claudio, Montenegro Max, Nahar Sultana, Palmeri Patrick, Pradhan Anil, Quinet Pascal, Ramsbottom Cathy, Saraph Hannelore, Scott Penny, Storey Peter, Wasson Ian, Withoeft Mike, Zeippen Claude,

https://cds.unistra.fr/topbase/home.html

DATABASES -QUANTEMOL DB



https://quantemoldb.com/

DATABASES - LXCAT

About the project

The **Plasma Data Exchange Project** is a community-based project which was initiated as a result of a public discussion held at the 2010 Gaseous Electronics Conference (GEC), a leading international meeting for the **Low-Temperature Plasma** community. This project aims to address, at least in part, the well-recognized needs for the community to organize the means of collecting, evaluating and sharing data both for modeling and for interpretation of experiments.
At the heart of the Plasma Data Exchange Project is **LXCat** (pronounced "elecscat"), an open-access website for collecting, displaying, and downloading electron and ion scattering cross sections, swarm parameters (*mobility, diffusion coefficient, etc.*), reaction rates, energy distribution functions, etc. and other data required for modeling low temperature plasmas. The available data bases have been contributed by members of the community and are indicated by the contributor's chosen title.

> This is a dynamic website, evolving as contributors add or upgrade data. Check back again frequently.

Supporting organizations

FAST NAVIGATION

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PROJECT STATISTICS

Scattering cross sections: 30 databases I 106 x 648 species I 31.5k records I updated: 27 March 2023
Differential scattering cross sections: 4 databases I 29 species I 517 records I updated: 12 March 2019
Interaction potentials: 1 database I 104 x 7 species I 705 records I updated: 30 December 2021
Oscillator strengths: 1 database I 65 species I 150 records I updated: 25 November 2013
Swarm / transport data: 18 databases I 198 x 152 species I 24.2k records I updated: 1 October 2023
Publications, notes and reports: 5 databases I 37 records I updated: 15 February 2022

https://us.lxcat.net/home/

HOW TO GENERATE COLLISION DATA

- Collaborate (have someone do it for you)
  - Experiment
  - Theory

- Do it yourself!
  - Probably just theory

EXPERIMENT

- Few active experimental groups
- Experiments are difficult!
- Resource intensive
- (Sometimes) take longer to produce results than theory
- Fully-differential cross-sections
- Difficult to obtain absolute values

THEORY

- More common than experimental groups
- Difficult to chose which approach?
- Convergence, numerical issues
- Options available for small, fast calculations
- Some calculations are resource intensive, and/or slow to perform
- More complete data sets?

DO IT YOURSELF - OPEN REPOSITORIES

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zatsaroi / BSR3 Public

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Code Issues 1 Pull requests Actions Projects Security Insights

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zatsaroi BSR3 8daf7f4 on Jan 12, 2021 232 commits

BSR_BMAT4	BSR3	3 years ago
BSR_BREIT	BSR3	3 years ago
BSR_CI	HF,CI,MCHF	3 years ago
BSR_CONF3	BSR3	3 years ago
BSR_DMAT3	BSR3	3 years ago

About

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April 21, 2023

Software Open Access

UKRmol-scripts

Houfek, Karel; Benda, Jakub; Mašín, Zdeněk; Harvey, Alex; Meltzer, Thomas; Graves, Vincent; Gorfinkiel, Jimena

Researcher(s)

Darby-Lewis, Daniel

Perl scripts to automatically run the UKRMol+ codes for both inner (UKRMol-in) and outer (UKRMol-out) regions which use the R-matrix method to calculate fixed-nuclei electron- and positron-scattering and photoionization for polyatomic molecules. Using a number of parameters that describe both physical models and machine-dependent settings, the scripts produce all necessary input files and run all codes for electronic structure and scattering calculations as well as gather the more frequently required outputs. The scripts provide a simple way to run such calculations for many molecular geometries concurrently and collect the resulting data for easier post-processing and visualization. Several examples of various types of calculations are provided.

The scripts should be used with releases 3.2 of UKRMol+: UKRmol-in and UKRMol+: UKRmol-out.

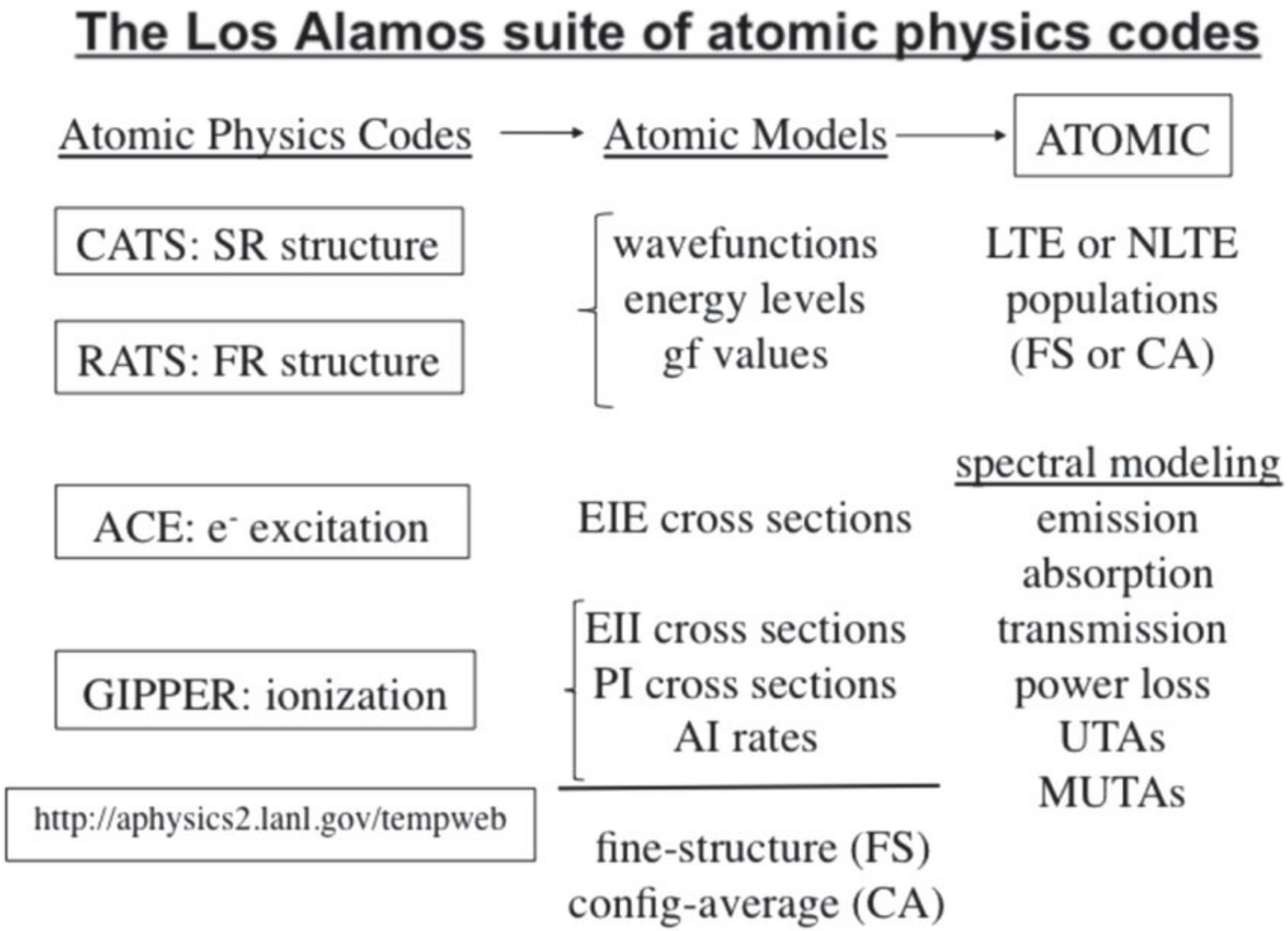
115 views

46 downloads

See more details...

Indexed in OpenAIRE

DO IT YOURSELF - LANL CODES



DO IT YOURSELF (BUT ITS A LITTLE BIT EASIER)

https://amosgateway.org/

AMOS GATEWAY US-BASED TEAM

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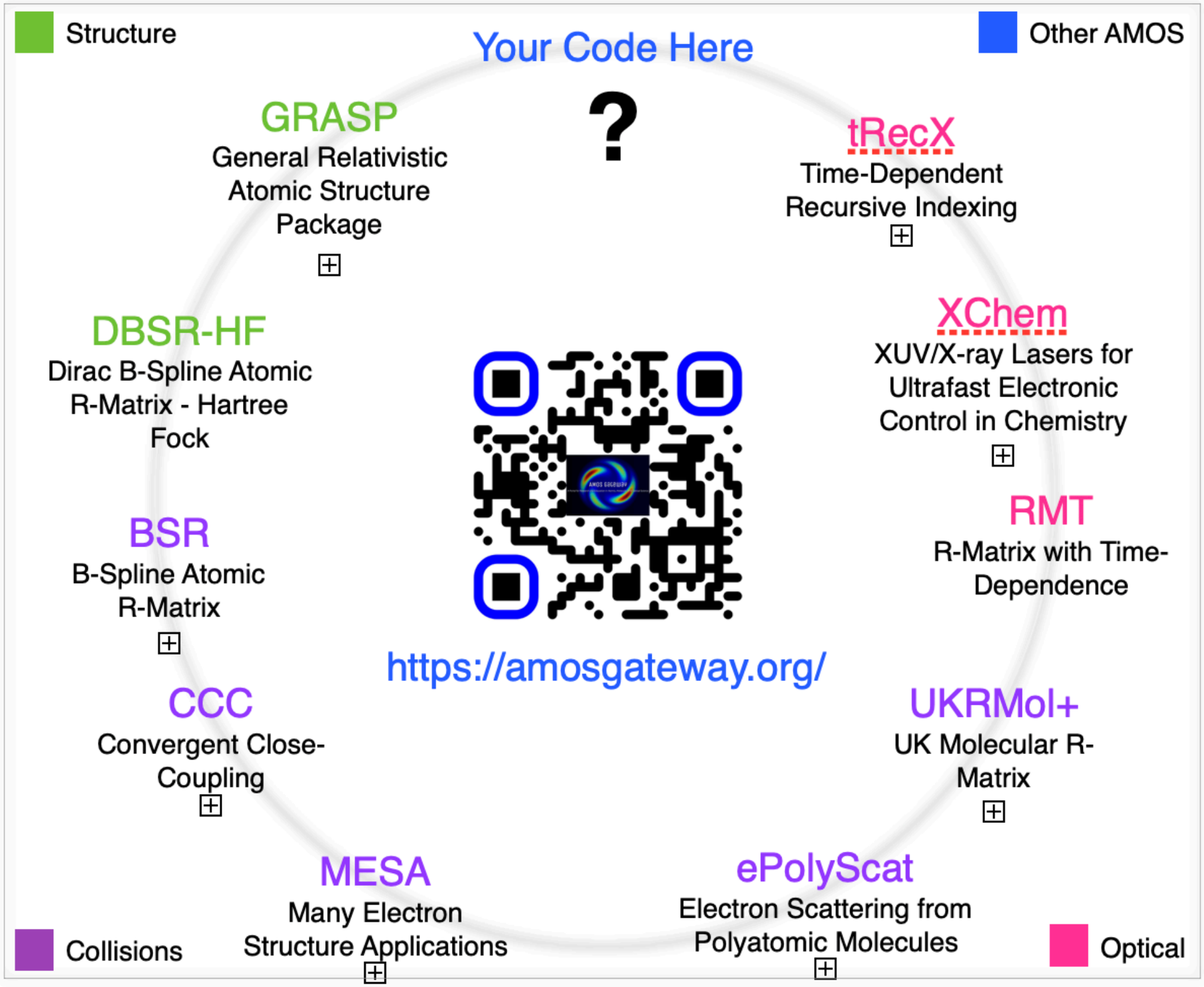
Jesus González-Vásquez, UAM, Spain

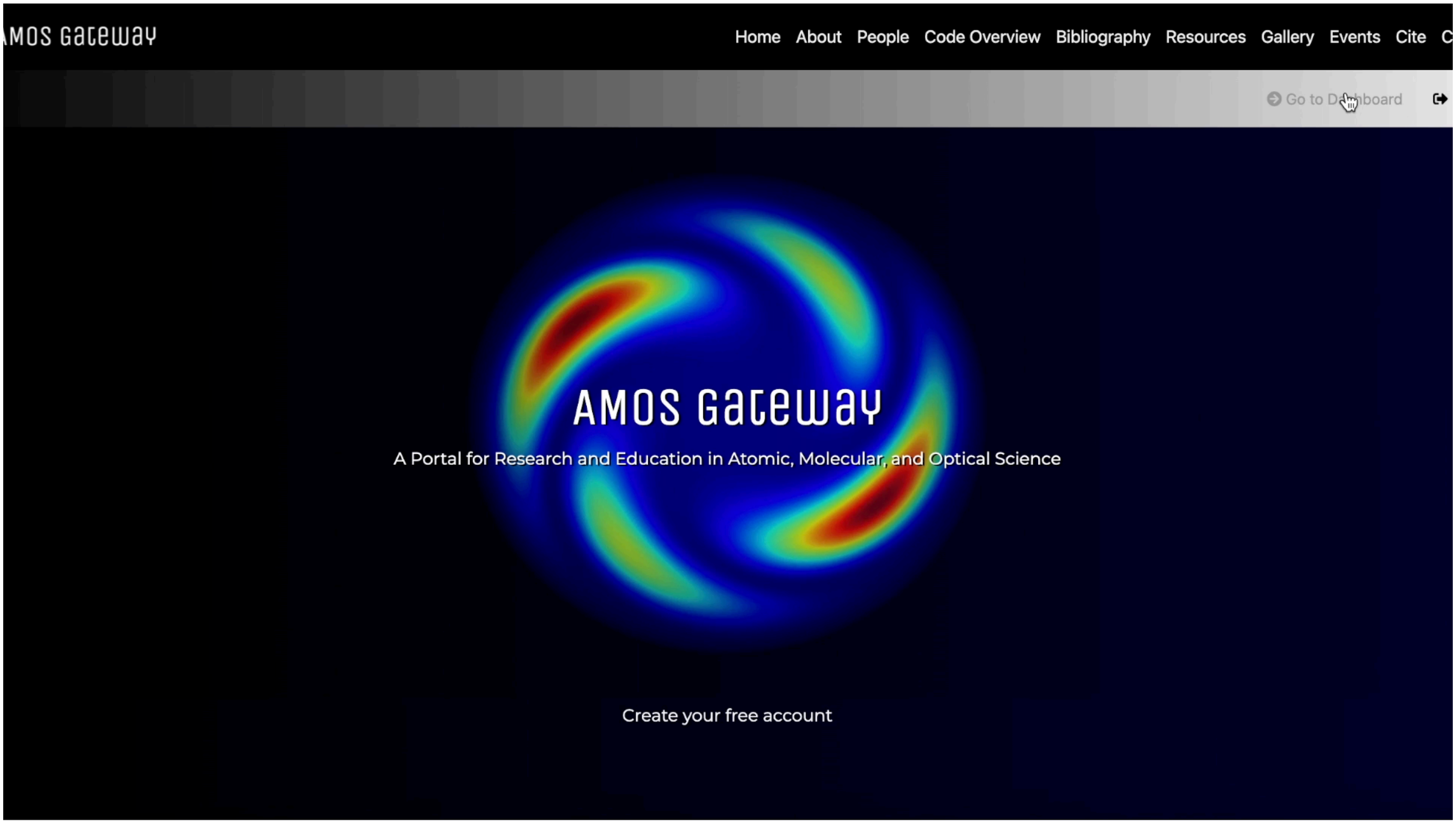
Fernando Martín, UAM, Spain

Armin Scrinzi, LMU, Germany

CURRENTLY HOSTED CODES



AMOS GATEWAY



CONCLUSIONS

- Lots of data out there!
- Important to know the limitations of data you choose to use
- Collaboration is always welcome
- AMOSGateway allows you to try out some scattering codes, even with minimal experience

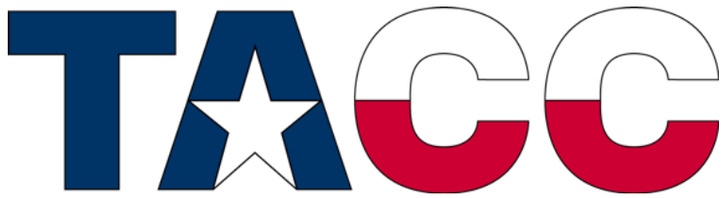
THANK YOU!


Drake
UNIVERSITY


NSF


University of Colorado
Denver


XSEDE


TACC


UK
AMOR

QUESTIONS?

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Slides available on request