



# The 14th International Colloquium on Atomic Spectra and Oscillator Strengths for Astrophysical and Laboratory Plasmas

ASOS14, July 10 – 13, 2023, Paris, France

## Programme and Abstracts



<https://asos2023paris.sciencesconf.org>

	Sunday	Monday July 10th	Tuesday July 11th	Wednesday July 12th	Thursday July 13th
8:00		Registration			
8:45		Opening			
9:00		IT 1 G. Nave	IT 10 C. Ballance	IT 22 J. Xiao	IT 33 A. Kramida
9:30		IT 2 C. Clear	IT 11 N. Badnell	IT 23 D. H. Kwon	IT 34 C. Mendoza
10:00		IT 3 C. Pagan	IT 12 P. Uylings	IT 24 N. Paul	IT 35 C. Zwolf
10:30		Coffee break	Coffee break	Coffee break	Coffee break
11:00		IT 4 F. Delahaye	IT 13 J. Mao	IT 25 Priti remote	IT 36 Dipti
11:30		IT 5 K. Hotokezaka	IT 14 J. Berengut remote	IT 26 A. Fairchild	IT 37 M. O'Mullane
12:00		IT 6 J. Deprince	IT 15 M. Murphy remote	IT 27 S. Kroger	C 6 M. Godefroid
12:15					Closure
12:30		Lunch	Lunch	Lunch	Lunch
13:45		IT 7 P. Hayden	IT 16 A. Ritchey	IT 28 W. Wen	
14:15		IT 8 A. Meftah Tribute to JF Wyart	C 2 N. De Olivera	IT 29 M. T. Belmonte	
14:30			IT 17 A. Amarsi		
14:45		IT 9 M. Lepers Tribute to JF Wyart		C 3 E. Takacs	
15:00			IT 18 W. Li	C 4 L. Duval	
15:15		C 1 G. Hovhannesian		C 5 H. Hartman	
15:30		Coffee break	Coffee break	Coffee break	
16:00		Poster session 16:00-18:00	IT 19 F. Pajot	IT 30 P. Young remote	
16:30			IT 20 L. Gastaldo	IT 31 A. Foster remote	
17:00			IT 21 H. Nilsson	IT 32 G. Berry remote Tribute to Larry Curtis	
17:30					
18:00	Regist.				
18:30 - 20:30	reception			Conf Dinner 19h30	

**Topics**

Laboratory Data

Theory & Calculations

Astrophysical plasmas

Laboratory plasmas and experiments

Fusion Plasmas

Databases & Data Assessment

**Location**  
**Scientific Sessions :**  
**R. Bilski-Pasquier**  
**Poster session:**  
**Cloister**  
 Reception, Lunch,  
 Coffee break:  
**R. Marie Curie**



# The 14th International Colloquium on Atomic Spectra and Oscillator Strengths for Astrophysical and Laboratory Plasmas

(ASOS14) Paris, July 10 – 13, 2023

The aim of the ASOS conference is to bring together scientists from atomic physics, plasma physics and astrophysics and to bring together the “producers” of fundamental atomic data and the “users” of this data. During the conference, atomic physicists present the development of their theoretical and experimental methods and the possibility of obtaining increasingly complete and precise data on the structures and the radiative and collisional properties of atomic systems. Astrophysicists and plasma physicists review the context of their research and their needs for atomic data for modelling the plasmas studied, such as stellar or solar plasmas, fusion plasmas or other laboratory plasmas.

The conference will be held on the campus "Les Cordeliers" of Sorbonne Université, located at 15, rue de l'Ecole de Médecine, 75006 Paris.

## Scientific Topics

- Need for atomic data from space and ground observations (solar and stellar plasmas, interstellar media, active nuclei of galaxies, quasars, kilonovas)
- Need for atomic data from laboratory experiments (diagnostics of fusion plasmas, plasmas produced by laser)
- Determination of lifetimes and oscillator strengths
- Hyperfine structures, isotopic shifts
- Theoretical modeling and numerical approaches
- Laboratory techniques
- Ion storage
- High resolution spectroscopy
- Variation of fundamental constants
- Collisional processes
- High energy density plasma spectra, opacities
- Spectral line profiles (broadening, shifts, nuclear effects, magnetic field effects, polarization)
- Atomic databases and connected subjects



## **Scientific Organising Committee**

Jorge Reyna Almandos	Optical Research Center (CIOP), Argentina
Beatriz Barbuy	Universidade de Sao Paulo, Brazil
Peter Beiersdorfer	Lawrence Livermore National Laboratory, USA
Thomas Brage (Co-Chair)	Lund University, Sweden
José Crespo-Urrutia	Max Planck Institute for Nuclear Physics (MPIK), Germany
Chen-zhong Dong	Northwest Normal University, China
Marie-Lise Dubernet	Observatoire de Paris-Meudon, France
Tao-tao Fang	Xiamen University, China
Steven Federman	University of Toledo, USA
Mathys Gautier	European Southern Observatory, Chile
Michel Godefroid	Université Libre de Bruxelles, Belgium
Elizabeth den Hartog	University of Wisconsin, USA
Alan Hibbert	Queen's University Belfast, UK
Roger Hutton (Co-Chair)	Fudan University, China
Paul Indelicato	Sorbonne Université and ENS-PSL
Daiji Kato	National Institute for Fusion Science (NIFS), Japan
Alexander Kramida	National Institute of Standards and Technology (NIST), USA
Duck-Hee Kwon	Korea Atomic Energy Research Center (KAERI), Rep. of Korea
Alla Safronova	University of Nevada, USA
Glenn Wahlgren	Space Telescope Science Institute, USA
Jun Xiao	Fudan University, China
Claude Zeppen	Observatoire de Paris-Meudon, France

## **Local Organising Committee**

Christian Balança	LERMA, Observatoire de Paris-PSL and Sorbonne Université
Emi Briquet	LERMA, Observatoire de Paris-PSL and Sorbonne Université
Norbert Champion	LERMA, Observatoire de Paris-PSL and Sorbonne Université
Franck Delahaye	LERMA, Observatoire de Paris-PSL and Sorbonne Université
Marie-Lise Dubernet	LERMA, Observatoire de Paris-PSL and Sorbonne Université
Paul Indelicato	LKB, Sorbonne Université and ENS-PSL
Richard Monier	LESIA, Observatoire de Paris-PSL and Sorbonne Université
Lydia Tchang-Brillet (Chair)	LERMA, Observatoire de Paris-PSL and Sorbonne Université

## Conference Programme

### Sunday 9 July

18:00        **Registration (Room Marie Curie, Campus “Les Cordeliers”)**

18:30 – 20:30 **Welcoming Reception (Room Marie Curie, Campus “Les Cordeliers”)**

### Monday 10 July

8:00 – 8:45    **Registration (Room Club, Campus “Les Cordeliers”)**

8:45 – 9:00    **Opening (Room Bilski-Pasquier)**

9:00 – 9:30    **Gillian Nave** **IT 1**  
(National Institute of Standards and Technology, Gaithersburg, MD, USA)  
*A New Approach to the Analysis of Experimental Atomic Spectra*

9:30 – 10:00 **Christian Clear** **IT 2**  
(Imperial College London, London, United Kingdom)  
*The Imperial College Spectroscopy Group: High Accuracy Atomic Data for Astrophysics*

10:00 – 10:30 **Cesar J. B. Pagan** **IT 3**  
(School of Electric and Computing Engineering of the University of Campinas, Campinas, Brazil)  
*Revised and Extended Analysis of Argon V – VII*

10:30 – 11:00 **Coffee break (Cloister)**

11:00 – 11:30 **Franck Delahaye** **IT 4**  
(LERMA, Observatoire de Paris-PSL, Sorbonne Université, Paris, France)  
*New Astrophysical Opacities from The Opacity Project*

11:30 – 12:00 **Kenta Hotokezaka** **IT 5**  
(University of Tokyo, Tokyo, Japan)  
*Kilonova and Neutron Star Merger Plasma*

12:00 – 12:30 **Jerôme Deprince** **IT 6**  
(Université Libre de Bruxelles & Université de Mons, Belgium)  
*Lanthanide and Actinides Opacity Computations for Kilonova Modeling*

12:30 – 13:45 **Buffet - Lunch (Room Marie Curie)**

13:45 – 14:15 **Patrick Hayden** **IT 7**  
(University College Dublin, Dublin, Ireland)  
*4f Photoabsorption in Pt II to Pt V*

14:15 – 14:45 **Ali Meftah** **IT 8**  
(Université Mouloud Mammeri, Algeria, & Observatoire de Paris, France)  
*Present Status of the Investigation on the Spectra of Moderately Charged Thulium Ions*  
*A tribute to Jean-François Wyart*

14:45 – 15:15 **Maxence Lepers** **IT 9**  
(CNRS & Université de Bourgogne Franche-Comté, Dijon, France)  
*Atomic-Structure Calculations for Ultracold Gases of Lanthanides*  
*A tribute to Jean-François Wyart*

15 :15 – 15 :30 **Gohar Hovhannesian** **OC 1**  
(CNRS & Université de Bourgogne Franche-Comté, Dijon, France)  
*Transition Intensities of Trivalent Lanthanide Ions in Solids:*  
*Extension of Judd-Ofelt Theory on  $\text{Eu}^{3+}$ ,  $\text{Nd}^{3+}$  and  $\text{Er}^{3+}$*

15:30 – 16:00 **Coffee Break (Cloister)**

16:00 – 18:00 **Poster Session (Arcades of the Cloister)**

## Tuesday 11 July

9:00 – 9:30 **Connor Ballance** **IT 10**  
(Queen's University of Belfast, Belfast, United Kingdom)  
*An Overview of Recent R-Matrix Developments with a Focus on*  
*Heavy Neutron-Star Merger and Magnetically-Confined Fusion Elements*

9:30 – 10:00 **Nigel Badnell** **IT 11**  
(University of Strathclyde, Glasgow, United Kingdom)  
*A FAC potential for AUTOSTRUCTURE*

10 :00 – 10:30 **Peter Uylings** **IT 12**  
(University of Amsterdam, Amsterdam, The Netherlands)  
*Orthogonal Operators: Extension to Hyperfine Structure*

10:30 – 11:00 **Coffee Break (Cloister)**

11:00 – 11:30 **Junjie Mao** **IT 13**  
(Tsinghua University, Beijing, China)  
*Electron-Impact Excitation Data for Astrophysical Plasma Diagnostics*

11:30 – 12:00 **Julian Berengut (remote)** **IT 14**  
(University of New South Wales, Sydney, Australia)  
*Atomic Structure Calculations for New Physics Searches*

12:00 – 12:30 **Michael Murphy (remote)** **IT 15**  
(Swinburne University of Technology, Melbourne, Australia)  
*Testing the Constancy of Electromagnetism's Strength with Dark*  
*Matter Density Using Stellar Twins*

12:30 – 13:45 **Buffet - Lunch (Room Marie Curie)**

13:45-14:15 **Adam Ritchey** **IT 16**  
(Eureka Scientific, USA)  
*Improvements in Oscillator Strengths and their Impact on*  
*Interstellar Abundances and Depletions*



- 14:15 – 14:30 **Nelson De Olivera** **OC 2**  
 (Synchrotron Soleil, Saint-Aubin, France)  
*High Resolution Vacuum Ultraviolet Absorption Spectroscopy:  
 Determination of Reactive Species' Oscillator Strengths*
- 14:30 - 15:00 **Anish Amarsi** **IT 17**  
 (Uppsala University, Uppsala, Sweden)  
*Atomic Data for 3D Non-LTE Solar and Stellar Spectroscopy*
- 15:00 – 15:30 **Wenxian Li** **IT 18**  
 (National Astronomical Observatories, Beijing, China)  
*Coronal Magnetic Field Measurements from EUV Wavelengths*
- 15:30 – 16:00 **Coffee Break (Cloister)**
- 16:00 – 16:30 **François Pajot** **IT 19**  
 (CNRS, Université Toulouse 3, Toulouse, France)  
*The Athena X-ray Observatory Integral Field Unit (X-IFU):  
 New Perspectives in the Study of the Universe Using High Resolution  
 X-ray Spectroscopy*
- 16:30 – 17:00 **Loredana Gastaldo** **IT 20**  
 (Heidelberg University, Heidelberg, Germany)  
*Metallic Magnetic Calorimeters for High Precision of  
 X-Ray Spectroscopy*
- 17:00 – 17:30 **Hampus Nilsson** **IT 21**  
 (Malmö University, Malmö, Sweden)  
*Laboratory Atomic Astrophysics at Malmö University with  
 Emphasis on the Infrared Spectral Region*

### Wednesday 12 July

- 9:00 – 9:30 **Jun Xiao** **IT 22**  
 (Fudan University, Shanghai, China)  
*Spectroscopy Studies of Moderately Charged Tungsten, Sulfur,  
 and Chlorine Ions at the SH-HTSCEBIT*
- 9:30 – 10:00 **Duck-Hee Kwon** **IT 23**  
 (Korea Atomic Energy Research Institute, Daejeon, Korea)  
*Modeling for Spectroscopic Diagnostics of CCP-ICP and  
 PBIF Plasmas in KAERI*
- 10 :00 – 10:30 **Nancy Paul** **IT 24**  
 (Sorbonne Université, Paris, France)  
*Probing Strong Field Quantum Electrodynamics through Precision  
 Spectroscopy of Highly Charged Ions and Exotic Atoms*
- 10:30 – 11:00 **Coffee Break (Cloister)**

- 11:00 – 11:30 **Priti (remote)** **IT 25**  
 (National Institute for Fusion Science, Gifu, Japan)  
*Hyperfine Resolved Laser Spectroscopy of Highly Charged  $I^{7+}$  Ions*
- 11:30 – 12:00 **Alexander Fairchild** **IT 26**  
 (Columbia University, New York, USA)  
*High-Resolution Laboratory Measurements of near Ar-like Fe EUV Line Emission Using EBIT-I*
- 12:00 – 12:30 **Sophie Kröger** **IT 27**  
 (Hochschule für Technik und Wirtschaft Berlin, Berlin, Germany)  
*Laboratory Measurements of Hyperfine Structure*
- 12:30 – 13:45 **Buffet - Lunch (Room Marie Curie)**
- 13:45 - 14:15 **Weiqiang Wen** **IT 28**  
 (IMPCAS, Lanzhou, China)  
*Storage Ring Measurements for Dielectronic Recombination of Na-like  $Fe^{15+}$*
- 14:15 - 14:45 **Maria Teresa Belmonte Sainz Ezquerro** **IT 29**  
 (University of Valladolid, Valladolid, Spain)  
*Measuring Transition Probabilities of Rare-Earths: Experimental Requirements and Challenges*
- 14:45 - 15:00 **Endre Takacs** **OC 3**  
 (Clemson University, Clemson, SC, USA)  
*Hyperfine Interaction Affecting the Charge-State Distribution of Highly Charged Ion Plasma*
- 15:00 – 15:15 **Louis Duval** **OC 4**  
 (LKB, Sorbonne Université, CNRS, ENS-PSL, Paris, France)  
*Study of B-Like Ions X-Ray Emission Spectra in an Electron-Cyclotron Resonance Ion Source Plasma*
- 15:15 - 15:30 **Henrik Hartman** **OC 5**  
 (Malmö University, Malmö, Sweden)  
*Experimental Metastable Lifetimes at DESIREE Storage Ring – First Stop : Barium*
- 15:30 – 16:00 **Coffee Break (Cloister)**
- 16:00 – 16:30 **Peter Young (remote)** **IT 30**  
 (NASA GSFC, Greenbelt, MD, USA)  
*Applications of Atomic Data to Studies of the Sun*
- 16:30 – 17:00 **Adam Foster (remote)** **IT 31**  
 (Center for Astrophysics, Harvard and Smithsonian, Cambridge, USA)  
*Evaluating Atomic Data Needs for X-RAY Astrophysics with the AtomDB Atomic Database*

17:00 – 17:30 **Gordon Berry (remote)** **IT 32**  
(Professor Emeritus, University of Notre Dame, Notre Dame, IN, USA)  
*Larry J Curtis 1935-2020: A Brief History: His Revelations in Atomic  
Structure and Dynamics*

**19:30 - Conference Dinner at the restaurant “Chez Françoise”**

### **Thursday 13 July**

9:00 – 9:30 **Alexander Kramida** **IT 33**  
(National Institute of Standards and Technology, Gaithersburg, MD, USA)  
*Evaluation of Uncertainties in Atomic Data on Spectral Lines  
and Transition Probabilities*

9:30 – 10:00 **Claudio Mendoza** **IT 34**  
(Venezuelan Institute for Scientific Research, Venezuela)  
*The XSTAR Atomic Database*

10 :00 – 10:30 **Carlo-Maria Zwolf** **IT 35**  
(Observatoire de Paris, Paris, France)  
*Assessment of the FAIRness of the Virtual Atomic and Molecular Data  
Centre Following the Research Data Alliance Evaluation Framework*

10:30 – 11:00 **Coffee Break (Cloister)**

11:00 – 11:30 **Dipti** **IT 36**  
(International Atomic Energy Agency, Vienna, Austria)  
*Charge Exchange Recombination Spectroscopy of W Ions for ITER Neutral  
H-Beam Diagnostics*

11:30 – 12:00 **Martin O’Mullane** **IT 37**  
(University of Strathclyde, Glasgow, United Kingdom)  
*Magnetically-Confined Nuclear Fusion and Atomic Data*

12:00 – 12:15 **Michel Godefroid** **OC 6**  
(Université libre de Bruxelles, Brussels, Belgium)  
*GRASP and COMPAS for ASOS*

12:15 – 12:30 **Closure of the conference**

12:30 – 13:45 **Buffet - Lunch (Room Marie Curie)**

**Poster Session**  
**(List of posters and presenting authors)**

**P1** Laser Spectroscopy of the Zeeman-hf Structure of Atomic Niobium  
Lukasz Sobolewski (University of Gdansk, Gdansk, Poland)

**P2** New Experimental Energy Levels, Lifetimes and Oscillator Strengths in Singly Ionised Zirconium  
Madeleine Burheim (Malmö University, Malmö, Sweden)

**P3** The Spectrum and Energy Levels of Doubly Ionised Neodymium  
Milan Ding (Imperial College London, London, UK)

**P4** Revised Energy Levels of Atomic Holmium Considering Hyperfine Structure in Fourier Transform Spectra  
Gönül Başar (Istanbul University, Istanbul, Turkey)

**P5** Characterization of a Hollow-Cathode Lamp to Measure Accurate Transition Probabilities of Rare-Earth Elements  
Pratyush Ranjan Sen Sarma (University of Valladolid, Valladolid, Spain)

**P6** A Joint Theoretical and Experimental Approach to Dielectronic Recombination Data for Photoionized Astrophysical Environments  
Michael Fogle (Auburn University, Auburn, AL, USA)

**P7** Extended Analysis of the VUV Emission Spectrum of the Free Ion  $\text{Er}^{+2}$  (Er III)  
Sofiane Ait Mammar (Université Mouloud Mammeri, Tizi-Ouzou, Algeria)

**P8** Energy Levels and Transition Data of Au IV  
Haris Kunari (Aligarh Muslim University, Aligarh, India)

**P9** Doubly-Ionised Iron: New Accurate Wavelengths and Energy Levels  
Florence Concepcion (Imperial College London, London, UK)

**P10** Multiplatform Determination of the Radiative Properties of the Seventh Spectrum of Tantalum (Ta VII)  
Patrick Palmeri (Université de Mons, Mons, Belgium)

**P11** JAC: A Community Platform for Just Atomic Computations  
Stephan Fritzsche (Helmholtz-Institut Jena, Jena, Germany)

**P12** Theoretical Study of Spectra of Hf VI Using a Multiplatform Approach  
Exaucé Bokamba Motoumba (Université Marien Ngouabi, Brazzaville, Congo)

**P13** The Effect of Electron Correlation on Trielectronic Recombination Rate Coefficients for Be-like Argon  
Chunyu Zhang (Fudan University, Shanghai, China & University of Strathclyde, Glasgow, UK)

**P14** The Fingerprints of Periodic Electric Fields on Line Shapes Emitted in Plasmas  
Ibtissem Hannachi (Batna 1 University, Batna, Algeria)

**P15** Semi-Empirical Determination of Radiative Parameters for Singly Ionized Atom of Cobalt  
Marcin Klempka (Poznan Univeristy of Technology, Poznan, Poland)

**P16** Hyperfine Splittings of Few-Electron Heliumlike Ions and Nuclear Properties  
Zongchao Yan (Wuhan Institute of Physics and Mathematics, Wuhan, China & University of New Brunswick, Fredericton, Canada)

**P17** Energy and Properties of Sb-Like  $\text{Nd}^{9+}$ , P-Like, As-Like, Sb-Like, Bi-Like and Mc-Like  $np^3$  Atoms and Ions  
Yanmei Yu (Institute of Physics, Chinese Academy of Sciences, Beijing, China)

**P18** Multiconfiguration Dirac-Hartree-Fock Calculations of the Hyperfine Structure in 137-Ba II for the  $^2S_{1/2}$  State  
Lucas Maison (Université De Mons, Mons, Belgium)

**P19** Alignment-Transfer Rate Coefficients for Electron Impact Excitation of O V  
Mokhtar Inal (Université Aboubekr Belkaid, Tlemcen, Algeria)

**P20** Calculated Oscillator Strengths for Spectral Lines in Re III-V Ions of Interest to Nuclear Fusion Research  
Pascal Quinet (Université De Mons & Université de Liège, Belgium)

**P21** Effect of the Breit Interaction on the Angular Distribution of Auger Electrons Following Electron-Impact Excitation of Be-Like Ions  
Zhongwen Wu (Northwest Normal University, Lanzhou, China, & Helmholtz-Institut Jena, Germany)

**P22** Quasi-Molecular Mechanism of Cosmological Recombination  
Tamaz Kereselidze (Tbilisi State University, Tbilisi, Georgia)

**P23** An Atomic Data Optimization Method for Improved Kilonova Opacity Modeling  
Ricardo Ferreira Da Silva (Universidade de Lisboa, Lisboa, Portugal)

**P24** Exploring Ab-Initio and Semi-Empirical Small-Scale Atomic Structure Models of Neutron-Capture Elements  
Sema Caliskan (Uppsala University, Uppsala, Sweden)

**P25** A Variational Atomic Model of Plasma Accounting for Ion Radial Correlations and Electronic Structure of Ions  
Robin Piron (CEA & Université Paris-Saclay, Bruyères-le-Châtel, France)

**P26** Stellar Opacities in Lab Using a High Intensity Laser  
Hanna Lahmar (Laboratoire pour l'Utilisation des Lasers Intenses, Palaiseau, France)

**P27** Erbium Optical Spectra From Pellet Ablation Cloud in the Large Helical Device for Laboratory Assessment of Atomic Data  
Priti (National Institute for Fusion Science, National Institutes of Natural Sciences, Toki, Japan)

**P28** Study of B-Like Ions X-Ray Emission Spectra in an Electron-Cyclotron Resonance Ion Source Plasma  
Louis Duval (Laboratoire Kastler Brossel, Paris, France)

**P29** Transition Probability Measurements for Lanthanide Elements Using Laser-Induced Breakdown Spectroscopy

Supriya Kodangil (University of Electro-Communication, Tokyo, Japan)

**P30** High-Resolution TALIF Spectroscopy for Optical Diagnostics in Cold Plasmas

Cyril Drag (Laboratoire de Physique des Plasmas, Palaiseau, France)

**P31** Development and Commissioning of the UNIST Electron Beam Ion Trap for X-Ray Spectroscopy of the Highly Charged Ions at PAL-XFEL

Sung Nam Park (Ulsan National Institute of Science and Technology, Ulsan, Korea)

**P32** Metastable Lifetime Measurements at the DESIREE Storage Ring - First Stop : Barium

Henrik Hartman (Malmö University, Malmö, Sweden)

**P33** Atomic Data and Opacity Calculations in Moderately Charged Lanthanide Ions in the Context of Kilonova Emission Modeling

Helena Carvajal Gallego (Université de Mons, Mons, Belgium)

**P34** Atomic Data and Opacity Calculations in Nb, Ag, Hf, Os and Au Ions for Kilonova Spectral Analyses

Sirine Ben Nasr (Université de Mons, Mons, Belgium)

**P35** Atomic Calculations for V - XI Ionized R-Process Elements for Early Kilonova

Smaranika Banerjee (Stockholm University, Stockholm, Sweden)

**P36** Detailed NLTE Abundance Analysis of 20 Nuclear Stellar Cluster/Disk Stars

Brian Thorsbro (Observatoire de La Côte d'Azur, Nice, France)

**P37** Transition Data for Neutral Carbon Rydberg Levels Benchmarked Against Solar UV Observations

Roger Dufresne (University of Cambridge, Cambridge, UK)

**P38** Japan-Lithuania Opacity Database for Kilonova

Daiji Kato (National Institute for Fusion Science, Toki, & Kyushu University, Japan)

## Invited Talks





## A New Approach to the Analysis of Experimental Atomic Spectra

Gillian Nave<sup>a\*</sup>, Christian P. Clear<sup>b</sup>, Jacob W. Ward<sup>c</sup>

<sup>a</sup>National Institute of Standards and Technology, Gaithersburg MD 20899, USA,

<sup>b</sup>Imperial College London, London SW7 2AZ, UK,

<sup>c</sup>Los Alamos National Laboratory, Los Alamos, NM 87545, USA.

Atomic spectroscopy is a vital field providing crucial reference data for applications ranging from astrophysics to fusion research and industrial applications. Despite its importance, the number of groups and people active in the field has been decreasing steadily over the past few decades and it is unlikely that this is going to change any time soon. Although we can, and should, advocate for more funding for atomic spectroscopy, it is incumbent on us to ensure that we are applying our limited resources in the most efficient way possible. One way we can do that is by sharing data and by improving the software tools that we use.

Many of the spectra recorded on our spectrometers can be used for multiple purposes – for example spectra recorded for the analysis of a neutral atom may include many lines of the singly-ionized atom, and can be used to measure wavelengths, oscillator strengths, and hyperfine structure. Reuse of these data has frequently relied on ad-hoc collaborations, but this has proved inefficient when the history of the data processing has been lost or inadequately documented, as is often the case when groups rely on summer students to boost their dwindling resources. Much of the software that is used to analyze atomic spectra is old, having been written in the 1970's and 1980's by titans of the field, who made the most of limited computer resources using computer languages that are rarely taught to students now. Since these codes contain valuable knowledge regarding the analysis of spectra, there is an unwillingness to re-write them, and instead, each researcher writes a custom wrapper to analyze their data, repeating the same basic tasks that have been done before. There is a better way.

We are working on new software and data formats using the Hierarchical Data Format 5 file format (HDF5 [1]). This format is designed for heterogeneous data and facilitates easy sharing, cross-platform support, version control, and the ability to store metadata with the data. We anticipate that this format will enable easier sharing of spectral data and better logging of analysis that has already been performed. Extensive python libraries are available that will enable us to embed previous knowledge in a way that can be understood and extended by future researchers. Our software is initially focusing on the measurement of branching fractions and oscillator strengths using spectra from Fourier transform spectrometers, but we plan to extend its scope to replace many of our current programs for analyzing other atomic data. This will require a more extensive team than the three coauthors of this paper, and thus we are actively seeking collaborators for this project. I shall describe our vision for the structure of the HDF5 files used for our data and the programs that we are developing for their analysis.

### References

[1] <https://hdfgroup.org/solutions/hdf5>

\*email: [gilliannave@gmail.com](mailto:gilliannave@gmail.com)

## The Imperial College Spectroscopy Group: High Accuracy Atomic Data for Astrophysics

Christian P. Clear<sup>a\*</sup>, Juliet C. Pickering<sup>a</sup>, Florence Concepcion<sup>a</sup> and Milan Ding<sup>a</sup>

<sup>a</sup>Physics Department, Imperial College London, London, SW7 2AZ, UK

Modern advancements in telescopes and astronomical spectroscopy have revolutionised our understanding of the universe, providing us with unprecedented high-resolution astronomical spectra across many spectral regions. However, the accurate interpretation of these spectra, collected at great effort and expenditure of resources, crucially depends on the availability of precise laboratory atomic data. The Imperial College (IC) Spectroscopy group has taken up the challenge of meeting this acute need by employing Fourier transform spectroscopy (FTS) to measure atomic spectra of many astrophysically important elements. Our analyses of these laboratory spectra have resulting in significant improvements in the breadth and accuracy of atomic data.

Our work focuses on measuring new atomic data and enhancing the precision of existing data for a wide range of astrophysically important elements, including the iron group elements, which hold special significance due to their high abundances and multitude of electronic transitions, and, more recently, the rare earth elements, which are involved in r-process nucleosynthesis. Through the analysis of high-resolution spectra, we have achieved substantial reductions in uncertainties for transition wavelengths and energy levels, often exceeding an order of magnitude, while transition probabilities can be measured with uncertainties of just a few percent. The high resolution of FTS also enables line broadening effects such as hyperfine and isotope structure, crucial data for accurate stellar abundance measurements, to be determined.

The significance of our work extends beyond the current state of astronomical research. As the field continues to advance, telescopes such as the Extremely Large Telescope and the James Webb Space Telescope will continue to drive the demand for further improvements in atomic data. To ensure that the IC spectroscopy group can continue our work providing the data vital for these instruments, we are expanding our measurement capability into the infrared with the addition of a new high-resolution Fourier transform spectrometer.

In this talk, we present some of the most recent results of our spectroscopic analyses, discuss our future research plans and emphasize the critical role of accurate atomic data in modern astronomical research.

\*email: christian.clear@imperial.ac.uk

## Revised and Extended Analysis of Argon V – VII

Cesar J B Pagan<sup>a,\*</sup>, Mónica Raineri<sup>b</sup>, Mario Gallado<sup>b</sup>, Jorge Reyna Almandos<sup>b</sup>

<sup>a</sup> School of Electric and Computing Engineering of the University of Campinas, Brazil

<sup>b</sup> Centro de Investigaciones Opticas, La Plata, Argentina

This project revisits the spectral analysis of argon's fourth to sixth ionization stages (Ar V-VII). We revised the experimental data's wavelengths, uncertainties, and intensity using the techniques for intensity and wavelength correction of the observed lines proposed by Alexander Kramida [1,2]. These techniques are used on data from a single set of experiments performed at the Centro de Investigaciones Opticas, La Plata, designed to cover the region from the vacuum ultraviolet to visible. We looked for all previously known lines in our reference spectrograms, which produced a table with wavelengths analyzed as a single set. This analysis also includes lines classified for the first time in this work.

Another work front is on atomic structure calculations. The increased computing power of the past decades offers possibilities that were not available when much of the original analysis work was done. More configurations have been used to elaborate isoelectronic sequences to compare experimental and theoretical values and to model least-squares fits with much more configurations. Other methodological additions include atomic core polarization effects in calculating energy and transition rates, statistical comparisons between observed line intensities, and transition rates corrected to take the population of the higher levels into account.

In this presentation, we will summarize the results obtained, including some new data on Ar VII and additions we made in our previous study of Ar V-VI [3,4].

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- \*email: pagan@unicamp.br

## New Astrophysical Opacities from The Opacity Project

Franck Delahaye<sup>a</sup>, C. Ballance<sup>b</sup>, N. Badnell<sup>c</sup>, C. Ramsbottom<sup>b</sup>, R. Smyth<sup>b</sup>, M. McCann<sup>b</sup>

<sup>a</sup>LERMA, Sorbonne Université - Paris Observatory, Meudon Campus, 92190 Meudon, France

<sup>b</sup>ARC, School of Mathematics and Physics, Queen's University, Belfast BT7 1NN, UK

<sup>c</sup>Department of Physics, University of Strathclyde, Glasgow G4 0NG, UK

A detailed comparison of the results between two methods used to calculate opacities has been assessed[1]. As well as trying to understand the underlying differences between the measured Fe opacities at the Sandia National Laboratory [2] and prior theoretical calculations, a new set of monochromatic opacities for key Fe ion stages have been calculated. These ion stages are important contributors to the Rosseland opacities for the physical conditions characterizing the base of the Solar convection zone, and have been calculated in the framework of the Opacity Project approach. These new data sets are being tested on solar models. These new results pave the way in defining the best way for future calculations to be integrated into the Opacity Project for a new updated release of monochromatic, Rosseland and Planck mean opacities as well as radiative accelerations.

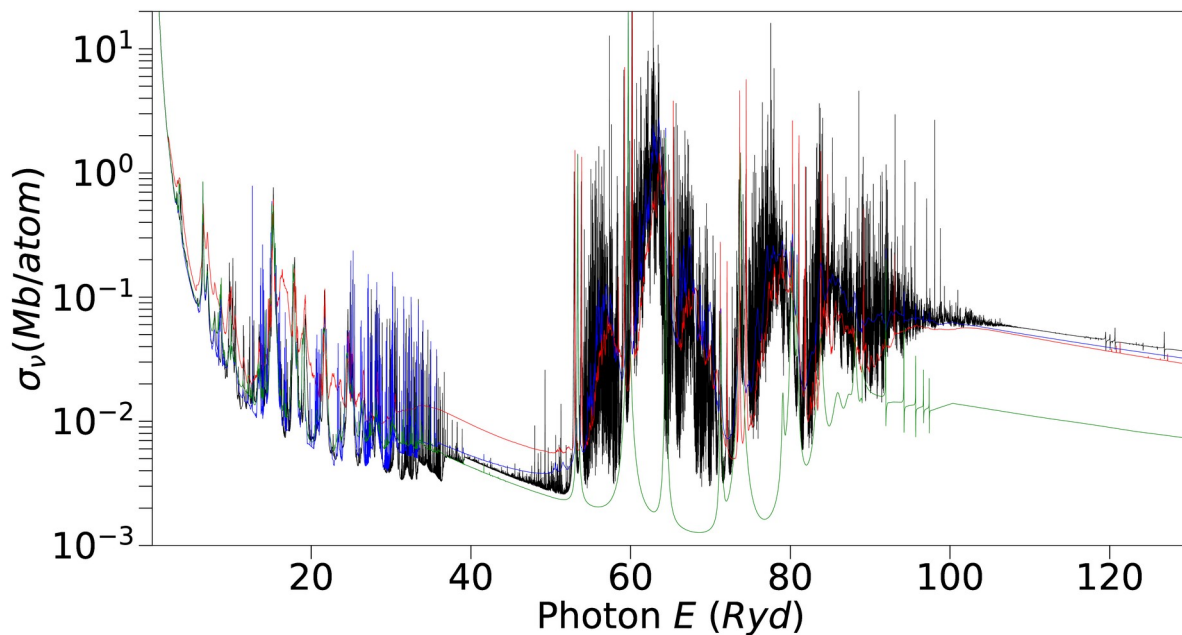


Figure 1: Fe XVII monochromatic opacity cross sections. R-Matrix n=6 (black), AutoStructure with autoionizing states (red), The Opacity Project 1<sup>st</sup> release 1996 (green), The Opacity Project 2<sup>nd</sup> release 2005 (blue).

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\*email: franck.delahaye@observatoiredeparis.psl.eu

## Kilonova and Neutron Star Merger Plasma

Kenta Hotokezaka<sup>a,\*</sup>

*<sup>a</sup>Research Center for the Early Universe, Graduate School of Science, University of Tokyo,  
Bunkyo, Tokyo 113-0033, Japan*

Neutron star mergers produce not only strong gravitational wave signals but also a substantial amount of neutron rich ejecta. The expanding neutron rich ejecta has been considered as a natural astrophysical environment of rapid neutron capture process (r-process) nucleosynthesis. Radioactive decay of freshly synthesized r-process nuclei continuously heats the ejecta and powers an optical-infrared transient, a so-called kilonova. A kilonova was detected after the first neutron star merger event, GW170817. To model the kilonova emission, we need to compute radiation transfer of the expanding ejecta composed of heavy elements and plasma condition of the ejecta. Here, we review the current status of the kilonova modeling and possible elemental identification in the spectra of the kilonova in GW170817. We also discuss the progress in the plasma modeling of kilonova nebulae [1,2].

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\*email: kentah@g.ecc.u-tokyo.ac.jp

## Lanthanide and Actinide Opacity Computations for Kilonova Modeling

J. Deprince<sup>a,b\*</sup>, H. Carvajal Gallego<sup>b</sup>, M. Godefroid<sup>c</sup>, S. Goriely<sup>a</sup>, P. Palmeri<sup>b</sup>, P. Quinet<sup>b,d</sup>

<sup>a</sup>Astronomy and Astrophysics Institute, Université Libre de Bruxelles, 1050 Brussels, Belgium

<sup>b</sup>Atomic Physics and Astrophysics, Université de Mons, 7000 Mons, Belgium

<sup>c</sup>SQUARES, Université Libre de Bruxelles, 1050 Brussels, Belgium

<sup>d</sup>IPNAS, Université de Liège, Sart Tilman, 4000 Liège, Belgium

The production of elements heavier than iron in the Universe still remains an unsolved mystery. About half of them are thought to be notably produced by the astrophysical r-process (rapid neutron-capture process) [1], for which one of the most promising production sites are neutron star mergers (NSMs), known as kilonova [2]. In August 2017, gravitational waves generated by a NSM event were detected by the LIGO detectors (event GW170817) [3], and the observation of its electromagnetic counterpart, the kilonova AT2017gfo, suggested the presence of heavy elements in the ejecta [4]. The luminosity and spectra of such kilonova emission depend significantly on the ejecta opacity, which is dominated by millions of lines from f-shell elements produced by the r-process, *i.e.* lanthanides and actinides [5]. Atomic data and opacities for these elements are thus sorely needed to model and interpret kilonova light curves and spectra.

In this context, the present work focusses on atomic data and opacity computations for lanthanides and actinides, for typical ejecta conditions expected one day post-merger, which correspond to the presence of the element first ionization stages only (neutral to trebly-ionized elements). We intend to discuss our new computations of atomic data and expansion opacities for weakly-charged lanthanides and actinides and compare them with previously reported studies (*e.g.*, [6-10]). In order to do so, we used the pseudo-relativistic Hartree-Fock (HFR) method as implemented in Cowan's codes [11], in which the choice of the interaction configuration model is of crucial importance [12]. In particular, we will also discuss the opacity sensitivity to several effects as the core polarization [13] as well as to a calibration procedure in which configuration average energies are adjusted to match data in the literature.

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\*email: [jerome.deprince@ulb.be](mailto:jerome.deprince@ulb.be)

## 4f Photoabsorption in Pt II to Pt V

Patrick Hayden\*, Eric Doyle, Gerry O’Sullivan, and Pdraig Dunne

School of Physics, University College Dublin, Belfield, Dublin 4, Ireland

Platinum is of significant astrophysical interest as it is one of the most abundant elements in the rapid process (r-process) nucleosynthesis peak around mass number  $A = 195$  [1,2]. Its detection in metal-poor stars provides evidence that r-process nucleosynthesis took place at some time in the environment of the star or the location of its formation. There is also interest in isotopic population anomalies [3] where heavier isotopes are seen to dominate the spectrum. The pattern of isotopic composition varies from the widely assumed fractionation formalism, and lighter isotopes are deficient compared to the prediction of a single-parameter fractionation model. While EUV stellar spectroscopy may not be able to unequivocally identify a given ion stage or excitation state of platinum, EUV studies will help laboratory astrophysicists to map laser produced plasma spectra of lowly-ionised platinum in the visible and near infra-red regions of the spectrum which are more accessible to high-resolution, ground and space-based, stellar spectroscopy. EUV photoabsorption of 6th row species is also of interest due to potential applications exploiting their photochemistry.

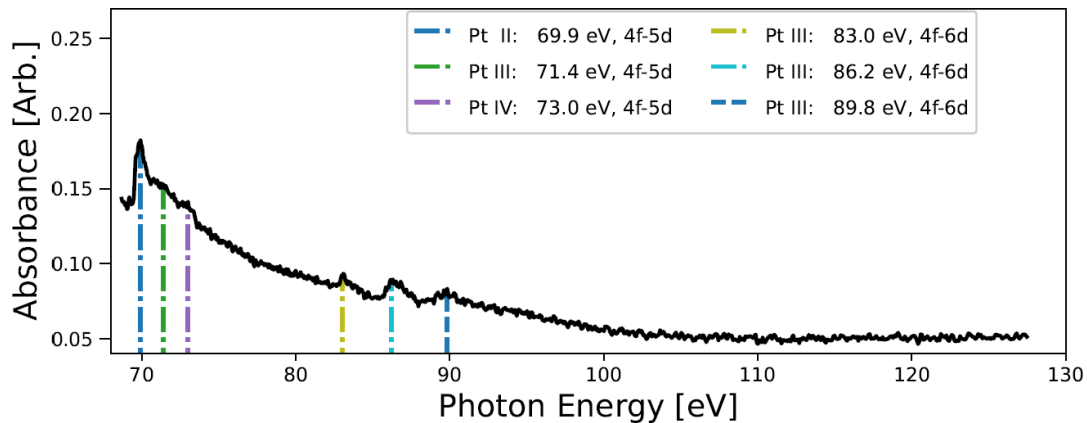


Figure 1: Experimental absorption spectra of laser produced plasmas of platinum, recorded at a delay of 300 ns, showing 4f-nd photoabsorption in  $\text{Pt}^+$ ,  $\text{Pt}^{2+}$  and  $\text{Pt}^{3+}$ .

In this work we present an investigation into the photoabsorption of platinum laser produced plasmas in the 69 - 128 eV region using the dual laser plasma (DLP) method. In this region  $4f \rightarrow 5d$ ,  $4f \rightarrow 6d$  and  $4f \rightarrow 7d$  transitions, broadened by autoionisation, are found in ions  $\text{Pt}^+$ ,  $\text{Pt}^{2+}$ ,  $\text{Pt}^{3+}$ , and  $\text{Pt}^{4+}$ . Analysis of the spectra was supported by atomic structure calculations using the Cowan suite of codes [4], by relativistic time-dependent local-density approximation (RTDLDA) calculations [5].

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\*email: patrick.hayden@ucd.ie

## Present Status of the Investigation on the Spectra of Moderately Charged Thulium Ions

A. Meftah<sup>a,b</sup>, W.-Ü L. Tchang-Brillet<sup>b</sup>, M. Sabri<sup>a</sup>, C. Balança<sup>b</sup>, N. Champion<sup>b</sup>, C. Blaess<sup>b</sup>, E. Bokamba Motoumba<sup>b,c</sup>, J.-F. Wyart<sup>b,d†</sup>

<sup>a</sup>LPCQ, University Mouloud Mammeri, BP17 RP, Tizi-Ouzou, 15000 Algeria

<sup>b</sup>LERMA, Sorbonne Université and Paris Observatory - PSL, CNRS8112, 92190 Meudon, France

<sup>c</sup>Faculté des Sciences et Technique, Université Marien Ngouabi, Brazzaville, BP 69, Congo

<sup>d</sup>Laboratoire Aimé Cotton, CNRS UMR9188, Univ Paris-Sud, ENS Cachan, Univ Paris-Saclay, bâtiment 505, 91405 Orsay CEDEX, France

The present contribution reports recent progress on the analyses of vacuum ultraviolet spectra of several thulium ions. The analyses are based on high resolution spectra emitted by a vacuum spark source recorded in the wavelength range of 350-2960Å on the 10m vacuum ultraviolet spectrograph of the Meudon Observatory. On these spectrograms, lines from the three neighbouring ionisation stages,  $Tm^{2+}$  (Tm III),  $Tm^{3+}$  (Tm IV) and  $Tm^{4+}$  (TmV), are present allowing parallel analyses to be carried on. All spectral analyses are supported by parametric calculations using the package of Cowan's codes [1] and provide level compositions, and consequently, transition probabilities and Landé factors.

For the  $Tm^{4+}$  ion (TmV), more than 300 lines have been identified for the first time as transitions involving 14 levels of the  $4f^{11}$  ground configuration, 37 levels of  $4f^{10}5d$ , 9 levels of  $4f^{10}6p$  and 2 levels of  $4f^{10}6s$ , all previously unknown. The results confirm the very preliminary report [2] on a few levels of this ion.

The first analysis of  $Tm^{3+}$  (Tm IV) was achieved in 2007 [3]. It resulted in the determination of 176 energy levels belonging to the  $4f^{12}$ ,  $4f^{11}5d$ ,  $4f^{11}6s$  and  $4f^{11}6p$  configurations. However, levels of small J values were missing due to weak intensities of the corresponding transitions. In the present work, we extended the analysis and determined additional levels for these configurations and moreover, new levels belonging to the  $4f^{11}6d$  configuration.

The spectrum of  $Tm^{2+}$  (Tm III) analyzed by Sugar [4] has been reinvestigated through his unpublished line list ( $\lambda > 2000\text{Å}$ ), supplemented by the new experimental data in shorter wavelength region.

For the Tm II spectrum that lies in longer wavelength region, a parametric interpretation of the available experimental levels [5, 6] has been carried out. Calculated Landé g-factors values are compared with experimental values when available.

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\*email: [ali.meftah@obspm.fr](mailto:ali.meftah@obspm.fr)

†Passed away in November 2021



## Atomic-Structure Calculations for Ultracold Gases of Lanthanides

Maxence Lepers<sup>a,\*</sup>

<sup>a</sup>Laboratoire Interdisciplinaire Carnot de Bourgogne, CNRS & Université Bourgogne  
Franche Comté, Dijon, France

Lanthanide elements are widely used as trivalent cations in many modern technological applications. Moreover, some neutral lanthanides, like erbium or dysprosium, have been cooled down to the nanokelvin regime by lasers since about 15 years. Indeed, their magnetic moments make them suitable candidates for *e.g.* quantum simulation of solid-state physics [1,2]. Laser-cooling and trapping require that the atoms are submitted to several electromagnetic fields, and so the detailed knowledge of the atomic spectroscopy – excited energy levels and transition probabilities.

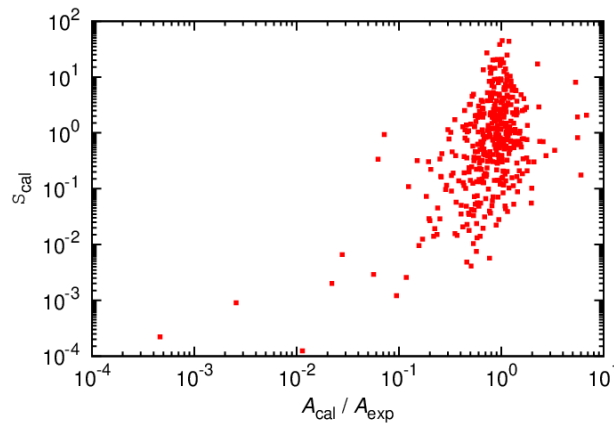


Figure 1: Calculated line strengths  $S_{\text{cal}}$  of  $\text{Er}^+$  as functions of the ratios between our calculated Einstein coefficients and the experimental ones of Ref. [3].

In this presentation, I will describe the work in which I was involved over the last years, regarding the calculations of atomic properties of interest for laser-cooling experiments, like energies, Landé  $g$ -factors, transition probabilities or dynamic dipole polarizabilities. In particular, I will present the *FitAik* program [4], that I have written to calculate  $A_{ik}$  Einstein coefficients, using least-square fitting with experimental values. I will focus on the example of  $\text{Er}^+$  ( $\text{Er II}$ ), see Figure 1, relevant for experiments with ultracold Rydberg  $\text{Er}$  atoms [5].

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\*email: maxence.lepers@u-bourgogne.fr

## An Overview of Recent R-Matrix Developments with a Focus on Heavy Neutron-Star Merger and Magnetically-Confined Fusion Elements

Connor Ballance<sup>a\*</sup>, Ryan Smyth<sup>a</sup>, Nicole Dunleavy<sup>a</sup> and Michael McCann<sup>a</sup>, Stuart Loch<sup>b</sup>,  
Curtis Johnson<sup>b</sup> and David Ennis<sup>b</sup>

<sup>a</sup>School of Maths and Physics, Queen's University of Belfast, Belfast, U.K., BT7 1NN

<sup>b</sup>Department of Physics, Auburn University, Auburn, United States, AL 36849

Both magnetically-confined fusion and astrophysical neutron-star merger plasmas require detailed atomic structure and subsequent collisional calculations (electron-impact excitation/ionization) for heavy atomic elements of the periodic table.

For electron-impact excitation we employ the parallel DARC version of the R-matrix codes (see R-matrix review book of P. G. Burke [1]) and this provides sufficiently accurate electron-impact rates to identify lines for near-neutral tungsten targets [2,3]. However, for electron-impact ionization major revision of the codes has been required to address groundstate and metastable ionization of open-shell heavy systems, such as tungsten. This directly impacts one particular fusion application, as by putting higher accuracy constraints known effective ionization will allow us to determine the impurity influx from tokamak plasma facing components.

From an astrophysical perspective, kilonova observations[4] have identified lines of gold and platinum for which parallel DARC codes are ideally suited to explore the LTE/NLTE assumptions of most previous modelling. I shall report upon this within the talk.

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\*email: C.Ballance@qub.ac.uk

## A FAC POTENTIAL FOR AUTOSTRUCTURE

N. R. Badnell<sup>a</sup> and Chun Yu Zhang<sup>a</sup>

<sup>a</sup>Department of Physics, University of Strathclyde, Glasgow, G4 0NG, UK

General atomic structure and collision codes fall into two broad categories: those which describe multi-channel coupled equations which result from the application of a variational principle (Hartree-Fock, Dirac-Fock, and their extension to the continuum, e.g. R-matrix[1]) and those which use a single channel uncoupled equation (generically labelled distorted-wave) where the choice of distorting potential(s) is essentially a free parameter. Examples of the former include Grant and co-workers' GRASP[2], Froese-Fischer's MCHF[3] and Cowan's HFR[4]. Examples of the latter are AUTOSTRUCTURE (AS)[5], FAC[6], HULLAC[7] and the LANL suite[8]. We focus on the latter group. The FAC, HULLAC and LANL codes are very similar being fully-relativistic and utilize a factorization approach[7] for scattering. To a first approximation they only differ in their choice of a unique distorted-wave potential which leads to a set of orthogonal orbitals. Even here, the Dirac-Fock-Slater potential used by FAC and LANL differ only in their detail. AS is fundamentally different in its formulation of the structure problem. It can use multiple distorted-wave potentials which leads to non-orthogonal orbitals which are treated in the same fashion as Cowan's HFR approach for bound orbitals and include the resulting exchange overlaps for the continuum. (The scattering problem is factored using  $jK$ -coupling.) AS also solves an uncoupled kappa-averaged Dirac equation akin to Cowan's HFR. It can also use non-unique orbitals so that different charge-states can be described by the appropriate physical potentials, e.g. for autoionization. The potentials themselves are optimized by the minimization of an energy functional (a feature found also in HULLAC). The goal here is to accelerate the convergence of the configuration interaction expansion for increasingly low-charge ions. In principle, AS can generate a single unique potential corresponding to that used by FAC and LANL and obtain essentially the same results. (The situation with HULLAC is complicated by the need to choose the same optimization strategy, but in principle it can be mimicked by AS as well.)

FAC is a very popular code within the atomic physics user community. But, as discussed above, it actually uses a rather restricted and simple approach to atomic structure. However, it is difficult to cross compare it with other codes in general since users tend to be expert in one code base. To this end, we have incorporated the current FAC potential within AS. We have applied it to a study of the dielectronic recombination of Be-like Ar using an extensive configuration interaction expansion so as to describe the so called trielectronic recombination seen in measurements on CSR[9]. We will present results obtained from FAC itself, AS using the FAC potential and AS using its standard Thomas-Fermi potential.

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**ORTHOGONAL OPERATORS:  
EXTENSION TO HYPERFINE STRUCTURE**

**Peter Uylings<sup>a</sup>, Ton Raassen<sup>a,b</sup>**

<sup>a</sup>API, University of Amsterdam, Science Park 904, 1098 XH Amsterdam,  
The Netherlands

<sup>b</sup>SRON, Netherlands Institute for Space Research, Niels Bohrweg 4, 2333 CA Leiden,  
The Netherlands

Orthogonal operators are a next step in the semi-empirical description of complex spectra. Orthogonality yields optimal independence and thus least correlation between the operators. The increased stability of the fitting process is used to include higher order many-body as well as fully relativistic effects. The calculated eigenvalues are frequently an order of magnitude more accurate with respect to a conventional semi-empirical approach. The resulting eigenvectors may not only be put to use to calculate transition probabilities and g-factors, but also to calculate hyperfine structure constants. We illustrate our first steps in this field with some examples of first and second spectra of the iron group elements. The results are compared to current experimental A-values while strong and weak points of the method are discussed.

\*email: [p.uylings@contact.uva.nl](mailto:p.uylings@contact.uva.nl)

## Electron-Impact Excitation Data for Astrophysical Plasma Diagnostics

Junjie Mao<sup>a,b\*</sup>

<sup>a</sup> Department of Astronomy, Tsinghua University, Haidian DS 100084, Beijing, People's Republic of China.

<sup>b</sup> Department of Physics, Hiroshima University, 1-3-1 Kagamiyama, Higashi-Hiroshima, Hiroshima 739-8526, Japan.

Plasma models built on extensive atomic data are essential to interpret the observed astrophysical spectra. Improving the accuracy and completeness of atomic data are particularly relevant in the era of the next generation of high-resolution spectroscopic instruments (e.g., XRISM, Athena, HUBS, and Arcus). Electron-impact excitation is one of the fundamental atomic processes in astrophysical plasmas. In this talk, I will focus on some recent R-matrix intermediate-coupling frame transformation (ICFT) calculations of electron-impact excitation data of cosmic abundant elements [1-4]. I will illustrate the importance of data with improved accuracy in the context of a wide range of astrophysical plasmas, including solar corona, dwarf nova, ionized winds driven away from black holes, hot plasmas in individual galaxies and galaxy assemblies.

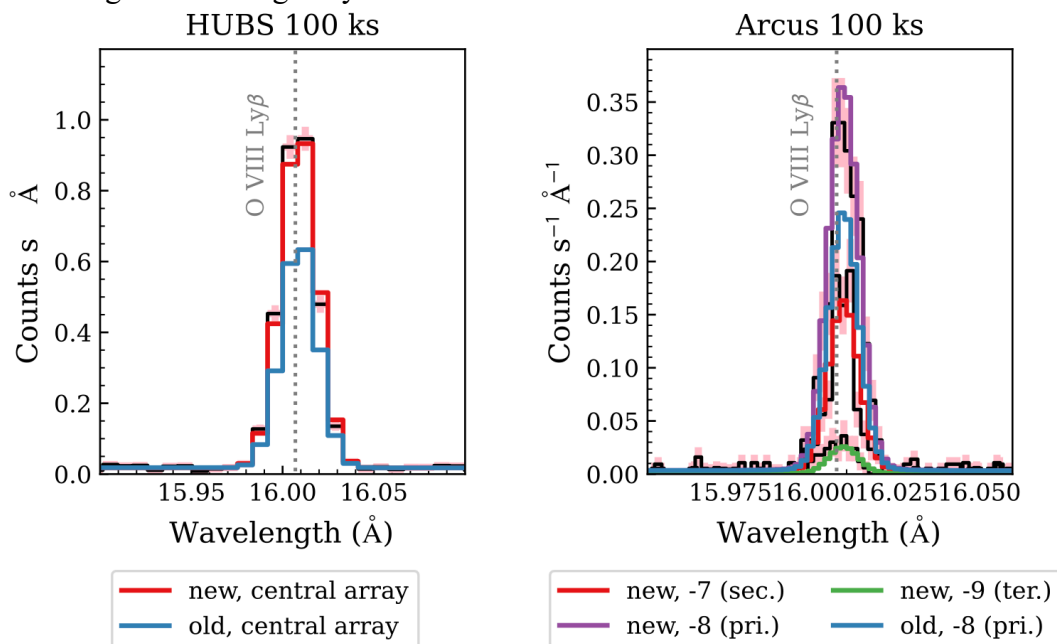


Figure 1: Simulated HUBS (left) and Arcus (right) spectra in the O VIII Ly beta neighborhood using old and new electron-impact excitation data.

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\*email: jmao@tsinghua.edu.cn

## Atomic Structure Calculations for New Physics Searches

Julian C. Berengut\*

School of Physics, University of New South Wales, Sydney NSW 2052, Australia

Precision laboratory and astronomical measurements of atomic spectra can be used to search for new physics including dark matter, dark energy, new forces, variations of fundamental constants, and violations of fundamental symmetries. Accurate atomic calculations are required for planning and supporting experiments, understanding and removing systematics, and interpreting the results as limits on new physics. However, open-shell systems still pose a challenge for atomic structure theory.

As an example, comparison of astronomical and laboratory spectra can be used to constrain variations in the fine-structure constant (see, e.g. review [1]). This dimensionless constant, which measures the strength of the electromagnetic interaction, might change of time and space as suggested by some unification theories, or could couple to dark matter and hence vary according to the local dark matter density. Atomic calculations are used to determine how the spectra depend on the value of the fine-structure constant.

Measured atomic spectra also depend on the isotope abundances via the isotope shift. This is a significant potential systematic effect for astrophysical studies of fundamental constant variation, but it is also an opportunity to extract the isotope abundances, with implications for stellar evolution models [2]. In the laboratory, precise measurement of isotope shift has been used to place limits on hypothetical force-carrying bosons that couple electrons and neutrons [3]. Calculations of isotope shift in complex atoms are based on precise *ab initio* atomic structure methods and finite-field formulation of the relativistic isotope shift operators.

A promising route to calculations of spectra, isotope shifts, and other properties of complicated atoms is the particle-hole configuration interaction with many-body perturbation theory (CI+MBPT) method [4]. This extends the CI+MBPT method [5] to non-perturbatively include configurations with electron holes below the designated Fermi level. The method has been implemented in AMBiT [6], a software package for fully relativistic, *ab initio* atomic structure calculations. The software is written in modern C++, and can make use of both OpenMP and MPI to achieve demonstrated scalability from a personal notebook all the way up to state-of-the-art supercomputer clusters.

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\*email: julian.berengut@unsw.edu.au

## Testing the Constancy of Electromagnetism's Strength with Dark Matter Density Using Stellar Twins

Michael T. Murphy<sup>a,\*</sup>, Daniel A. Berke<sup>a</sup>, Brett C. Addison<sup>a</sup>, Fan Liu<sup>a,b</sup>, Chris Flynn<sup>a,c</sup>,  
Christian Lehmann<sup>a</sup>, Vladimir A. Dzuba<sup>d</sup>, Victor V. Flambaum<sup>d</sup>

<sup>a</sup>Centre for Astrophysics and Supercomputing, Swinburne University of Technology,  
Hawthorn, Victoria 3122, Australia

<sup>b</sup>School of Physics and Astronomy, Monash University, Melbourne, Victoria 3800, Australia

<sup>c</sup>ARC Centre of Excellence for Gravitational Wave Discovery, Swinburne University of  
Technology, Hawthorn, Victoria 3122, Australia

<sup>d</sup>School of Physics, University of New South Wales, Sydney, NSW 2052, Australia

The Standard Model of nature's laws provides no explanation for the fundamental constants, like electromagnetism's strength,  $\alpha$ . It is therefore up to experiments to test whether fundamental constants are, indeed, constant and universal, or instead vary and depend on other physical parameters. I will describe a new probe of  $\alpha$ 's constancy within our Galaxy – stellar twins – and show our first results from solar twins which have an ensemble precision of 12 parts-per-billion. This is already the best astronomical measurement of any fundamental constant so far. I will also show that red clump stars also provide precise measurements with this approach. The results derive from archival high-resolution optical spectra (HARPS) from the ESO 3.6-m telescope, so there is considerable scope for extending them using larger facilities. Our goal is to map  $\alpha$  across the Milky Way and, importantly, its widely-varying dark matter density field. This will be a completely new, direct test of physics beyond the Standard Model.

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\*email: mmurphy@swin.edu.au

## Improvements in Oscillator Strengths and their Impact on Interstellare Abundances and Depletions

Adam M. Ritchey<sup>a,b,\*</sup>

<sup>a</sup>Eureka Scientific, 2452 Delmer Street, Suite 100, Oakland, CA 96402, USA

<sup>b</sup>Department of Physics and Astronomy, University of Toledo, Toledo, OH 43606 USA

In this talk, I will discuss how recent improvements in the oscillator strengths of astrophysically-relevant atomic transitions have impacted our understanding of interstellar gas-phase abundances and dust-grain depletions. The abundances of neutral and ionized atomic species in interstellar clouds are typically derived by measuring the strengths of absorption lines that correspond to electronic transitions out of the ground state, using stars or quasars as background continuum sources. The absorption strength can be converted into a column density only if the oscillator strength of the transition is well determined. For atomic species that represent the dominant ionization stage of an element in neutral diffuse gas, such measurements yield the gas-phase abundance of the element. Many of the more highly refractory elements are found to be severely underabundant in interstellar gas (when their abundances are compared to those derived for the Sun or local B stars), indicating that large fractions of those elements are locked up in interstellar dust grains. Thus, accurate oscillator strengths are needed not only to understand gas-phase elemental abundances but also to correctly identify and characterize the depletion properties of different elements that yield clues to the formation and evolution of interstellar dust grains.

In recent years, new experimental oscillator strengths have been determined for commonly observed transitions in P II [1,2], Cl I [3], Cl II [4], Cu II [5], Ge II [6], and Pb II [7]. In these experiments, lifetimes and oscillator strengths are derived using beam foil techniques at the Toledo Heavy Ion Accelerator (THIA). I will discuss how the improvements in the oscillator strengths afforded by these measurements have given us new perspectives on the abundances and depletions of neutron-capture elements [8] and on the growth of dust grains in interstellar clouds [9]. I will also highlight cases where further experimental results may be needed to resolve discrepancies in existing determinations of oscillator strengths for astrophysically important atomic species.

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\*email: ritchey.astro@gmail.com

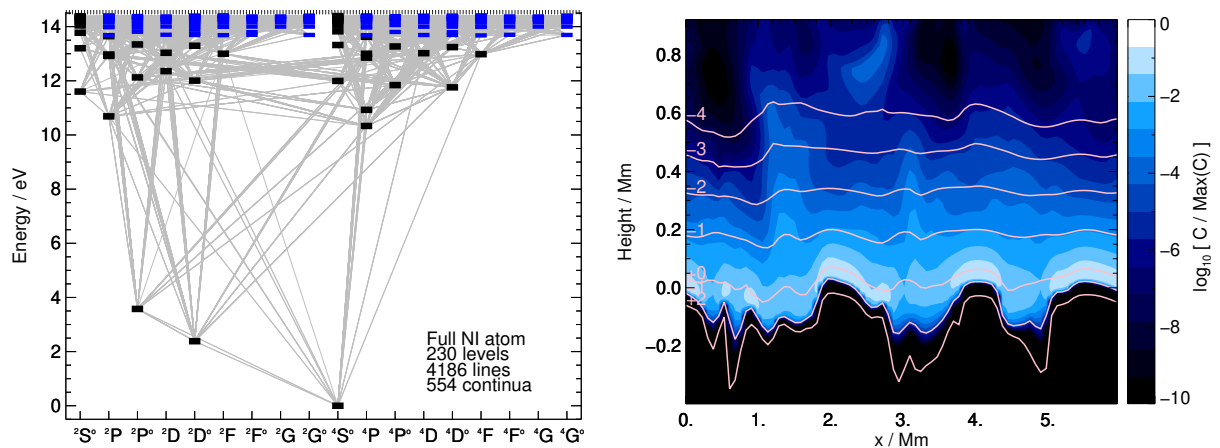


# Atomic Data for 3D Non-LTE Solar and Stellar Spectroscopy

A. M. Amarsi\*

Theoretical Astrophysics, Department of Physics and Astronomy, Uppsala University, Box 516, 751 20, Uppsala, Sweden

Stars leave their signatures on the light they emit from their atmospheres, in the form of absorption and emission lines. By comparing with model stellar spectra, we can decode these signatures to reveal the physical properties of stars, in particular their chemical compositions. This information sheds light on the structure and evolution of the stars themselves, as well as their planets, and even the Galaxy as a whole... provided that the model spectra are sufficiently realistic [1].



**Figure 1:** 3D non-LTE modelling of N I lines in the solar atmosphere [2]. *Left:* Term diagram illustrating the levels and transitions considered in statistical equilibrium. *Right:* Contribution function for the N I 868.34nm line in a vertical slice of a snapshot of the solar atmosphere.

I shall describe the state-of-the-art in modelling the spectra of late-type stars like our Sun. Such models are based on three-dimensional (3D) radiation-hydrodynamics and take into account departures from local thermodynamic equilibrium (non-LTE) [2,3]. I shall illustrate some of their successes, as well as their limitations, and thereby try to make the case for more reliable atomic data, in particular oscillator strengths, photoionisation cross-sections, and inelastic collision rates [4].

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\*email: anish.amarsi@physics.uu.se

## Coronal Magnetic Field Measurements from EUV Wavelengths

Wenxian Li\*

National Astronomical Observatories, Chinese Academy of Sciences, Beijing 100101, China

Coronal magnetic fields are at the heart of most of the unsolved problems in solar physics. The lack of precise measurements of coronal magnetic field has limited our investigation of many important topics in solar physics research including the driving mechanism of solar eruptions and the heating process of corona. In the past several decades, a number of techniques have been developed for coronal magnetic field diagnostics. Recently, a novel method by using unexpected transitions induced by external magnetic fields, so called magnetic-field-induced transitions (MITs) has been proposed for the magnetic field measurements in the solar and stellar coronae and subsequently received attention from the solar physics community. The most promising MIT candidate for coronal magnetic field measurements existed in EUV spectral lines of Fe X, in which the MIT is enhanced due to accidental close degeneracy between levels of short and long lifetimes [1-3]. It has been demonstrated that the Fe X MIT in EUV wavelength has great potential for solar and stellar coronal magnetic field diagnostics [4-9]. In this talk, I will report recent progress on the solar and stellar coronal magnetic field measurements from MIT method.

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\*email: wxli@nao.cas.cn

## **The Athena X-ray Observatory Integral Field Unit (X-IFU): New Perspectives in the Study of the Universe Using High Resolution X-ray Spectroscopy**

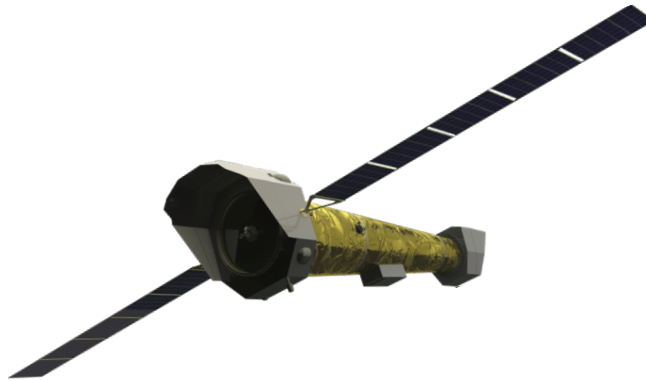
**François Pajot<sup>a</sup>**, on behalf of the X-IFU Consortium

<sup>a</sup>IRAP, Université de Toulouse, CNRS, CNES, 9 av. du Colonel Roche, 31400 Toulouse,  
France

The Advanced Telescope for High ENergy Astrophysics (Athena) is the second large mission of the ESA Cosmic Vision science program. The X-ray Integral Field Unit (X-IFU), on board Athena, will provide spatially resolved high resolution spectroscopy from 0.2 to 12 keV with 5 arc second pixels over a nominal field of view of 4 arc minute equivalent diameter and a goal spectral resolution of 3 eV up to 7 keV, thanks to a  $\sim 1.5$  kpixel array of microcalorimeters cooled down to 55 mK.

The core scientific objectives of Athena are defined in the science theme of the Hot and Energetic Universe:

- How does ordinary matter assemble into the large-scale structures we see today?
- How do black holes grow and shape the Universe?



Athena spacecraft artist's view (credit: IRAP, CNES, ESA).

Gas, heated to temperatures of tens of millions of degrees, resides in groups and clusters of galaxies. Stars in galaxies are collapsing at the end of their life, generating supernova explosions. These explosions generate heavy chemical elements, feeding galactic winds which, in turn, mix and push matter within and outside galaxies, triggering the birth of new stars.

X-IFU unique X-ray spectral images will give access to the nature of the emitting elements and their physical conditions such as temperature, speed and turbulence. The study of the associated astrophysical processes will require new model and laboratory data, as well as a careful calibration of the instrument and observational data.

The X-IFU will be provided by an international consortium led by France, The Netherlands and Italy, with ESA member state contributions from Belgium, Czech Republic, Finland, Germany, Poland, Spain, Switzerland, with additional contributions from the United States and Japan.

\*email: [francois.pajot@irap.omp.eu](mailto:francois.pajot@irap.omp.eu)

## Metallic Magnetic Calorimeters for High Precision of X-Ray Spectroscopy

Loredana Gastaldo<sup>a,\*</sup>

<sup>a</sup>Kirchhoff Institute for Physics, Heidelberg University, INF 227, 60126 Heidelberg Germany

Metallic magnetic calorimeters (MMCs) are high energy resolution detectors operated at mK temperatures [1]. The achieved performance, like the energy resolution of 1.6 eV full width at half maximum (FWHM) at 6 keV and the reliable and stable energy calibration as well as the possibility to optimize the detector geometry for the particle/energy to be detected, motivated the use of MMCs for a large variety of applications. Figure 1 shows the energy spectrum acquired with a *maXs-30* array while using an  $^{241}\text{Am}$  calibration source. The photo of the 2D *maXs-30* MMC array is shown in the inset of figure 1. The number of pixels is 64, covering an active area of  $4\text{ mm} \times 4\text{ mm}$ . The baseline resolution was determined to be 7.5 eV FWHM while at 60 keV the energy resolution was 9.8 eV FWHM indicating only a slight dependence of the energy resolution on the energy of the photon [2]. MMCs have also been optimized for measurements with radioactive sources fully contained in the absorber so that the emitted radiation can be detected with quantum efficiency close to unity. These measurements allow for the determination of the absolute intensities of different excitations. An example is the electron capture spectrum of  $^{163}\text{Ho}$  whose interpretation has triggered several theoretical works [3].

After a short introduction on MMCs, a few key measurements will be presented with focus on the detector performance and the achieved results.

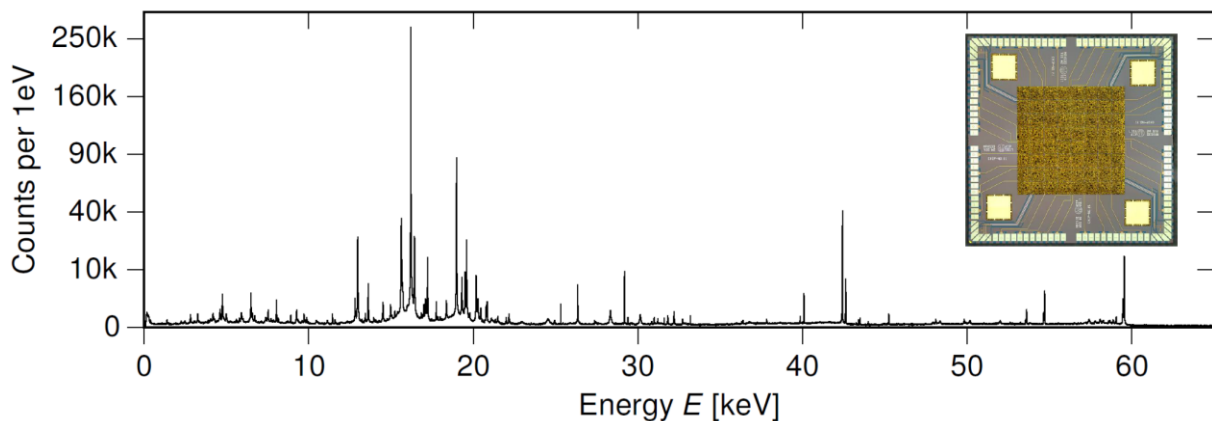


Figure 1:  $^{241}\text{Am}$  spectrum acquired with the 2D *maXs-30* MMC array showed in the inset of the spectrum. The chip size is  $8\text{ mm} \times 8\text{ mm}$  while the detection area in the middle, formed by 64 MMC pixels, has size  $4\text{ mm} \times 4\text{ mm}$  [2].

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\*email: Loredana.Gastaldo@kip.uni-heidelberg.de

## Laboratory Atomic Astrophysics at Malmö University with Emphasis on the Infrared Spectral Region

Hampus Nilsson<sup>a,\*</sup>

<sup>a</sup>Department of Materials Science and Applied Mathematics, Malmö University,  
205 06 Malmö, Sweden

The infrared wavelength region continues to be the main focus of spectroscopic investigations of astrophysical plasmas. For example, the ESO ELT will have an echelle spectrograph (ANDES) with resolution of  $R \approx 100,000$  and a simultaneous spectral range of  $0.4 - 1.8 \mu\text{m}$  [1]. The infrared wavelength region is of particular interest due to the low scattering by particles, making it possible to observe stars in dust rich environments e.g., close to the Galactic center.

The important parameters needed for spectral analysis are wavelengths, energy levels, transition probabilities and line structures like hyperfine structure and isotopic shifts. However, atomic data in the infrared wavelength region is still scarce [2]. I will discuss laboratory measurements of wavelengths, energy levels, hyperfine structure and isotopic shifts in atoms and ions, with emphasis on the infrared spectral region. Furthermore, I will report recent and ongoing work at :

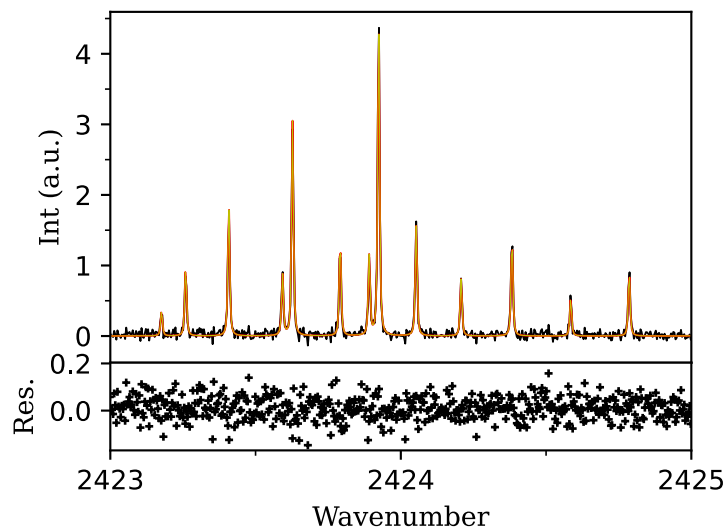


Figure 1: Infrared spectral line of In II showing large hyperfine structure. The black spectrum is recorded with a Bruker 125HR IR FTS, and the red spectrum is a fitted spectrum. Bottom panel shows the residual between the recorded and fitted spectra.

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\*email: Hampus.nilsson@mau.se

## Spectroscopy Studies of Moderately Charged Tungsten, Sulfur, and Chlorine Ions at the SH-HTSCEBIT

Q. Lu<sup>a</sup>, C. L. Yan<sup>a</sup>, N. Fu<sup>a</sup>, X. Liu<sup>a</sup>, F. H. Qu<sup>a</sup>, Y. M. Xie<sup>a</sup>, B. L. Li<sup>a</sup>, Y. Yang<sup>a</sup>, K. Wang<sup>b</sup>, J.G. Li<sup>c</sup>, W.Q. Wen<sup>d</sup>, A.V. Volotka<sup>e</sup>, Y.S. Kozhedub<sup>f</sup>, M. Y. Kaygorodov<sup>f</sup>, N. Nakamura<sup>g</sup>, C.Y. Chen<sup>a</sup>, R. Hutton<sup>a</sup>, Y. Zou<sup>a</sup>, **J. Xiao<sup>a,\*</sup>**

<sup>a</sup>Shanghai EBIT Laboratory, Key Laboratory of Nuclear Physics and Ion-Beam Application (MOE), Institute of Modern Physics, Fudan University, Shanghai 200433, China

<sup>b</sup>Department of Physics and Anhui Key Laboratory of Optoelectric Materials Science and Technology, Key Laboratory of Functional Molecular Solids, Ministry of Education, Anhui Normal University, Wuhu, Anhui 241000, China

<sup>c</sup>Institute of Applied Physics and Computational Mathematics, Beijing 100088, China

<sup>d</sup>Institute of Modern Physics, Chinese Academy of Sciences, 730000 Lanzhou, China

<sup>e</sup>School of Physics and Engineering, ITMO University, Kronverkskiy prospekt 49, 197101 St. Petersburg, Russia

<sup>f</sup>Department of Physics, St. Petersburg State University, Universitetskaya 7/9, 199034 St. Petersburg, Russia

<sup>g</sup>Institute for Laser Science, The University of Electro-Communications, Chofu, Tokyo 182-8585, Japan

In this talk, we present the spectroscopy studies of moderately charged tungsten, sulfur, and chlorine ions during the past several years. To provide atomic data needed for magnetically confined fusion plasma diagnostics, the visible spectra of  $W^{7+}$  -  $W^{12+}$  have been measured using the Shanghai high-temperature superconducting electron beam ion trap (SH-HtscEBIT[1]) at Fudan University. The atomic structures of tungsten ions are given by our large-scale FAC[2] and GRASP[3] calculations. We utilize two methods to calculate the energy levels and the transition rates: the relativistic configuration interaction method with the FAC code and the multi-configuration Dirac-Hartree-Fock method with the GRASP package. To simulate spectra under different plasma conditions, a collisional-radiative model implemented in FAC is adopted. The calculated FAC and GRASP wavelengths agree with the experimental ones, except for a few lines. We hope that in the future, more theoretical studies will be conducted to address this discrepancy. To test the QED effects, the fine-structure splittings in  $S^{7+}$ ,  $Cl^{8+}$ ,  $S^{11+}$ , and  $Cl^{12+}$  have been measured with high precision at the SH-HtscEBIT. Their M1 transition energies are evaluated within the ab initio QED framework. The present experimental results agree with the theoretical calculations and provide a possibility to test QED effects and correlation effects with high accuracy in few-electron highly charged ions.

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\*email: xiao\_jun@fudan.edu.cn

# Modeling for Spectroscopic Diagnostics of CCP-ICP and PBIF Plasmas in KAERI

Duck-Hee Kwon<sup>a,\*</sup>, Changmin Shin<sup>a,b</sup>, Haewon Shin<sup>a</sup>, Kil-Byoung Chai<sup>a</sup>

<sup>a</sup>Nuclear Physics Application Research Division, Korea Atomic Energy Research Institute, Daejeon, 34057, Republic of Korea

<sup>b</sup>Department of Nuclear and Quantum Engineering, Korea Advanced Institute of Science and Technology, Daejeon, 34057, Republic of Korea

We report optical emission spectroscopy and collisional-radiative modeling (CRM) for diagnostics of He ICP (inductively coupled plasma) [1] and KPBF (KAERI plasma beam irradiation facility) H/D plasmas [2], together with a Langmuir probe measurement, in low electron temperature regime ( $T_e \sim 5$  eV). The CRM solves non-linear steady state balance equations including processes such as radiation trapping and heavy particle collisions self-consistently. The sensitivities of line spectra intensities and densities of particles to used atomic and molecular (AM) data [3] in the CRM was investigated (Fig. 1).

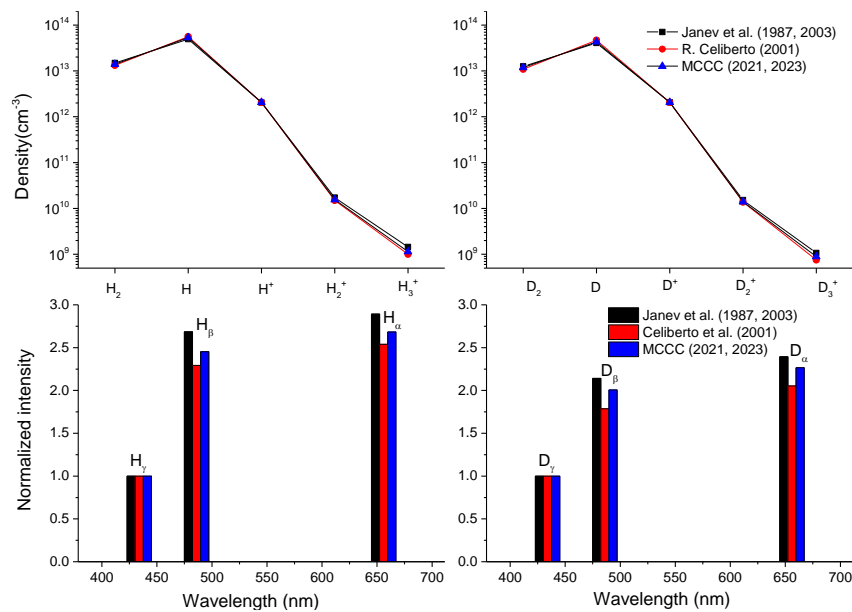


Figure 1: Population densities and line spectra intensities depending on various AM data.

In addition, measurements of S/XB ratios to determine sputtered flux of W I in KPBF and the calculations by modeling using various atomic data on electron impact ionization/excitation and radiative decay are presented.

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\*email: hkwon@kaeri.re.kr

# Probing Strong Field Quantum Electrodynamics Through Precision Spectroscopy of Highly Charged Ions and Exotic Atoms

Nancy Paul<sup>a</sup>

<sup>a</sup>Laboratoire Kastler Brossel, Sorbonne Université, CNRS, ENS-PSL Research University, Collège de France, Case 74; 4, place Jussieu, F-75005 Paris, France

Despite decades of effort, quantum electrodynamics (QED), the field theory that describes the interaction between light and charged particles, is poorly tested in the regime of strong coulomb fields. This is due to a confluence of difficulties linked to experimental limitations in highly-charged ion spectroscopy and nuclear uncertainties. I will show recent results from the Paris Double Crystal Spectrometer for He-like S [1] and Li-like Ar and S [2] for QED tests and astrophysics applications. The unique role of Bayesian analysis methods in untangling hidden contributions will be highlighted with a dedicated study of the influence of the atomic form factors on the response function of the Paris Double Crystal Spectrometer. I will then present a new paradigm for probing higher-order QED effects using spectroscopy of Rydberg states in exotic atoms, where orders of magnitude stronger field strengths can be achieved while nuclear uncertainties may be neglected [3]. Such tests are now possible due to the advent of quantum sensing detectors and new facilities providing low-energy intense beams of exotic particles for precision physics. I will present first results from experiments with muonic atoms at J-PARC within the context of the HEATES collaboration [4], and discuss a new project for antiprotonic atom spectroscopy at CERN.

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\*email: nancy.paul@lkb.upmc.fr



# Hyperfine Resolved Laser Spectroscopy of Highly Charged I<sup>7+</sup> Ions

Priti\*

National Institute for Fusion Science, Gifu, Japan

\*priti.priti@nifs.ac.jp

The study of hyperfine structures in many-electron highly charged ions (HCIs) can provide a deeper understanding of strongly correlated electrons and serve as a benchmark for advanced theoretical calculations. Additionally, the possibility of using HCIs as atomic clock candidates emphasize the importance of hyperfine structures in many-electron HCIs [1]. However, there has been limited progress in hyperfine spectroscopy of many-electron HCIs due to experimental challenges. We successfully performed hyperfine-structure resolved laser spectroscopy of HCIs in an electron beam ion trap plasma. Here, we present laser-induced fluorescence (LIF) spectra of palladium-like I<sup>7+</sup> in an electron beam ion trap (EBIT) plasma [2]. The electric quadrupole (E2) emissions ((4d3/2<sup>-1</sup>5s)J=2 → (4d<sup>10</sup>)J=0) induced by a pulse laser excitation via the magnetic dipole (M1) transition ((4d5/2<sup>-1</sup>5s)J=3 → (4d3/2<sup>-1</sup>5s)J=2) were observed by a time-resolving extreme ultraviolet spectrometer directly coupled to the EBIT chamber. The collisional and radiative processes in the EBIT plasma provide a high population in the long-lived metastable state (4d<sup>-1</sup>5s)J=3 and make it possible to continuously induce the E2 emission with the pulse laser irradiation. The small natural width of the transition between the metastable states without electric dipole (E1) decay paths enables to perform the high-precision wavelength measurement and reveals the hyperfine structure. Hyperfine structures were confirmed by theoretical calculations of hyperfine splittings and transition probabilities for (4d5/2<sup>-1</sup>5s)J=3 and (4d3/2<sup>-1</sup>5s)J=2 using the GRASP2018 [3].

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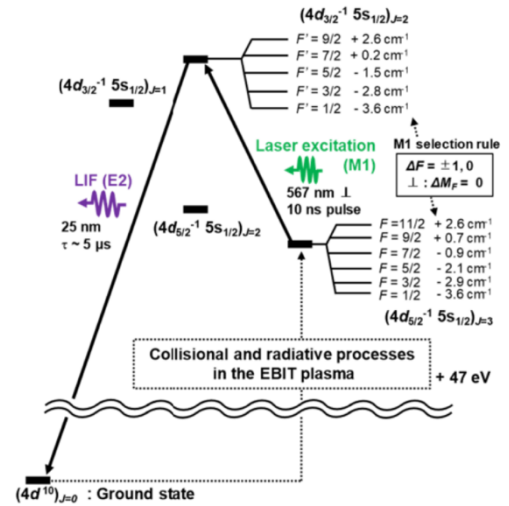


Figure 1. Schematic energy level diagram of  $^{127}\text{I}^{7+}$  with the laser-induced transition.

## High-Resolution Laboratory Measurements of near Ar-like Fe EUV Line Emission using EBIT-I

Alexander J. Fairchild<sup>a,\*</sup>, Natalie Hell<sup>b</sup>, Peter Beiersdorfer<sup>c</sup>, Greg Brown<sup>b</sup>, Michael Hahn<sup>a</sup>, Megan E. Eckart<sup>b</sup>, Daniel W. Savin<sup>a</sup>

<sup>a</sup>Columbia Astrophysics Laboratory, Columbia University, New York, NY 10027, USA

<sup>b</sup>Physics Division, Lawrence Livermore National Laboratory, Livermore, CA 94550, USA

<sup>c</sup>Space Science Laboratory, University of California, Berkeley, CA 94720, USA

Ar-like Fe IX is formed over a broad range of solar temperatures, probing many solar structures. Its peak formation temperature,  $\log[T(K)] = 5.9$ , is at the boundary between the transition region and the corona, making Fe IX a critical ion in understanding energy and mass flow into the corona. The Fe IX 241.74/244.91 Å intensity ratio is also predicted to be one of the best EUV density diagnostics for the solar corona. Despite this, the diagnostic is not commonly used, in part because previous observations by Orbiting Solar Observatory (OSO) 5, OSO 7, and Skylab, showed that the inferred electron densities differ significantly from those obtained from other ions. Uncertainties in the underlying atomic data have been proposed as one possible reason for the disagreement. Density diagnostics are very sensitive to uncertainties in the atomic data because they depend on many factors, such as collisional excitation and de-excitation rates, radiative transition rates, and cascade contributions from higher energy levels. Additionally, line blends, including those from other ions, can impact the accuracy of density diagnostics. In order to benchmark the density sensitive line ratio of the Fe IX line pair, we have measured the EUV line emission from Fe VII-Fe X in the wavelength range 238 to 258 Å at the Lawrence Livermore National Laboratory electron beam ion trap (EBIT-I). Here we report a new line survey of Fe VII-Fe X emission in this wavelength range and the implications for the 241.74/244.91 Å density diagnostic.

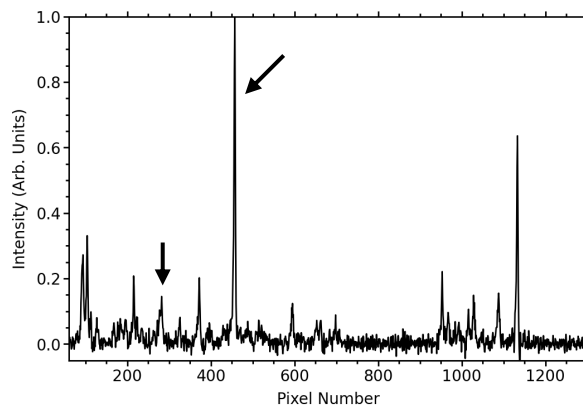


Figure 1: EBIT-I Fe VII-Fe X EUV line emission spectrum from 238 to 258 Å. The Fe IX 241.74 Å and 244.91 Å lines are indicated with arrows.

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\*email: [ajf2236@columbia.edu](mailto:ajf2236@columbia.edu)

## Laboratory Measurements of Hyperfine Structure

Sophie Kröger

Hochschule für Technik und Wirtschaft Berlin, Fachbereich 1, Wilhelminenhofstr. 75A,  
Berlin, D-12459 Germany

The theory of atomic hyperfine structure has been known for almost a hundred years and nearly 50 years ago, continuous-wave tunable single mode lasers heralded a new era in the study of atomic spectra. Since this time, a very large number of experimental and theoretical studies have been carried out. Despite these numerous studies, the data of hyperfine structure of almost all elements are still far from being fully known.

This lecture will give an overview of the current state of research and insight into recent studies on the hyperfine structure of atoms and atomic ions, which are carried out in recent years in collaboration with my cooperation partners at Istanbul University (Türkiye), Istanbul Technical University (Türkiye), University of Latvia (Latvia), Technical University Graz (Austria) and with other partners. Different spectroscopic methods and different spectral ranges were used in the different laboratories. By combining the experimental results of these different methods in different spectral ranges and by also include experimental and theoretical results from other research groups, new results could be obtained, which will be presented here by means of examples. A few examples of experimental atomic hyperfine structure spectra are already shown in Figure 1.

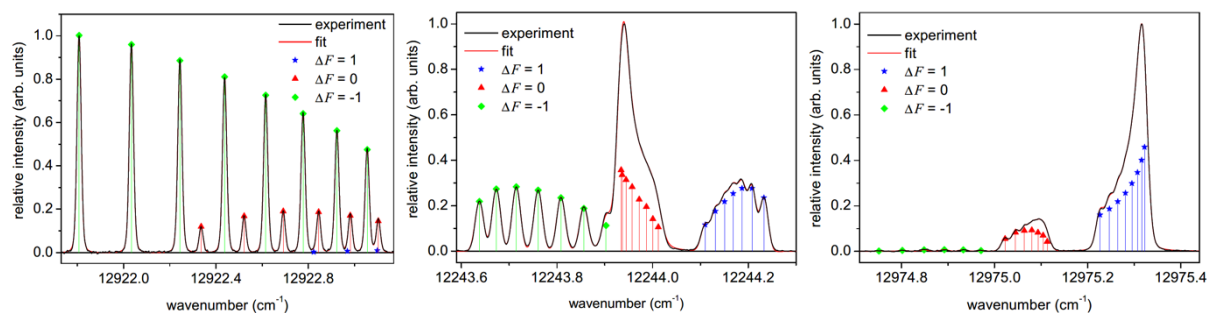


Figure 1: Examples of hyperfine structures of atomic Ho measured with laser-induced fluorescence spectroscopy [1]; experimental spectra together with the best fitted curves; the components are assigned by the difference  $F$  of the total angular momentum between the upper and lower hyperfine levels (for more details see [1])

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\*email: Sophie.kroeger@htw-berlin.de

# Storage Ring Measurements for Dielectronic Recombination of Na-like Fe<sup>15+</sup>

H.K. Huang<sup>1</sup>, Z.K. Huang<sup>1</sup>, **W.Q. Wen**<sup>1</sup>, W.L. Ma<sup>2</sup>, S.X. Wang<sup>2</sup>, H.B. Wang<sup>1</sup>, S.J. Wu<sup>3</sup>, C.Y. Chen<sup>3</sup>, C.Y. Zhang<sup>4</sup>, N.R. Badnell<sup>4</sup>, L.F. Zhu<sup>2</sup>, X. Ma<sup>1</sup> and DR collaboration

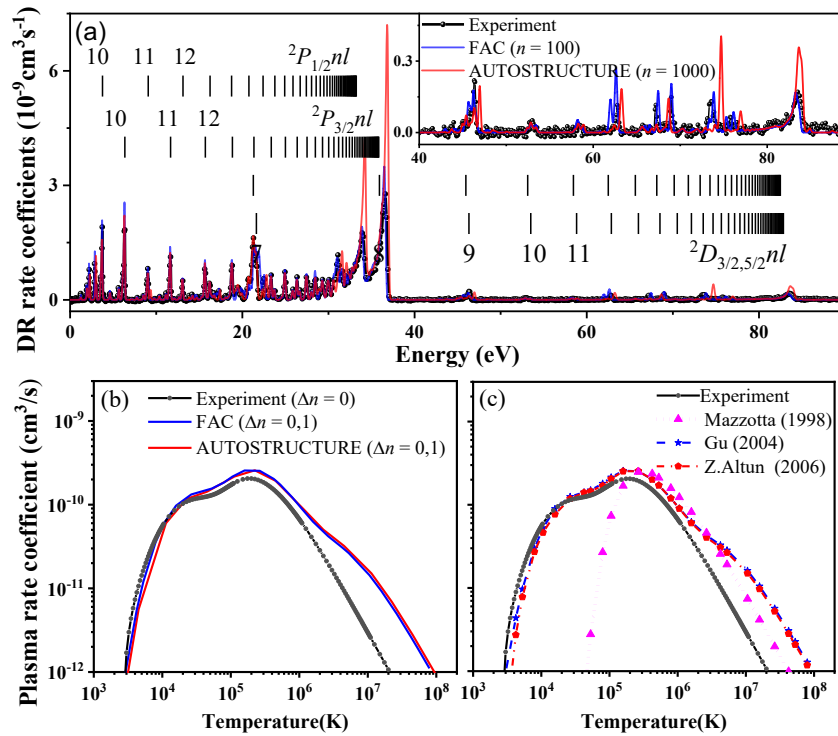
<sup>1</sup>*Institute of modern physics, Chinese Academy of Sciences, 730000, Lanzhou, China*

<sup>2</sup>*University of Science and Technology of China, 230026, Hefei, China*

<sup>3</sup>*Shanghai EBIT Laboratory, Fudan University, Shanghai 200433, China*

<sup>4</sup>*Department of Physics, University of Strathclyde, Glasgow G4 0NG, United Kingdom*

Dielectronic recombination (DR) is an important atomic process governing the charge balance in astrophysical and fusion plasmas, therefore, the accurate DR rate coefficients are required for interpretation of the plasma observations [1,2]. The absolute DR rate coefficients for sodium-like Fe<sup>15+</sup> forming magnesium-like Fe<sup>14+</sup> have been measured using the electron-ion merged-beam technique at the heavy ion storage ring CSRm at IMP, China. The measured DR rate coefficients, as shown in Figure 1, cover most of the DR resonances associated with the  $3s \rightarrow 3p$  and  $3s \rightarrow 3d$  core excitations ( $\Delta N = 0$ ). In the range of 0-40 eV, our results agree very well with the previously DR measurement at the TSR [3]. Furthermore, we observed a clear signature in the range of 40-90 eV which belongs to  ${}^2D_{3/2,5/2} nl$  resonances. We compare the experimental results with the calculations from AUTOSTRUCTURE and FAC and have a good agreement (comparison with JAC calculation is in progress). In addition, temperature dependent plasma recombination rate coefficients are derived from the measured DR rate coefficients and compared with the recommended atomic data from the literature [4].



**Figure 1.** DR rate coefficients and plasma recombination rate coefficients of Na-like Fe<sup>15+</sup>.

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Email: wenweiqiang@impcas.ac.cn, x.ma@impcas.ac.cn

## Measuring Transition Probabilities of Rare-Earths: Experimental Requirements and Challenges

M. T. Belmonte<sup>a\*</sup>, P. R. Sen Sarma<sup>a</sup>, S. Mar<sup>a</sup>

<sup>a</sup>University of Valladolid, Department of Theoretical and Atomic Physics and Optics,  
Paseo de Belén 7, 47011 Valladolid, Spain.

Transition probabilities (Einstein coefficient for spontaneous emission,  $A_{ul}$ -values,  $\log(gf_i)$ ) are essential atomic parameters that play a key role in a wide range of applications, from the lighting and laser development industry to the analysis of astrophysical spectra.

The Atomic Spectroscopy Laboratory at the University of Valladolid (Spain) has extensive experience in the measurement of transition probabilities using emission spectroscopy. After more than 30 years working on the noble gases, we have changed our focus to the measurement of transition probabilities of rare-earths given their current importance after the detection of the first kilonova [1]. As a light source, we use an in-house made water-cooled continuous hollow-cathode lamp under different conditions of carrier gas pressure and current (between 0.1 and 1 A). The radiation emitted by the lamp is analysed using a 1.5 m Jobin-Yvon monochromator with a 2400 lines/mm holographic diffraction grating (resolving power of 150 000 at 450 nm).

The determination of accurate spectral line intensities (area under the profile) is key to provide high-quality transition probabilities. We have conducted a detailed analysis of all the potential causes of uncertainty when measuring line intensities of rare-earth spectra with our experimental set-up. Key factors are: correct identification of lines, ability to resolve blends, stability of the hollow-cathode lamp, intensity calibration of the spectra and self-absorption correction for strong lines.

Due to the very crowded spectra of the rare-earths, knowledge of the intrinsic width of the spectral lines we want to observe (due to natural, Doppler and pressure broadening) is key to define our experimental requirements. The width of the monochromator's entrance slit, the resolving power of the diffraction grating and the spatial resolution of the detector must work together to ensure that the total instrumental width is below the intrinsic width of the lines.

We have carried out a careful study of line widths for neodymium to define the minimum requirements our experimental set-up must meet to resolve these lines. We are currently using these findings to upgrade our laboratory for the measurement of the very rich rare-earth element spectra.

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\*email: [mariateresa.belmonte@uva.es](mailto:mariateresa.belmonte@uva.es)

## **Applications of Atomic Data to Studies of the Sun**

**Peter Young\***

NASA Goddard Space Flight Center, Heliophysics Division, Greenbelt Road, Greenbelt, MD  
20771, USA

Department of Mathematics, Physics and Electrical Engineering, Northumbria University,  
Newcastle upon Tyne, NE1 8ST, UK

The wide range of temperature exhibited by the solar atmosphere, from 6000 K in the photosphere to over 20 MK in solar flares, makes it an important testing ground for atomic data of ionized ions. High signal-to-noise coupled with the ability to spatially discriminate a wide range of plasma structures has been valuable for identifying new atomic transitions and for assessing the accuracy of atomic data. The extreme ultraviolet (EUV: 10-91 nm) is of particular interest as it is very rich in emission lines but is mostly absorbed by the interstellar medium for other stars in the Milky Way. In this talk I summarize current and upcoming Solar Physics instrumentation and identify atomic data needs. Techniques for analyzing solar spectra are described, with a particular focus on how the CHIANTI atomic database is used by Solar Physicists. CHIANTI is an open-source database and software package for modeling emission line spectra and continuum emission.

\*email: [peter.r.young@nasa.gov](mailto:peter.r.young@nasa.gov)

## Evaluating Atomic Data Needs for X-Ray Astrophysics with the AtomDB Atomic Database

Adam R Foster<sup>a,\*</sup>, Priyanka Chakraborty<sup>a</sup>, Stuart Loch<sup>b</sup>, Hans Werner van Wyk<sup>b</sup>, Randall Smith<sup>a</sup>

<sup>a</sup>Center for Astrophysics | Harvard and Smithsonian, 60 Garden St, Cambridge, MA 02138  
USA

<sup>b</sup>Auburn University, Auburn, AL 36849 USA

The AtomDB project ([www.atomdb.org](http://www.atomdb.org)) is a combination of a large atomic database and several spectral models designed for modeling emission from optically thin, X-ray emitting plasmas. The code and database are optimized in the EUV and X-ray ranges ( $1 < \lambda < 1240\text{\AA}$ ), although the models cover a wider range of spectra.

The upcoming launch of high resolution X-ray calorimeter on the NASA XRISM mission, which will have unprecedented spectral resolution in the  $2 < E_{\text{phot}} < 10$  keV range, creates a new impetus for updating and interpreting X-ray spectra. In addition, other proposed instruments in the soft X-ray and EUV will place tighter requirements on the accuracy of atomic data to enable accurate interpretation of results.

We present here a general outline of the AtomDB project, including the range of plasmas which it is designed to model including equilibrium, non-equilibrium, charge exchange and non-Maxwellian plasmas. We then discuss ways to identify the limitations to diagnostic accuracy imposed by the current knowledge of atomic data using our *variableapec* software. Finally, we outline ways of estimating the uncertainties on atomic data and resulting line diagnostics from first principles, enabling us to identify which diagnostics may only be effective with improved experimental measurements.

\*email: [afoster@cfa.harvard.edu](mailto:afoster@cfa.harvard.edu)

**Larry J Curtis 1935-2020: A Brief History: His Revelations in Atomic Structure and Dynamics**

**Gordon Berry**

University of Notre Dame, Notre Dame IN 46556, USA

I will very briefly review the 40-year career of Larry Curtis and his discoveries both experimental and theoretical. The focus will be limited to three atomic physics areas in which he played a principal part: these include the first observations of light from oriented atoms; observations of light from doubly-excited states in light atoms (helium and lithium). These include the verification of the only light ever observed from a negative atomic ion; thirdly, his theoretical analysis multiple exponential decays, enhancing the precision of beam-foil measurements of atomic lifetimes. Finally, some reminiscences about his personal life, his Swedish honorary doctorate, his wife Maj Rosander, and other European adventures.

\*email: [hgb@att.net](mailto:hgb@att.net)



## **EVALUATION OF UNCERTAINTIES IN ATOMIC DATA ON SPECTRAL LINES AND TRANSITION PROBABILITIES**

**Alexander Kramida<sup>a</sup>**

<sup>a</sup>National Institute of Standards and Technology, Gaithersburg, MD 20899, USA

This talk will discuss some recent advances in methods of critical evaluation of experimental data on wavelengths of spectral lines and theoretical data on transition probabilities and oscillator strengths for atoms and atomic ions. In particular, recently developed new statistical approaches to estimation of uncertainties of weighted means of multiple measurements are described, and a numerical toolbox implementing these new approaches is presented. There are also some new developments in estimation of uncertainties of theoretical transition probabilities. A short review of literature implementing these new procedures is provided, including a description of the methodology.

## The XSTAR Atomic Database

Claudio Mendoza\*

Physics Center, Venezuelan Institute for Scientific Research (IVIC),  
Caracas 1020, Venezuela

XSTAR [1] is a spectral modeling code of photoionized plasmas widely used in X-ray astronomy. It relies on an extensive atomic database for elements with atomic number  $Z \leq 30$  [2, 3], which has taken over 20 years to compute in-house and collect from diverse sources. The XSTAR database emphasizes the descriptions of the recombination spectra of H- and He-like ions [4, 5] and the transition arrays associated with the K edge (namely,  $K\alpha$  and  $K\beta$  lines) due to their plasma diagnostic potential (see [3] and references therein), but the database also includes radiative and collisional rates for processes involving the valence shell. In this presentation, we bring to the fore the perspective of the atomic-data user and the adaptations that must be made to the atomic datasets, e.g., line positions and high-density effects, to be able to model astrophysical systems reliably [6, 7, 8]. We are particularly concerned with the modeling of the reflection spectrum of the high-density ( $n_e > 10^{18} \text{ cm}^{-3}$ ) inner region of AGN accretion disks to deduce the black-hole spin. In this respect, the consistently high iron abundances currently obtained from the flagship Fe  $K\alpha$  lines are believed to be indicators of missing atomic processes [9].

We will also briefly discuss database maintenance difficulties that have led to the development of the Python module PyXstarDB to automate atomic data collecting from online databases (e.g., CHIANTI [10]. and NIST [11]) into an SQLite environment, which may also be of interest to prospective modelers.

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\*email: claudiom07@gmail.com

## Assessment of the FAIRness of the Virtual Atomic and Molecular Data Centre following the Research Data Alliance Evaluation Framework

Carlo Maria Zwölf<sup>a</sup>, Nicolas Moreau<sup>a</sup>

<sup>a</sup>LERMA, Sorbonne Université and Paris Observatory, Meudon Campus, 92190 Meudon, France

We will present the result of the analysis [1] made on the Virtual Atomic and Molecular Data Centre infrastructure [1], following the FAIR Data Maturity Model framework defined by the Research Data Alliance [2]: after recalling the technical architecture of the VAMDC infrastructure, we will introduce the RDA FAIR evaluation framework and define the methodology we adopt to perform our analysis. After having presented the results, we will conclude with some lines of work aimed at improving the FAIRness of VAMDC, together with some ideas for further development of this work.

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\*email: carlo-maria.zwolf@obspm.fr

## Charge Exchange Recombination Spectroscopy of W Ions for ITER Neutral H-Beam Diagnostics

Dipti<sup>a,\*</sup>, D. R. Schultz<sup>b</sup>, and Yu. Ralchenko<sup>a</sup>

<sup>a</sup>National Institute of Standards and Technology, Gaithersburg, MD 20899, USA

<sup>b</sup>Northern Arizona University, Flagstaff, AZ 86011, USA

\*Present address: International Atomic Energy Agency, Vienna A-1400, Austria

Charge-exchange recombination spectroscopy (CXRS) remains one of the most important diagnostic methods for existing and future magnetic fusion devices. In particular, the CXRS with energetic neutral beams of hydrogen will be a key diagnostic tool for ITER where interactions with its important impurity, namely, tungsten, should result in new spectral features to be analyzed. The results of the present spectral synthesis are based on the new set of *nl*-resolved CX cross sections for recombination of the  $W^{q+}$  ions ( $q = 61-66$ ) with atomic hydrogen calculated using the classical trajectory Monte Carlo method for the planned ITER neutral beams (diagnostic beam of 100 keV/u and heating beam of  $\sim 1$  MeV/u). These calculated CX cross sections, along with the atomic data needed for other relevant physical processes, were used in a large-scale collisional-radiative model to study the population kinetics of atomic states of the tungsten ions and to generate the synthetic spectra across a wide range of photon energies. The simulations demonstrated that the CX-induced emission drastically modifies the observed spectrum in the visible and VUV ranges for the interaction with diagnostics neutral beam, which can provide important predictions for interpretation and evaluation of the CXRS diagnostics on ITER. Details of the theoretical calculations and results will be presented and discussed.

\*email: d.dipti@iaea.org

**Magnetically-Confined Nuclear Fusion and Atomic Data****M G O'Mullane<sup>a\*</sup>, N R Badnell<sup>a</sup>, C P Ballance<sup>b</sup>, S D Loch<sup>c</sup>, S S Henderson<sup>d</sup>**<sup>a</sup> Department of Physics, University of Strathclyde, Glasgow, G4 0NG, UK<sup>b</sup> Centre for Theoretical Atomic, Molecular and Optical Physics, Queen's University Belfast, University Road, Belfast BT7 1NN, UK<sup>c</sup> Department of Physics, Auburn University, Auburn, AL 36849, USA<sup>d</sup> CCFE, Culham Science Centre, Abingdon, OX14 3DB, UK

Atomic physics and spectroscopy are intertwined in the history of fusion. Unlike astrophysical plasmas, laboratory fusion experiments, such as tokamaks, have independent measurements of the local electron temperature and density. They are therefore less reliant on traditional line ratio methods for diagnosing the plasma environment but these plasmas cover a very wide parameter range and present demanding challenges to atomic physics. High magnetic fields, large gradients in electron temperature and density, fast fluctuations and non-Maxwellian electrons and conditions which favour both highly charged ions and un-dissociated molecules in the same plasma are some of the interesting situations which must be considered when using atomic physics to model the radiation properties of fusion plasmas and to interpret spectroscopic measurements as diagnostics of the plasma. Many of the atomic based measurements are needed in terms of engineering or operational parameters and are therefore the result of a synthesis and reduction of large amounts of fundamental atomic data via, primarily, collisional-radiative models. The uses for machine protection, operating scenario design, impurity content detection and understanding plasma transport places demands on the availability and precision of atomic data.

This talk will give an overview of the quality of atomic and molecular data used in magnetically confined fusion analysis. The basis for all calculated data is a good atomic structure and how this influences the many processes involved is explored. The choices, and comprises, made in calculating cooling curves for low, medium and high-Z elements is examined from the point of view of controlling the radiated power and spectroscopy. The specific challenges for the atomic data and models of tungsten in its journey from a neutral influx species to X-ray emitter in the core illustrates the successes of recent work but also highlights that significant and essential work is needed in fundamental atomic physics.

\*email: martin.omullane@strath.ac.uk

# Oral Contributions



# TRANSITION INTENSITIES OF TRIVALENT LANTHANIDE IONS IN SOLIDS: EXTENSION OF JUDD-OFELT THEORY ON $\text{Eu}^{3+}$ , $\text{Nd}^{3+}$ AND $\text{Er}^{3+}$

Gohar Hovhannesian<sup>a</sup>, Vincent Boudon<sup>a</sup>, Maxence Lepers<sup>a</sup>

<sup>a</sup>Laboratoire Interdisciplinaire Carnot de Bourgogne, UMR 6303 CNRS-Univ. Bourgogne Franche-Comté,  
9 Avenue Alain Savary, BP 47 870, Dijon cedex, F-21078 , France

Lanthanides are widely used in the industry. For example, they are used as the active ions in luminescent materials used in optoelectronics applications, most notably the Nd:YAG laser. Erbium-doped fiber amplifiers are significant devices in optical-fiber communication systems. These and other applications are based on optical transitions between levels of the ground configuration of the trivalent lanthanide ions. Being forbidden in the electric-dipole approximation, those transitions are activated by the crystal-field potential created by the host material. The Judd-Ofelt (JO) theory has been successfully applied since 60 years, to interpret the intensities of absorption and emissions lines of crystals and glasses doped with trivalent lanthanide ions. Despite the fact that it is remarkably efficient for many cases, the standard version of the JO theory cannot reproduce some of the observed transitions, because of its strong selection rules [1-2].

In order to overcome this issue we present a modified version of the JO theory, where the properties of the dopant are calculated with well-established atomic-structure techniques, while the influence of the crystal-field potential is described as a perturbation, by three adjustable parameters [3]. In the extension we introduce also the wavelength-dependence of the refractive index of the host material with the help of the Sellmeier equation. We test the validity of our model on three ions:  $\text{Eu}^{3+}$ ,  $\text{Nd}^{3+}$  and  $\text{Er}^{3+}$ . The results of the extension are very good (see figure 1). We are able to give a physical insight into all the transitions within the ground electronic configuration, and also to reproduce quantitatively experimental absorption oscillator strengths.

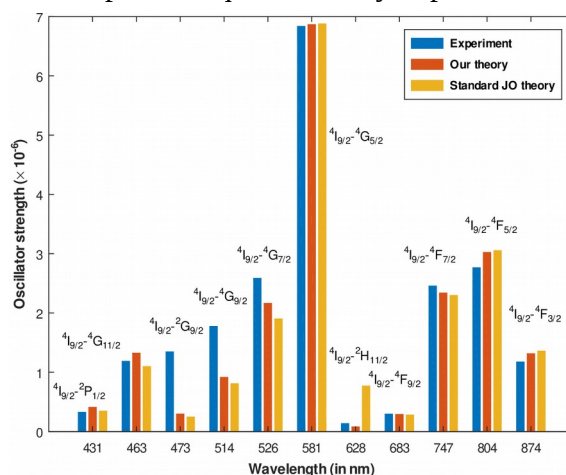


Figure 1: Comparison between experimental [4] and theoretical oscillator strengths of absorption, plotted as function of the transition wavelength (not at scale) for  $\text{Nd}^{3+}$ .

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\*email: gohar.hovhannesian@u-bourgogne.fr



## High resolution vacuum ultraviolet absorption spectroscopy: determination of reactive species' oscillator strengths

Nelson De Oliveira<sup>a\*</sup>, Denis Joyeux<sup>a</sup>, Laurent Nahon<sup>a</sup>

<sup>(a)</sup> Synchrotron SOLEIL - L'Orme des Merisiers-Saint-Aubin / BP 48 91192 Gif sur Yvette cedex France

DESIRS is a VUV (Vacuum UltraViolet) beamline at the synchrotron SOLEIL facility characterized by high flux, high resolution, spectral purity, and variable polarization. DESIRS is equipped with several state-of-the-art instruments, including an i2PEPICO set-up and an ion trap, for the study of VUV photon-induced processes on isolated gas phase samples, such as cold molecules, radicals, (chiral) biomolecules, large ionic biopolymers, clusters and nanoparticles[1]. In addition, the VUV-FTS (VUV-Fourier Transform Spectrometry) experimental branch has been designed to provide both high spectral resolution and broad band capability[2,3]. In operation since 2008, this permanent endstation has permitted the study of small molecules, revisiting the spectroscopy of fundamental stable molecules such as CO, N<sub>2</sub>, O<sub>2</sub>, CO<sub>2</sub> or H<sub>2</sub>O presenting an evident astrophysical interest. Recently, various set-ups aiming at the production of transient species such as radicals have been developed and led to an increased knowledge including band oscillator strengths on key radical species such as OH, S<sub>2</sub>, CH<sub>3</sub> and SO, VUV spectroscopic studies of atomic species [4,5], or application to plasma modelization[6]. An overview of the most significant achievements will be shown, with a highlight on the OH radical[7].

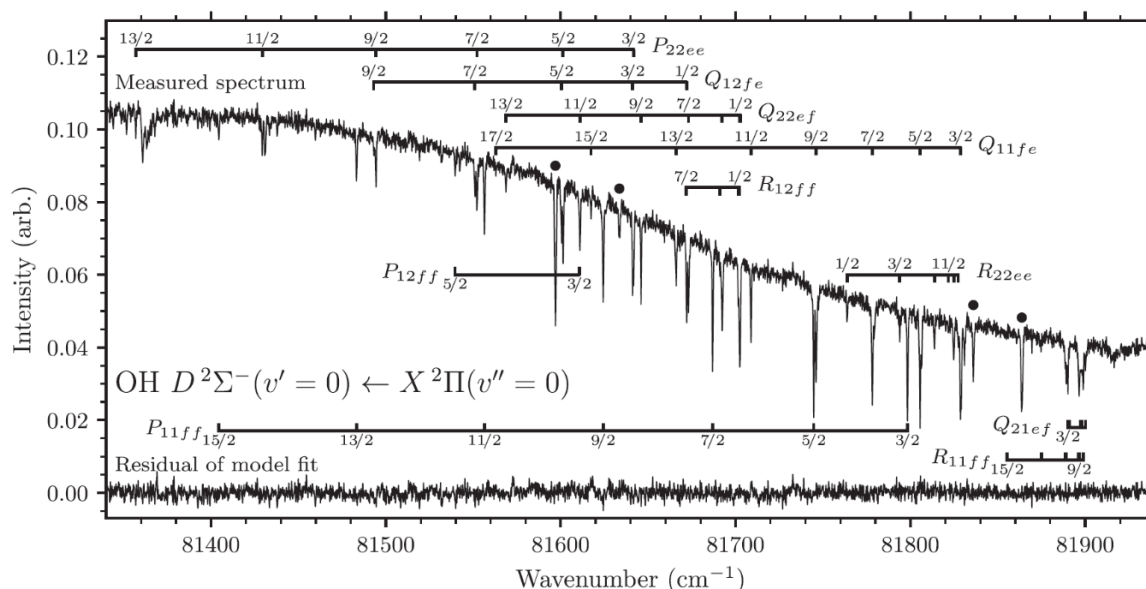


Figure 1: Assigned experimental spectrum showing the OH  $D^2\Sigma^-(v' = 0) \leftarrow X^2\Pi(v'' = 0)$  absorption band (RF discharge, FTS spectral resolution:  $0.27 \text{ cm}^{-1}$ ).

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\*email : nelson.de.oliveira@synchrotron-soleil.fr

## HYPERFINE INTERACTION AFFECTING THE CHARGE-STATE DISTRIBUTION OF HIGHLY CHARGED ION PLASMA

**Endre Takacs**<sup>a,b,\*</sup>, Dipti<sup>b,c</sup>, Adam Hosier<sup>a</sup>, Timothy Burke<sup>a</sup>, Galen C. O'Neil<sup>d</sup>, Joseph .N. Tan, Aung S. Naing, Joan P. Marler<sup>a</sup>, Yuri Ralchenko<sup>b</sup>

<sup>a</sup>Department of Physics and Astronomy, Clemson University, Clemson, SC 29634

<sup>b</sup>National Institute of Standards and Technology, Gaithersburg, MD 20899

<sup>c</sup>Present address: International Atomic Energy Agency, A-1400 Vienna, Austria

<sup>d</sup>National Institute of Standards and Technology, Boulder, CO 80305

In a recent electron beam ion trap (EBIT) experiment we have found that the charge state distribution of highly charged ions can be strongly affected by metastable energy levels that accumulate considerable population [1]. In an EBIT, where the ion cloud in its equilibrium generally consists of a narrow distribution of charge states, the effect strongly depends on the density of the electrons. Ultimately the population distribution among levels of the different ions, together with the transition rates from these levels determine the emitted spectra of plasmas. As a result, these spectra can serve as sensitive diagnostic tools for environments where metastable ions are present.

In a series of measurements, we used the EBIT of the National Institute of Standards and Technology (NIST) to confine and probe Pr and Nd lanthanide ions at different electron beam energies and densities [1-3]. Spectra were recorded by a recently installed transition edge (TES) sensor x-ray microcalorimeter with good energy and photon arrival time resolution [4]. The non-Maxwellian plasma was modeled by collisional-radiative calculations [5] to reliably predict the spectral emission of the ion cloud [1-3]. Our analysis showed that the finely tuned charge state distribution near the Ni-like charge state is strongly affected by the metastable population fraction at  $10^{10}$ - $10^{12}$  cm<sup>-3</sup> densities. The time evolution and the equilibrium intensity ratio of spectral lines showed that isotope-dependent hyperfine interaction strongly influences the population dynamics in these systems.

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## STUDY OF B-LIKE IONS X-RAY EMISSION SPECTRA IN AN ELECTRON-CYCLOTRON RESONANCE ION SOURCE PLASMA

Louis Duval <sup>a,b,\*</sup>, Emily Lamour <sup>b</sup>, Stéphane Macé <sup>b</sup>, Jorge Machado <sup>c</sup>, Nancy Paul <sup>a</sup>,  
Christophe Prigent <sup>b</sup>, Martino Trassinelli <sup>b</sup>, Paul Indelicato <sup>a</sup>.

<sup>a</sup> *Laboratoire Kastler-Brossel, Sorbonne Université, CNRS, ENS-PSL Research University, Collège de France, Case 74; 4, place Jussieu, F-75005 Paris, France*

<sup>b</sup> *Institut des NanoSciences de Paris, CNRS, Sorbonne Université, 4 Place Jussieu, 75005 Paris, France*

<sup>c</sup> *Universidade Nova de Lisboa Laboratório de Instrumentação Engenharia Biomédica e Física da Radiação, Departamento de Física, Faculdade Ciências e Tecnologia, Universidade Nova de Lisboa, 2829-516 Caparica, Portugal*

Chandra and XMM-Newton brought astrophysical x-ray spectroscopy to a new era by providing the first high-resolution (0.5% in the X-ray band) measurements. These improvements have led to a need for more precise atomic data to interpret the astrophysical measurements. Later measurements, showing unknown x-ray contributions, drew the question of new physics [1], which was finally resolved by new measurements using ion sources [2]. The extensive usage of microcalorimeters in recent (Hitomi) and future (Athena/XFU and XRISM) missions give new perspectives for x-ray measurements of astrophysical objects [3]. Concurrently, thanks to modern intense ion sources [4], in-lab precise measurements of transitions in highly-charged ions, like in sulfur, allow to improve the modelling of the measurements [5]. We present here new reference-free high-precision measurements of x-ray transitions in boron-like argon and sulfur. The measurements were performed with an Electron Cyclotron Resonance Ion Source and a double-crystal spectrometer installed in Paris at Sorbonne Université [6]. These spectra show multiple transitions, which required the use of Bayesian model selection methods to determine the number of spectral components and their characteristic profile. This is performed using the nested sampling method implemented in the nested fit code [7] which will be also introduced.

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\*email: [louis.duval@lkb.upmc.fr](mailto:louis.duval@lkb.upmc.fr)

## EXPERIMENTAL METASTABLE LIFETIMES AT DESIREE STORAGE RING – FIRST STOP : BARIUM

Uldis Berzins<sup>a</sup>, Jose Navarette<sup>b</sup>, Paul Martini<sup>b</sup>, Arturs Ciniņš<sup>a</sup>, Dag Hanstorp<sup>c</sup>, Henning Schmidt<sup>b</sup>, **Henrik Hartman**<sup>d,\*</sup>

<sup>a</sup>University of Latvia, Institute of Atomic Physics and Spectroscopy, Latvia

<sup>b</sup>Stockholm University, AlbaNova University Centre, SE-10691 Stockholm, Sweden

<sup>c</sup>Gothenburg University, Department of Physics, SE-10691 Gothenburg, Sweden

<sup>d</sup>Malmö University, Faculty of Technology, SE-20506 Malmö, Sweden

We are developing a laser probing technique at the Double Electrostatic Cryogenic Storage Ring DESIREE at Stockholm university, Sweden [1]. The excellent vacuum and temperature conditions allows to store the barium ions  $Ba^+$  with a beam lifetime of 500s. We present our first measurements of the  $5d\ ^2D_{3/2}$  metastable state of Ba II with a lifetime around 80 s with a 1% uncertainty.

We apply a pump and probe technique utilizing two lasers. One red laser emptying the metastable state and probing the population, and a blue laser repopulating the state by transferring all the population from the ground state  $6s\ ^2S_{1/2}$  to the  $5d\ ^2D_{3/2}$  state investigated. By varying the time delay between pump and probe, the lifetime curve is built up.

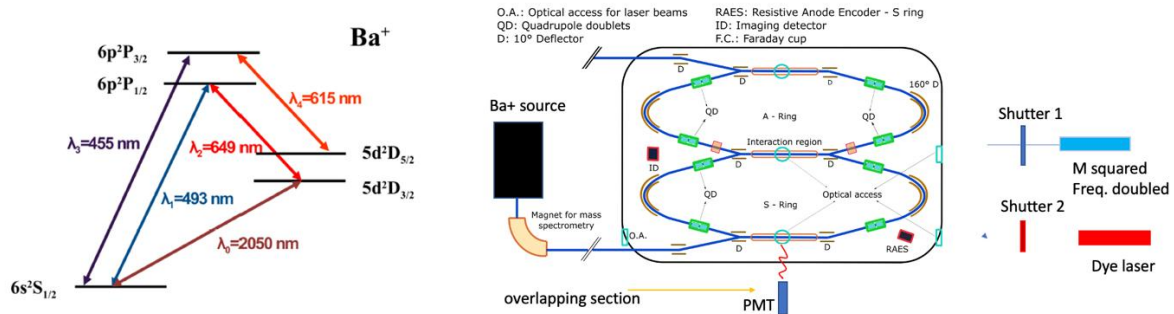


Figure 1: *left*: Energy level diagram of Ba II, with metastable  $5d\ ^2D_{3/2}$ . *Right*: The DESIREE storage ring and the experimental setup

Thanks to the excellent storage conditions, we see only very small systematic effects such as repopulation and collisional quenching. Future studies will include more complex spectra such as Fe II.

A consortium consisting of Stockholm University (SU), the University of Gothenburg (UGOT) and Malmö University (MaU) operate DESIREE as a national infrastructure since January 2018 with support from the Swedish research Council VR. Authors from UL were supported by ERDF project No. 1.1.1.5/19/A/003: and ERDF project No. 1.1.1.1/19/A/144.

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\*email: Henrik.Hartman@mau.se

## GRASP and COMPAS for ASOS

Jacek Bieroń<sup>a</sup>, Tomas Brage<sup>b</sup>, Chong Yang Chen<sup>c</sup>, Jörgen Ekman<sup>d</sup>, Charlotte Froese Fischer<sup>e</sup>,  
Gediminas Gaigalas<sup>f</sup>, Ian P. Grant<sup>g</sup>, Per Jönsson<sup>d</sup>, **Michel Godefroid**<sup>h\*</sup>, Jon Grumer<sup>i</sup>,  
Wenxian Li<sup>j</sup>, Yan Ting Li<sup>c,d</sup>, Jiguang Li<sup>k</sup>, Ran Si<sup>c</sup>, Kai Wang<sup>c</sup>

<sup>a</sup>Institut Fizyki Teoretycznej, Uniwersytet Jagielloński, 30-348 Kraków, Poland

<sup>b</sup>Division of Mathematical Physics, Dpt of Physics, Lund University, 22100 Lund, Sweden

<sup>c</sup>EBIT Lab, IMP, Dpt of Nuclear Science & Technology, Fudan U., Shanghai 200433, China

<sup>d</sup>Dpt of Materials Science and Applied Mathematics, Malmö U., 20506 Malmö, Sweden

<sup>e</sup>Dpt of Computer Science, University of British Columbia, Vancouver, BC V6T 1Z4, Canada

<sup>f</sup>Institute of Theoretical Physics and Astronomy, Vilnius U., LT-010222 Vilnius, Lithuania

<sup>g</sup>Dpt Mathematical Institute, University of Oxford, Oxford OX2 6GG, UK

<sup>h</sup>SQUARES, Université libre de Bruxelles, 1050 Brussels, Belgium

<sup>i</sup>Theoretical Astrophysics, Dpt of Physics & Astronomy, Uppsala U., 75120 Uppsala, Sweden

<sup>j</sup>Key Lab. of Solar Activity, NAO, Chinese Academy of Sciences, Beijing 100101, China

<sup>k</sup>No. 6 Huayuan Road, Haidian District, Beijing 100088, China

There is a well-established interest in the General(-purpose) Relativistic Atomic Structure Package (GRASP) [1] for the ASOS community. To celebrate the 10<sup>th</sup> anniversary of the international collaboration on Computation Atomic Structure (CompAS) [2], a Special Issue of Atoms dedicated to GRASP was recently published [3].

The most important contribution to this issue is the GRASP manual describing the application of the package for evaluating various properties of atomic systems, supported by a paper that describes the underlying theory as it is implemented in the code. This complete documentation provides useful guides for new groups of users from the ASOS community to produce reliable atomic data that meet the accuracy requirements.

To illustrate the capacity of the GRASP package and the underlying role of the CompAS community in methodological and computational developments, new features of the code and recent extensions will be described, together with examples of calculations of relevance for astrophysics, plasma physics, and nuclear physics.

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\*email: mrgodef@ulb.ac.be

# Poster Contributions

Laboratory Data (LD)

Theory and Calculations (TC)

Laboratory Plasmas and Experiments (LPE)

Astrophysical Plasmas (AP)

Databases and Data Assessment (DBA)



## Laser spectroscopy of the Zeeman-hf structure of atomic niobium

Ł. M. Sobolewski<sup>a,\*</sup>, L. Windholz<sup>b</sup>, J. Kwela<sup>a</sup>

<sup>a</sup>Institute of Experimental Physics, University of Gdańsk,  
ul. Wita Stwosza 57, 80-308 Gdańsk, Poland

<sup>b</sup>Institute of Experimental Physics, Graz University of Technology, Petersgasse 16, A-8010  
Graz, Austria

The hyperfine and Zeeman structures of 36 lines of Nb I covering the 573.7-649.4 nm spectral region have been measured [1,2]. We used three techniques of laser spectroscopy: optogalvanic spectroscopy (OG), laser induced fluorescence (LIF) and fluorescence depletion spectroscopy (FDS). The source of free niobium atoms was a hollow cathode discharge lamp. In spectral analysis, we used software that takes into account the saturation effect. One of the measured structure and their computer analysis is presented in the figure below.

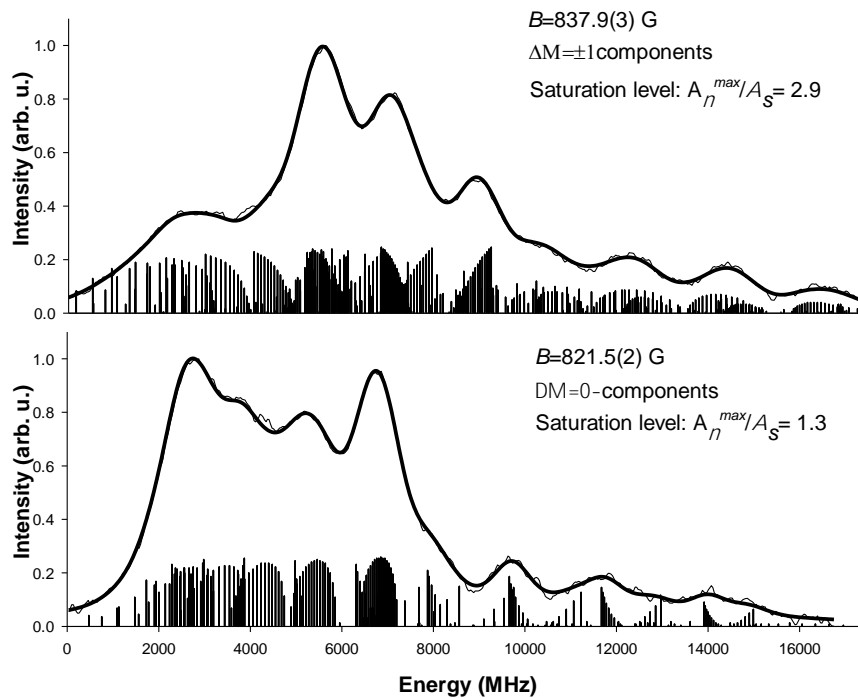


Figure 1: FDS spectra of the Zeeman-hf structures ( $\pi$  and  $\sigma$  patterns) of the 586.493 nm line in the magnetic field above 800 G. The computer generated profiles (thick lines) take into account the saturation effect. As it can be seen the saturation effect appears and the ratio for the  $M, M'$  component of the highest intensity  $A_v^{max}$  to the saturation rate  $A_S$  equals 2.9 and 1.3 for  $\Delta M = \pm 1$  and  $\Delta M = 0$  components, respectively.

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\*email: lukasz.sobolewski@ug.edu.pl



## **New experimental energy levels, lifetimes and oscillator strengths in singly ionised zirconium**

**M. Burheim<sup>1,2</sup>, H. Nilsson<sup>2</sup>, L. Engström<sup>3</sup>, H. Lundberg<sup>3</sup>, H. Hartman<sup>2</sup>, P. Palmeri<sup>4</sup>,  
P. Quinet<sup>4,5</sup>**

<sup>1</sup>Lund Observatory, Division of astrophysics, Department of physics, Box 43, 221 00 Lund, Sweden

<sup>2</sup>Material Science and Applied Mathematics, Malmö University, 205 06 Malmö, Sweden

<sup>3</sup>Department of physics, Lund University, Box 118, 221 00, Lund, Sweden

<sup>4</sup>Physique Atomique et Astrophysique, Université de Mons, B-7000 Mons, Belgium

<sup>5</sup>IPNAS, Université de Liège, B-4000 Liège, Belgium

Recent advances in resolution and spectral range of ground-based and space-based astronomical spectrographs, call for accurate atomic data in order to reliably interpret and model astrophysical spectra. Correctly interpreted, stellar spectra allow for precise abundance analysis which, in turn, makes it possible to study the Galactic formation and evolution. To meet this demand, we study the complex atomic system of singly ionised zirconium, Zr II. Zirconium is predominantly found in cool giants and sub-dwarfs, as well as in kilonova spectra, providing a way to study the s-process and r-process elements.

In this project we report completely new experimental energies for 20 highly excited states belonging to the  $4d^26s$  and  $4d^25d$  configurations in Zr II. We have also measured radiative lifetimes for these levels, and combined with branching fractions we have derived experimental transition probabilities (oscillator strengths) for 104 lines between the first odd  $4d^25p$  and  $4d5s5p$  configurations and the new levels. The energy levels were identified from lines in spectra recorded with a Chelsea Instruments FT500 Fourier transform spectrometer, using a hollow cathode as light source, and the branching fractions were measured in the same intensity calibrated spectra. The lifetimes were measured with a laser induced fluorescence technique at the Lund Laser Centre.

## THE SPECTRUM AND ENERGY LEVELS OF DOUBLY IONISED NEODYMIUM

Milan Ding<sup>a,\*</sup>, Juliet C. Pickering<sup>a</sup>, Alexander Ryabtsev<sup>b</sup>, Edward Y. Kononov<sup>b</sup>,  
and Tanya Ryabchikova<sup>c,d</sup>

<sup>a</sup>Dept. of Physics, Imperial College London, Prince Consort Road, SW7 2AZ, London, UK

<sup>b</sup>Institute of Spectroscopy, Russian Academy of Sciences, Troitsk, 108840, Moscow, Russia

<sup>c</sup>Dept. of Astronomy, University of Vienna, Türkenschanzstrasse 17, 1180 Wien, Austria

<sup>d</sup>Institute of Astronomy, Russian Academy of Sciences, Pyatnitskaya 48, 119017, Moscow, Russia

Radiative properties of the neutral, singly, and doubly ionized rare-earth element neodymium ( $Z = 60$ ) are of astrophysical interest, particularly in the spectra of chemically peculiar stars [1] and kilonovae of neutron star mergers [2,3]. Experimentally, little is known of the atomic structure of doubly ionised neodymium (Nd III), only 40 energy levels were previously published [1]. Using the Imperial College VUV Fourier transform spectrometer, intensity and wavenumber calibrated spectra of a pure Nd cathode Penning discharge lamp were recorded in the region  $11500\text{-}54000\text{ cm}^{-1}$  ( $8695\text{-}1852\text{ \AA}$ ) at resolving powers of up to  $10^6$ . Fourier transform spectra of Nd hollow cathode discharges, Nd vacuum spark grating spectra, and UVES stellar spectra were used to aid the line and energy level classification of lower-lying levels of the  $4f^4$ ,  $4f^35d$ ,  $4f^36s$ ,  $4f^36p$ ,  $4f^37s$ , and  $4f^36d$  configurations. New and more accurate semi-empirical calculations were made using the Cowan code for these configurations. In total, 184 energy levels and 570 transitions of Nd III have been classified and measured with accuracies up to a few parts in  $10^8$ , the classified transitions are presented in Figure 1. Analysis of the  $4f^35f$  configuration by grating spectroscopy is ongoing, from which an additional 68 levels have been classified so far.

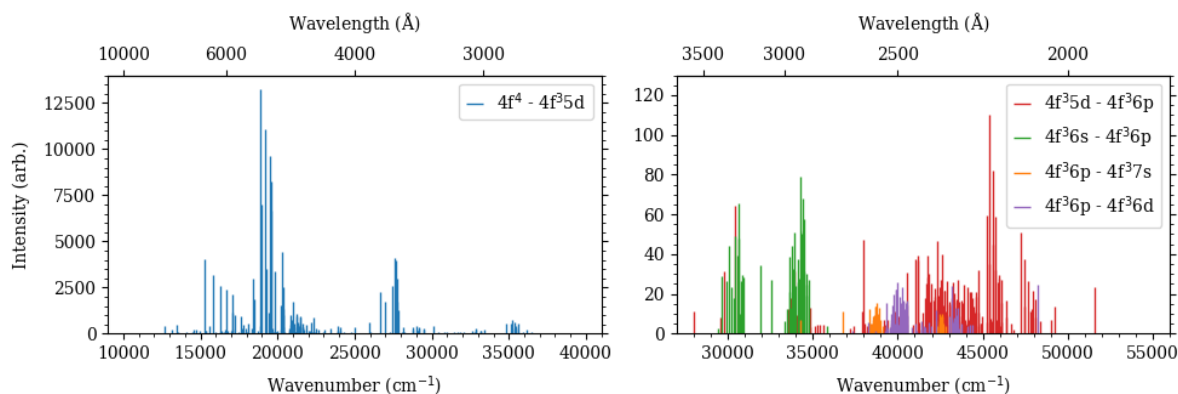


Figure 1: Classified Nd III lines from the Penning discharge lamp spectra. Three lines of the  $4f^4 - 4f^36s$  transitions were also observed (not shown). The two intensity scales are the same.

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\*email: [milan.ding15@imperial.ac.uk](mailto:milan.ding15@imperial.ac.uk)

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## REVISED ENERGY LEVELS OF ATOMIC HOLMIUM CONSIDERING HYPERFINE STRUCTURE IN FOURIER TRANSFORM SPECTRA

Gö Başar<sup>a</sup>, M. Zengin<sup>b</sup>, S. Kröger<sup>c</sup>

<sup>a</sup> Istanbul University, Faculty of Science, Physics Department, TR-34134 Vezneciler, Istanbul, Türkiye

<sup>b</sup> Graduate School of Engineering and Sciences, Istanbul University, TR-34452 Beyazıt, Istanbul, Türkiye

<sup>c</sup> Hochschule für Technik und Wirtschaft Berlin, Fachbereich 1, Wilhelminenhofstr. 75A, Berlin D- 12459, Germany

Holmium (Ho) is the fifth to last element in the series of lanthanides. The atomic spectrum of Ho is characterized by a broad hyperfine structure (hfs) of the only stable isotope, <sup>165</sup>Ho, which has a nuclear spin of  $I = 7/2$ , a large nuclear magnetic dipole moment as well as a large electric quadrupole moment. As a result, the hfs of most spectral lines of the Ho atoms and ions can be resolved using Doppler-limited spectroscopic methods such as Fourier spectroscopy.

Numerous studies of fine and hyperfine structure have been carried out in recent years (of which only the most recent publications are listed here, see [1-4] and citations therein). Several of these previous papers have revealed large uncertainties in the energy values of the fine structure levels of atomic Ho.

In this study, revised values for the fine structure level energies of atomic Ho are presented. Based on the experimental wavenumbers of more than 1400 spectral lines from calibrated Fourier transform (FT) spectra, the energy of fine structure levels of atomic Ho has been revised by weighted global fits. Various spectroscopic techniques have previously been used by different researchers and also our group to classify the Ho spectral lines before and to provide data for the hfs constants. The line classifications have been reviewed and for the high accurate determination of the center of gravity wavenumbers from the FT spectra, the hfs constants of the involved levels have been taken into account.

When checking the classification, each spectral line was assigned a weighting factor depending on its intensity in the spectrum, whether its hfs is well resolved or not, and whether it is blended with other lines. Based on these data, an overdetermined linear equation system was built up. Subsequently the revised energy levels were obtained by solving the weighted linear equation system using a self-written GNU Octave script.

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## CHARACTERIZATION OF A HOLLOW-CATHODE LAMP TO MEASURE ACCURATE TRANSITION PROBABILITIES OF RARE-EARTH ELEMENTS

P. R. Sen Sarma<sup>a\*</sup>, M. T. Belmonte<sup>a</sup>, S. Mar<sup>a</sup>, N. Lorenzana<sup>a</sup>

<sup>a</sup>University of Valladolid, Department of Theoretical and Atomic Physics and Optics, Paseo de Belén 7, 47011 Valladolid, Spain.

Rare-earths like neodymium (Nd) have a very wide range of applications. Nd is used, for example, in Nd:YAG LASER and as a dopant in metal-halide high-intensity discharge (MH-HID) lamps, which are more efficient than incandescent lamps [1]. Accurate atomic data of neodymium, such as transition probabilities, are used not only by lighting scientists to model and diagnose MH-HID [2], but also by astrophysicists to calculate chemical abundances of stars [3].

Over the last 30 years, the Atomic Spectroscopy Laboratory at the University of Valladolid (Spain) has reported transition probabilities of noble gases [4]. Due to contemporary needs [5], the laboratory has reopened with the new objective of measuring transition probabilities ( $A_{ki}$ ) of rare-earths. Our aim is to obtain accurate  $A_{ki}$ -values of rare-earths, like Nd, with a hollow-cathode lamp (HCL) and a diffraction grating spectrometer of 150 000 resolving power (at 450 nm) in the UV-visible spectral range. To achieve this goal, the HCL is operated in the abnormal glow region of the carrier gas [6] and it is ensured that the spectra emitted does not vary with time.

In this poster, we will present the voltage-current curve of the lamp also known as the gas discharge characteristic curve of the carrier gas (which is argon in our case) at different pressure inside the lamp to ensure that the lamp is operating in the abnormal glow region. We will also study the stability of the hollow-cathode lamp by studying the variation of line intensities over time. For this, we have measured spectra for a set of selected lines ranging from 300 nm to 700 nm from different upper energy levels for different ionization stages of argon (Ar I, Ar II) and iron (Fe I, Fe II, used as a test cathode) over a period of several hours. We have performed this study under different conditions of pressure and current to analyse the behaviour of the hollow-cathode lamp with different measuring conditions

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# A JOINT THEORETICAL AND EXPERIMENTAL APPROACH TO DIELECTRONIC RECOMBINATION DATA FOR PHOTOIONIZED ASTROPHYSICAL ENVIRONMENTS

M. Fogle<sup>a,\*</sup>, S. Loch<sup>a</sup>, I. Garcia<sup>a</sup>, S. Bromley<sup>a</sup>, P. Stancil<sup>b</sup>

<sup>a</sup>Department of Physics, Auburn University, Auburn, Alabama, USA 36849

<sup>b</sup>Department of Physics and Astronomy, University of Georgia, Athens, Georgia, USA 30602

Uncertainties in dielectronic recombination (DR) rate coefficients that are used in current modeling and diagnostic codes represent a obstacle for the accurate determination of elemental and charge state abundances of low-temperature astrophysical plasmas. This in turn has an impact on cosmological models of elemental abundances and evolution. Accurate data for low temperature DR remains sparse from experiments, while theoretical rates have large uncertainties due to the difficulty in calculating many-body effects for low-energy resonances, particularly for elements beyond the second row of the periodic table. These same theoretical uncertainties also contribute to uncertainties in DR satellite line wavelengths and intensities. The new DR data generated as a part of the proposed project will have an impact on the study of several areas of astronomy, e.g., galaxy evolution, H II regions, gas-rich dwarfs and planetary nebulae.

In this work, we address the issue of low temperature DR rate coefficients for astrophysical photoionized plasmas, where the DR rates are known to have large uncertainties in their calculated values. A commonly used code for computing DR rates is AUTOSTRUCTURE, which uses the multi-configuration Breit-Pauli approach. The current approach makes use of large configuration-interaction (CI) calculation using the AUTOSTRUCTURE code. Although effective in the high temperature case, current theoretical methods are known to have large uncertainties in the low temperature regime due to uncertainties in calculating low-n doubly excited states. This can be observed via comparison with ion storage ring measurements. We have developed an algorithmic method for the generation of large configuration sets to improve the low temperature DR modeling through CI. These new theoretical DR rate coefficients are then compared to existing storage ring measurements and will also be compared to new measurements being performed at the heavy ion storage ring CRYRING@ESR at the FAIR facility in Darmstadt, Germany.

\*email: fogle@auburn.edu

## EXTENDED ANALYSIS OF THE VUV EMISSION SPECTRUM OF THE FREE ION Er<sup>+2</sup> (Er III)

S. Ait Mammam<sup>1,2</sup>, W-Ü L. Tchang-Brillet<sup>3\*</sup>, A. Meftah<sup>1,3</sup>, J-F. Wyart<sup>3,4</sup>, A. Chikh<sup>1,3</sup>, D. Deghiche<sup>1</sup>, C. Balança<sup>3</sup>, N. Champion<sup>3</sup>, C. Blaess<sup>3</sup>.

<sup>1</sup>LPCQ, UMMTO BP 17 RP, 15000 Tizi-Ouzou, Algeria.

<sup>2</sup>Université d'Alger 1 - Benyoucef Benkhedda, 2 Rue Didouche Mourad, Alger 16000, Algeria.

<sup>3</sup> LERMA, Observatoire de Paris-PSL, Sorbonne Université, CNRS8112, 92190 Meudon, France.

<sup>4</sup>Laboratoire Aimé Cotton, CNRS9025, Université Paris-Saclay, Orsay, France.

Lanthanides have multiple applications, notably in astrophysics and in photonics. The complexity of their spectra implies a systematic study by isoelectronic or isoionic sequences. The first study of the spectrum of the Er<sup>+2</sup> ion, concerning the 5p<sup>6</sup>4f<sup>12</sup>, 4f<sup>11</sup>5d, 4f<sup>11</sup>6s and 4f<sup>11</sup>6p configurations by Nissan Spector [1] was summarized in the NBS critical compilation in 1978 [2]. An extended study of these configurations in Er<sup>+2</sup> ion was taken up by Wyart et al [3], and led to increase the number of known energy levels from 45 to 115, and to identify 470 new spectral lines in the spectral range between 2000 and 7000Å. Our objective is to further extend the analysis of this spectrum to the VUV wavelength region below 2000Å, where identification of new spectral lines could allow the determination of higher energy levels. The analysis is based on the VUV emission spectrum of erbium produced in the spectral region of 705-2460 Å, already used for the Er IV analysis [4,5]. All the spectrograms have been recorded on photographic plates (PP) or image plates (IP), using the high-resolution normal incidence spectrograph at Meudon Observatory with a vacuum spark emission source.

Theoretical predictions of energy levels and transition probabilities were carried out by means of Cowan codes (RCN, RCG, and RCE) with relativistic corrections (HFR option) [6]. Configuration interactions were investigated in the calculations, including in the even parity (5p<sup>6</sup>4f<sup>12</sup>, 4f<sup>11</sup> 6p, 4f<sup>10</sup>5d<sup>2</sup>, 4d<sup>10</sup>5d6s, 4f<sup>11</sup>5f and 5p<sup>5</sup>4f<sup>13</sup>) and in the odd parity, (4f<sup>11</sup>5d, 4f<sup>11</sup>6s, 4f<sup>11</sup>6d, 4f<sup>11</sup>7s, 5p<sup>5</sup>4f<sup>12</sup>5d and 5p<sup>5</sup>4f<sup>12</sup>6s). The parameters calculated at the HFR step were corrected with scaling factors of the Tm<sup>+3</sup> [7] and Yb<sup>+4</sup> [8] ions when available, which allowed us to improve the initial predictions of energies and transition probabilities. Results on spectral line identifications and new energy levels will be presented, together with parametric fits of energy parameters.

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\* [lydia.tchang-brillet@obspm.fr](mailto:lydia.tchang-brillet@obspm.fr);

**ENERGY LEVELS AND TRANSITION DATA OF Au IV**

**Haris Kunari**<sup>1\*</sup>, Aashna Zainab<sup>1</sup>, Sebastien Gamrath<sup>2</sup>, Pascal Quinet<sup>2</sup>, Tauheed Ahmad<sup>1</sup>

<sup>1</sup>Department of Physics, Aligarh Muslim University, Aligarh 202002, India.

<sup>2</sup>Physique Atomique et Astrophysique, Université de Mons, B-7000 Mons, Belgium

In this contribution, reliable atomic data for triply ionized gold (Au IV) were presented with the help of its spectrum investigated in the wavelength region of 500–2106 Å. The spectra of gold were photographed on 10.7-m normal incidence vacuum spectrograph using a sliding spark source at the National Institute of Standards and Technology (NIST, USA) as well as on a 3-m NIVS at the Antigonish laboratory in Canada with a triggered spark source. A total of 139 energy levels of Au IV were established with the help of 1031 classified transitions. The theoretical support for the present observations was made with the use of extended Cowan's codes (HFR) calculations for Au IV and HFR+CPOL (core-polarization effects). Several astrophysically relevant transitions, forbidden (M1- and E2-type) transitions of  $5d^8$  and  $5d^76s$  configurations are provided with their Ritz wavelengths and radiative parameters. The transition data for forbidden types were computed within the frameworks of HFR, HFR+CPOL and GRASP2K codes. A critically evaluated set of the Au IV's energy levels, observed and Ritz wavelengths along with their uncertainties, and transition rates were presented.

\*Email: [kharisphy@gmail.com](mailto:kharisphy@gmail.com)

## DOUBLY-IONISED IRON : NEW ACCURATE WAVELENGTHS AND ENERGY LEVELS

F. Concepcion<sup>a\*</sup>, J. C. Pickering<sup>a</sup>, M. T. Belmonte<sup>a</sup>, C. P. Clear<sup>a</sup>

<sup>a</sup>Department of Physics, Imperial College London, London, SW7 2AZ, UK

Presented here is new laboratory-measured doubly-ionised iron (Fe III) transition wavelengths and energy level values, to meet the need for higher quality atomic data. These data will be invaluable to astronomers as the spectral lines of iron are present in, and dominate opacities of, many astrophysical sources, due to its complex spectrum and high relative abundance.

Fe III spectra were generated using a Penning discharge lamp (PDL) and recorded on the high-resolution vacuum-ultraviolet (VUV) Fourier transform (FT) spectrometer at Imperial College (IC) London, UK. This instrument has a resolving power of up to  $\sim 2$  million at 200 nm, resulting in the most accurate Fe III linelist produced to date in the UV-VUV (152.7 nm to 295.6 nm). The strongest Fe III spectral lines recorded had uncertainties between 0.000027 nm and 0.00012 nm.

As our FT spectrometer has a lower wavelength limit of  $\sim 135$  nm, these accurate wavenumbers were supplemented with grating spectra in the lower wavelength region. The grating spectra (90 nm to 181 nm) were recorded on the 10.7 m normal incidence vacuum spectrograph (NIVS) at the National Institute of Standards and Technology (NIST) in Gaithersburg, Maryland, USA. Both the FT and grating spectra were wavenumber calibrated using Fe II Ritz wavelengths published by [1]. The FT data were calibrated to an accuracy of 5 - 8.5 parts per  $10^8$ .

Using the observed transition wavelengths, an extensive term analysis of the lower-lying energy levels of Fe III has been conducted. The results include the revision of 313 previously published atomic energy level values and 1890 Ritz wavenumbers identified as Fe III transitions in the UV-VUV, which are at least an order-of-magnitude more accurate than previous publications. The atomic data reported here have numerous applications in astronomy. These accurate Fe III transition wavelengths will be used as wavelength standards to calibrate VUV spectra of hot stars and for the identification of spectral lines.

Additionally, 400 parity-forbidden Fe III Ritz wavelengths have been calculated between the lowest-lying configurations,  $3d^6$  and  $3d^5(ML)4s$ . These findings will assist astronomers in analysing spectra obtained from diluted astrophysical plasmas.

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\*email: f.concepcion@imperial.ac.uk

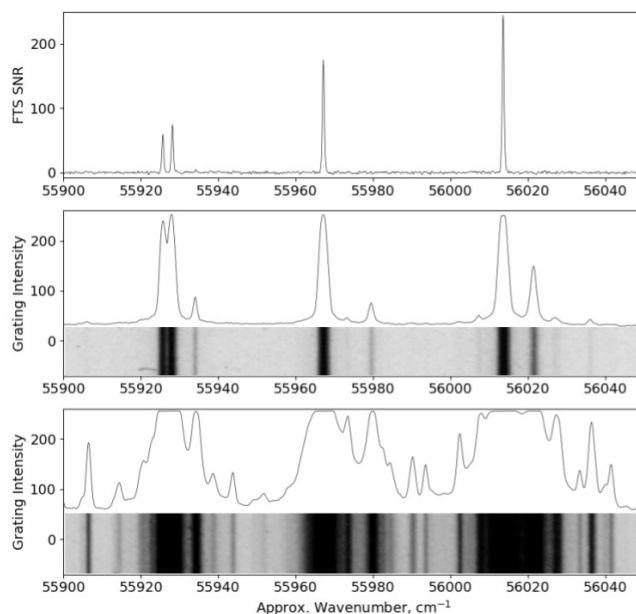


Figure 1: The iron spectrum observed on the IC FT spectrometer [top], and on the NIST NIVS with 5-minute [middle] and 45-minute exposure [bottom].



## Multiplatform determination of the radiative properties of the seventh spectrum of tantalum (Ta VII)

E. Bokamba Motoumba<sup>a</sup>, S. Enzonga Yoca<sup>a,b</sup>, P. Quinet<sup>c,d</sup>, and **P. Palmeri<sup>c,\*</sup>**

<sup>a</sup>Faculté des Sciences et Techniques, Université Marien Ngouabi, Brazzaville, BP 69, Congo

<sup>b</sup>Conseil Africain et Malgache pour l'Enseignement Supérieur - CAMES, Ouagadougou 01, 01 BP 134, Burkina Faso

<sup>c</sup>Physique Atomique et Astrophysique, Université de Mons – UMONS, Mons, B-7000, Belgium

<sup>d</sup>IPNAS, Université de Liège, Liège, B-4000, Belgium

Tantalum ( $Z=73$ ) is an element that is produced in the neutron-induced transmutation of tungsten ( $Z=74$ ) which in turn will compose the divertors in Tokamaks [1]. As a consequence, their sputtering may generate ionic impurities of all possible charge states in the deuterium-tritium plasma that could contribute to radiation losses in controlled nuclear devices. The radiative properties of these ions have therefore potential important applications in this field.

In this context, a multiplatform approach has been adopted in order to compute the Ta VII radiative rates and estimate their accuracy. The oscillator strengths and transition probabilities have been calculated for the 237 E1 transitions in Ta VII as classified in 2014 by Ryabtsev *et al* [2]. Three independent atomic structure models have been used; one based on the semi-empirical pseudo-relativistic Hartree-Fock (HFR) method [3] and two based on the fully relativistic *ab initio* multiconfiguration Dirac-Hartree-Fock (MCDHF) method [4,5].

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\*email: Patrick.Palmeri@umons.ac.be

# JAC: A community platform for just atomic computations

Stephan Fritzsche

GSI Helmholtzzentrum für Schwerionenforschung, Darmstadt, Germany

Helmholtz-Institut Jena, Jena, Germany

Institut für Theoretische Physik, Friedrich-Schiller-Universität Jena, Germany

Electronic structure calculations of atoms and ions have a long tradition in physics with applications in basic research and spectroscopy. With the Jena Atomic Calculator (JAC), I here present a new implementation of a (relativistic) electronic structure code for the computation of atomic amplitudes, properties as well as a large number of excitation and decay processes for open-shell atoms and ions across the periodic table. JAC [1] is based on Julia, a new programming language for scientific computing, and provides an easy-to-use but powerful platform to extent atomic theory towards new applications.

A primary guiding philosophy in designing JAC was to develop a general and easy-to-use toolbox for the atomic physics community, including an interface that is equally accessible for working spectroscopists, theoreticians and code developers. In addition, I also wish to provide a modern code design, a reasonable detailed documentation of the code and features for integrated testing [2].



Figure 1: Overview of the JAC toolbox.

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\*email: s.fritzsche@gsi.de

# THEORETICAL STUDY OF SPECTRA OF Hf VI USING A MULTIPLATFORM APPROACH

Exaucé BOKAMBA MOTOUMBA<sup>a,\*</sup>, S.E. YOCA<sup>b</sup>, P. QUINET<sup>c,d</sup>, P. PALMERI<sup>c</sup>

<sup>a</sup> Faculté des Sciences et Techniques, Université Marien Ngouabi, Brazzaville, BP 69, Congo

<sup>b</sup> Conseil Africain et Malgache pour l'Enseignement Supérieur – CAMES, Ouagadougou BP 134, Burkina-Faso

<sup>c</sup> Physique Atomique et Astrophysique, Université de Mons – UMONS, Mons, BP 7000, Belgium

<sup>d</sup> IPNAS, Université de Liège, Liège, BP 4000, Belgium

Hafnium ( $Z = 72$ ) is an element that could be employed in plasma-facing materials in Tokamaks [1,2] and is also produced in neutron-induced transmutation of tungsten ( $Z = 74$ ) and its alloys that will compose the divertors in these fusion reactors [3]. As a consequence, their sputtering may generate ionic impurities of all possible charge states in the deuterium-tritium plasma. These impurities could contribute to radiation losses in controlled nuclear fusion devices. The radiative properties of these ions have therefore potential important applications in this field [4,5,6].

**Many lines of Hf VI in UV range, precisely from 193 Å to 474 Å, have been calculated. As no experimental determination of radiative rates is available in the literature, a multiplatform approach has been adopted to carry out the present calculations so as to estimate the accuracy of the computed rates.**

From the comparisons of our three independent models based on both the HFR [7] and MCDHF [8,9] methods along with the calculations published by Ryabtsev et al. [5] that they used for line classification purpose, it was found that the uncertainties affecting the theoretical rates range from a few percent (for our HFR model) to ~40 % (for our MCDHF-RCI-A model) for the strong E1 transitions with  $S \geq 1$  a.u. With respect to the other lines, they can be highly inaccurate with uncertainties far more than 100 % due to strong cancellation effects and important gauge disagreements that render the rates highly model sensitive. This is essentially caused by the strong mixing affecting most of the Hf VI atomic states. **Finally, we recommend our HFR rates except for the two lines at 223.172 Å and at 231.451 Å where the  $gA$ -values of Ryabtsev et al. [5] should be used instead with an uncertainty indicator *Unc.* equal to  $E$  ( $> 50\%$ ), due to strong cancellation effects affecting the former for these two transitions.**

We have plotted in 3 figures the difference between the level energy calculated in our three independent models and the one determined experimentally by Ryabtsev et al [5]; also plotted in 3 figures the comparison of our transition probabilities, with respect to the calculation of Ryabtsev et al. [5], The ratio,  $gA_{HFR}/gA_{RYA}$ , is plotted versus our HFR line strength,  $S_{HFR}$ , both in logarithmic scale. Similar plots are displayed for our MCDHF-RCI-A and our MCDHF-RCI-B models.

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## **The effect of electron correlation on trielectronic recombination rate coefficients for Be-like argon**

**Chunyu Zhang<sup>a,\*</sup>, Chongyang Chen<sup>b</sup>, Nigel Badnell<sup>a</sup>**

<sup>a</sup>Department of Physics, University of Strathclyde, Glasgow G4 0NG, UK

<sup>b</sup>Shanghai EBIT Lab, Key Laboratory of Nuclear Physics and Ion-beam Application, Institute of Modern Physics, Department of Nuclear Science and Technology, Fudan University, Shanghai 200433, China

The merged-beam rate coefficients of dielectronic and trielectronic recombinations (DR and TR) within  $\Delta N = 0$  channels for Be-like Ar14+ were measured by Huang et al. [Astrophys. J. Supp. Ser. 235, 2 (2018)] with the cooler storage ring at Lanzhou, China. Meanwhile, theoretical data were also calculated with AUTOSTRUCTURE (AS) code for comparison with the measured resonance spectrum. However, the AS calculations in most cases significantly underestimated TR resonance strengths. In the present work, we find that the electron correlation between DR and TR resonance states with different captured electron principal quantum numbers  $n$  can lead to an obvious enhancement in TR resonance strengths, which is cross-validated via the relativistic distorted-wave (RDW) approximation implemented in the Flexible Atomic Code (FAC) and the semi-relativistic distortedwave (SRDW) approximation implemented in the AS code. Previous theoretical calculations for this system, however, did not include this form of electron correlation.

\*email: [chunyu.zhang@strath.ac.uk](mailto:chunyu.zhang@strath.ac.uk)

## **THE FINGERPRINTS OF PERIODIC ELECTRIC FIELDS ON LINE SHAPES EMITTED IN PLASMAS**

**Ibtissem HANNACHI<sup>a,\*</sup>, Roland STAMM<sup>b</sup>**

<sup>a</sup>Batna 1 University, LRPRIM, 05000 Batna, Algeria

<sup>b</sup>Aix Marseille University and CNRS, PIIM UMR 7345, 13013 Marseille, France

Periodic electric fields are found in many kinds of plasmas and result from the presence of collective fields amplified by plasma instabilities, or are created by external sources such as microwave generators or lasers. Spectral lines emitted by atoms or ions in a plasma exhibit a frequency profile characteristic of plasma conditions such as the temperature and density of charged particles. The fingerprints of periodic electric fields appear clearly on the line shape for a large range of frequencies and magnitudes of the oscillating electric field. Satellite structures appear near to multiples of the oscillation frequency and redistribute the intensity of the line far from the line center. The modeling of the simultaneous effects of the plasma microfield and of a periodic electric field has been active since the seventies, but remains difficult to be done accurately since the quantum emitter is submitted to several time dependent electric fields, each with its own characteristic time. We describe here a numerical approach which couples a simulation of the motion of charged plasma particles with an integration of the emitter Schrödinger equation. Resulting line shapes are presented for different plasmas and periodic fields encountered in laboratory and astrophysical plasmas.

\*email: [ibtissam.hannachi@univ-batna.dz](mailto:ibtissam.hannachi@univ-batna.dz)

## SEMI-EMPIRICAL DETERMINATION OF RADIATIVE PARAMETERS FOR SINGLY IONIZED ATOM OF COBALT

**Marcin Klempka<sup>a\*</sup>**, Jarosław Ruczkowski<sup>b</sup>, Magdalena Elantkowska<sup>a</sup>

<sup>a</sup>Institute of Materials Research and Quantum Engineering, Faculty of Materials Engineering and Technical Physics, Poznan University of Technology, Piotrowo 3, Poznan 60-965, Poland

<sup>b</sup>Institute of Robotics and Machine Intelligence, Faculty of Control, Robotics and Electrical Engineering, Poznan University of Technology, Piotrowo 3a, 60-965 Poznan, Poland

Cobalt belongs to iron group elements with an open 3d-shell, which structure is interesting in various fields, astrophysics in particular. There is a noticeable interest in determining the overall abundance trend of Co for testing stellar atmosphere models, evaluating galactic chemical evolution and examining the cobalt nucleosynthesis process.

In our earlier works [1, 2] we carried out semi-empirical calculations of the fine and hyperfine structure for both Co II parity configuration systems. In these articles, we made an attempt to resolve significant discrepancies in some experimental results recently published by two research teams [3, 4]. The fine-structure eigenvectors, determined in those studies, were applied in the presented work for the determination of the radiative parameters. Predicting the values of radiative lifetimes and oscillator strengths was the final way to verify the accuracy of the calculated eigenvectors.

The aim of our research is to determine the values of radiative lifetimes and oscillator strengths for Co II based on available experimental data, using a semi-empirical method. A total of 118 values of the oscillator strengths were calculated and compared with the empirical data. Among the lines with small measurement uncertainties, very good agreement was achieved. The largest differences are mainly related to the values specified with an error greater than 20%. The results of our calculations are shown in comparison to experimental data and other theoretical research published by Raassen et al. [5], Quinet et al. [6] and Kurucz [7]. Additionally, lifetime values for 185 levels were calculated, with 34 of them compared to the experimental data. The similarity of our calculated lifetimes to the experimental values indicates good agreement.

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\*email: marcin.klempka@doctorate.put.poznan.pl

## HYPERFINE SPLITTINGS OF FEW-ELECTRON HELIUMLIKE IONS AND NUCLEAR PROPERTIES

Xiao-Qiu Qi<sup>a,b</sup>, Pei-Pei Zhang<sup>b</sup>, **Zong-Chao Yan**<sup>c,b,\*</sup>, Ting-Yun Shi<sup>b</sup>, G. W. F. Drake<sup>d</sup>, Ai-Xi Chen<sup>a</sup>, and Zhen-Xiang Zhong<sup>b,e</sup>

<sup>a</sup> Zhejiang Sci-Tech University, Hangzhou 310018, China

<sup>b</sup> Wuhan Institute of Physics and Mathematics, Wuhan 430071, China

<sup>c</sup> University of New Brunswick, Fredericton, New Brunswick, Canada E3B 5A3

<sup>d</sup> University of Windsor, Windsor, Ontario, Canada N9B 3P4

<sup>e</sup> Hainan University, Haikou 570228, China

The hyperfine structures of the  $2^3S$  and  $2^3P$  states of  $7\text{Be}^{2+}$  and  $9\text{Be}^{2+}$  are investigated within the framework of the nonrelativistic quantum electrodynamics (NRQED), including relativistic and radiative corrections up to order  $m\alpha^6$ . The uncertainties of the calculated hyperfine splittings are on the order of tens of ppm, and for  $9\text{Be}^{2+}$  our results improve the previous theoretical and experimental values by at least two orders of magnitude. The improved sensitivity of the hyperfine splittings of  $7,9\text{Be}^{2+}$  to the nuclear Zemach radius and electric quadrupole moment opens the way to future measurements to extract the atomic physics values of these two nuclear properties to an accuracy of 5% or better.

\*email: zyan@unb.ca

## Energy and Properties of Sb-like Nd<sup>9+</sup>, P-like, As-like, Sb-like, Bi-like and Mc-like np<sup>3</sup> Atoms and Ions

Hongxu LIU<sup>a,b</sup> and Yanmei YU<sup>a\*</sup>

<sup>a</sup> Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

<sup>b</sup> State Key Laboratory of Metastable Materials Science and Technology & Key Laboratory for Microstructural Material Physics of Hebei Province, School of Science, Yanshan University, Qinhuangdao, 066004, China

The rich energy configuration of multiply ionized atoms offers numerous optical transitions between the ground state and the long-lived excited states. These transitions have numerous practical applications, including identifying and characterizing astronomical objects like stars and galaxies, diagnosing plasma composition, temperature, and density, and serving as frequency standards for precision measurement and testing fundamental constants [1-4]. In this study, we present accurate calculations of the energies and properties of Sb-like Nd<sup>9+</sup> ion and a group of P-like, As-like, Sb-like, Bi-like and Mc-like np<sup>3</sup> atoms and ions (n=3-7), which are useful for making high-accuracy optical clocks as well as for astronomical identification and plasma diagnosis. To achieve this, we used the relativistic multi-reference configuration interaction (MRCI) method under both four-component Dirac-Coulomb all-electron and relativistic effective core potential frameworks, while considering various types of correlation consistent basis sets. Our calculations predicted wavelengths, quality factors, lifetimes, gJ factors, electric quadrupole moment, electric dipole and quadrupole polarizabilities, and hyperfine structure constants for Nd<sup>9+</sup> [5] and the np<sup>3</sup> atoms and ions [6], including many previously unmeasured energies and atomic properties. This study also provides a theoretical benchmark for complex multi-valent systems and expands our understanding of astrophysical spectroscopy, plasma diagnosis, and precision measurement based on optical forbidden transitions.

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\*email: ymyu@iphy.ac.cn



## Multiconfiguration Dirac-Hartree-Fock calculations of the hyperfine structure in 137-Ba II for the $^2S_{1/2}$ state

L. Maison<sup>a,\*</sup>, M. Godefroid<sup>b</sup>, P. Palmeri<sup>a</sup> and P. Quinet<sup>a,c</sup>

<sup>a</sup>Physique Atomique et Astrophysique, Université de Mons, B-7000 Mons, Belgium

<sup>b</sup>SQUARES, Université Libre de Bruxelles, B-1050 Brussels, Belgium

<sup>c</sup>IPNAS, Université de Liège, B-4000 Liège, Belgium

One of the most dominant processes for the creation of heavy elements in our universe is the r-process. In order to explain their abundance, astrophysicists have developed the theory of nucleosynthesis. Most of the nucleosynthesis signatures can be found in the isotopic abundances. This isotopic mixture for the r-process elements can be determined at the stellar surface of r-process enriched stars by measuring the odd-to-even isotopic ratio of these r-process elements [1]. However, the r-process models predict isotopic mixtures that are difficult to constrain observationally because the lines of odd nuclei are affected by hyperfine splitting which can be hard to resolve in a spectrum. If the hyperfine structure can be determined it is thus possible to measure the fraction of the odd-mass isotopes and to relate it to a given nucleosynthetic process. Barium is a r-process element which has a great interest in astrophysics [2]. Its spectrum for different stage of ionization is therefore well known. If one plans to measure the abundance for this element it is therefore crucial to know its hyperfine structure.

In this work, ab initio atomic calculations of the magnetic dipolar hyperfine constant A for the  $5s^25p^66s\ ^2S_{1/2}$  ground state of singly ionized 137-barium were performed. The preliminary results presented here were determined by means of the multiconfiguration Dirac-Hartree-Fock (MCDHF) method [3] with the GRASP2018 code [4]. Three strategies of orbital optimization were used to probe the effect of different electronic correlation effects on the A constant. After that, for each strategy, a series of relativistic configuration interaction calculations (RCI) were carried out by considering other types of correlation effects. Finally, the preliminary results obtained were compared with the experimental value [5] and others theoretical computations [6,7].

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\*email: lucas.maison@umons.ac.be

# ALIGNMENT-TRANSFER RATE COEFFICIENTS FOR ELECTRON IMPACT EXCITATION OF O V

M.K. Inal\* and M. Benmouna\*\*

Department of Physics, Faculty of Sciences, University of Tlemcen, 13000 Tlemcen, Algeria

The multipole rate coefficients  $C_0^{KK'}$  for electron impact excitation of ions are required in the analysis of intensity and polarization of lines emitted from non-thermal plasmas with a cylindrically symmetric electron velocity distribution [1]. Among them, the alignment-transfer rate coefficients, corresponding to non-zero even values of  $K$  and  $K'$ , include quantum coherences between magnetic sublevels within the initial and final ion levels, via integration of a linear combination of alignment-transfer  $\sigma_{Q=0}^{KK'}$  and coherence-transfer  $\sigma_{Q\neq 0}^{KK'}$  cross sections [2]. However, the few calculations of the alignment-transfer rate coefficients  $C_0^{KK'}$  published so far consider only the contribution from  $\sigma_{Q=0}^{KK'}$ . This was the case of Ref. [3] where significant discrepancies were observed between theoretical predictions and measurements in the WT-3 tokamak for certain UV lines of Be-like ion O V.

In an attempt to evaluate the effects of coherence-transfer, we report here calculated data of  $C_0^{22}$  for excitations of O V from the metastable levels  $2s2p\ ^3P_1$  and  $^3P_2$  to the  $2s3p$  and  $2p3d$  configuration levels, using the same electron velocity distribution as in [3]. The  $\sigma_{Q=0,\pm 1,\pm 2}^{22}$  cross sections are computed in the relativistic distorted-wave approximation using an extended version [4] of the flexible atomic code. Table 1 gives selected results that illustrate the important contribution of the coherence-transfer cross sections  $\sigma_{Q=\pm 1,\pm 2}^{22}$ , which could be a clue to explain, at least partly, the discrepancies mentioned above.

Table 1: Selected results of  $C_0^{22}$  (in  $\text{cm}^3\text{s}^{-1}$ ) for excitations of O V with and without coherence-transfer.

Excitation	with $\sigma_{Q=\pm 1,\pm 2}^{22}$	without $\sigma_{Q=\pm 1,\pm 2}^{22}$
$2s2p\ ^3P_1 \rightarrow 2s3p\ ^3P_1$	$5.85 \times 10^{-10}$	$1.03 \times 10^{-10}$
$2s2p\ ^3P_2 \rightarrow 2s3p\ ^3P_2$	$5.84 \times 10^{-10}$	$1.04 \times 10^{-10}$
$2s2p\ ^3P_1 \rightarrow 2s3p\ ^3P_2$	$-2.21 \times 10^{-11}$	$-3.00 \times 10^{-12}$
$2s2p\ ^3P_2 \rightarrow 2s3p\ ^3P_1$	$-2.24 \times 10^{-11}$	$-3.18 \times 10^{-12}$

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\* email: mokhtar.inal@univ-tlemcen.dz

\*\* Retired

# CALCULATED OSCILLATOR STRENGTHS FOR SPECTRAL LINES IN Re III-V IONS OF INTEREST TO NUCLEAR FUSION RESEARCH

Maxime Brasseur<sup>a</sup>, Sébastien Gamrath<sup>a</sup>, **Pascal Quinet**<sup>a,b,\*</sup>

<sup>a</sup>Physique Atomique et Astrophysique, Université de Mons, B-7000 Mons, Belgium

<sup>b</sup>IPNAS, Université de Liège, B-4000 Liège, Belgium

It is now well established that tungsten will be one of the main divertor components of the ITER nuclear fusion reactor. When D-T fusion will take place, very energetic neutrons will strike the walls of the reactor and cause the transmutation of tungsten atoms by irradiation. The primary transmutation products for tungsten are rhenium, osmium and tantalum. In particular, the calculations revealed that, after 5-year irradiation under first wall fusion power-plant conditions in ITER, Re, Os and Ta would reach concentrations of 3.8, 1.4, and 0.8 atomic percentage, respectively [1]. As with tungsten, during fusion operations, these atoms, and more particularly rhenium atoms, will be torn from the reactor wall and enter the plasma where they will constitute impurities contributing to the energy loss by radiation but can also be used for plasma temperature and density diagnostics from the analysis of their spectra in all ionization stages. Therefore the radiative properties of these ions have potential important applications in this field. The purpose of the present work is to provide a new set of atomic data (oscillator strengths and transition probabilities) for electric dipole lines in rhenium ions, from Re III to Re V, obtained using two independent theoretical approaches, i.e. the pseudo-relativistic Hartree-Fock method [2] including core-polarization effects (HFR+CPOL) [3,4] and the fully relativistic Dirac-Hartree-Fock (MCDHF) method [5,6].

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\*email: pascal.quinet@umons.ac.be

# EFFECT OF THE BREIT INTERACTION ON THE ANGULAR DISTRIBUTION OF AUGER ELECTRONS FOLLOWING ELECTRON-IMPACT EXCITATION OF BE-LIKE IONS

Z W Wu <sup>a, b, c, \*</sup>, Y Li <sup>a</sup>, Z Q Tian <sup>a</sup>, C Z Dong <sup>a</sup>, and S Fritzsche <sup>b, c, d</sup>

<sup>a</sup>Northwest Normal University, Lanzhou, P. R. China

<sup>b</sup>Helmholtz-Institut Jena, Jena, Germany

<sup>c</sup>GSI Helmholtzzentrum für Schwerionenforschung GmbH, Darmstadt, Germany

<sup>d</sup>Friedrich-Schiller-Universität Jena, Jena, Germany

Electron-impact excitation (EIE) of atoms or ions is one of fundamental atomic processes in astrophysical and laboratory plasmas. Chen *et al.* studied the relativistic effect on the angular distribution of Auger electrons following EIE of Be-like ions [1]. However, as a main part of the relativistic effect, the Breit interaction was not considered.

In the present work [2], we studied the angular distribution of Auger electrons following the EIE  $1s^2 2s^2 J=0 \rightarrow 1s 2s^2 2p_{1/2} J=1$  of Be-like  $Mg^{8+}$ ,  $Fe^{22+}$ ,  $Mo^{38+}$ ,  $Nd^{56+}$ ,  $Au^{75+}$ , and  $U^{88+}$  ions using the multi-configurational Dirac-Fock method and the relativistic distorted-wave theory. Special attention was paid to the effect of the Breit interaction on the angular distribution of the emitted Auger electrons. It was found that for low- $Z$  Be-like ions such as  $Mg^{8+}$  the Breit interaction hardly contributes to the angular distribution of the Auger electrons, whereas for medium- and high- $Z$  ions it makes the angular distribution less anisotropic. To be specific, such an effect becomes first more prominent with increasing nuclear charge  $Z$  and, then, less and less when it further increases, as shown in Figure 1 as an example for the impact electron energy of 3.0 times their respective excitation thresholds, where NB and B denote the results without and with consideration of the Breit interaction, respectively.

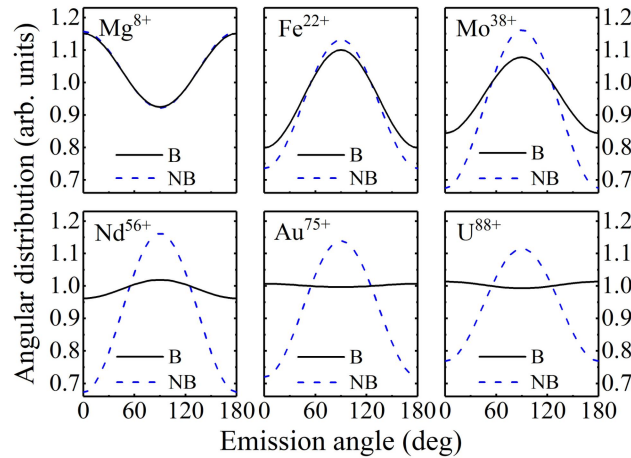


Figure 1: Angular distribution of the Auger electrons emitted from the Auger decay  $1s 2s^2 2p_{1/2} J=1 \rightarrow 1s^2 2s J=1/2$  of Be-like ions for an impact energy of 3.0 times their respective excitation thresholds. Results are given for both NB (blue dashed lines) and B (black solid lines) cases.

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# QUASI-MOLECULAR MECHANISM OF COSMOLOGICAL RECOMBINATION

Tamaz Kereselidze<sup>a</sup>, Irakli Noselidze<sup>b</sup>

<sup>a</sup>Faculty of Exact and Natural Sciences, Tbilisi State University, Chavchavadze Avenue 3, 0179 Tbilisi, Georgia

<sup>b</sup>School of Science and Technology, University of Georgia, Kostava Str. 77a, 0171 Tbilisi, Georgia

According to the standard mechanism of recombination two charged particles an electron, and a proton participated in the formation of atomic hydrogen. An electron and a proton combined efficiently into the hydrogen atom only in a highly excited state, from which a rapid cascade occurred into a state with the principal quantum number  $n = 2$ .

In our study, we assume that an electron collides with two protons situated one far from another, emits a photon, and creates a quasi-molecule,  $H_2^+$  in a highly excited state [1]. If  $H_2^+$  is formed in a repulsive state, it rapidly dissociates into a proton and the excited hydrogen atom, which then cascades downward. This mechanism is analogous to the standard mechanism of recombination. However, if  $H_2^+$  is formed in an attractive state, the protons involved in recombination approach each other, and the quasi-molecule descends into a low-lying state which might be repulsive or attractive (see Fig.1 in [2]). The quasi-molecular mechanism of recombination (QMR) thus produces  $H$  as well as  $H_2^+$  in the ground state.

Obviously, the QMR was significant at the pre-recombination stage of the evolution of the Universe (redshift  $z > 2000$ ) when the temperature and density of matter were higher than subsequently. The estimation shows that at that period the average distance between protons in the primordial plasma was about  $10^6 a_0$ , where  $a_0$  is the radius of the first Bohr orbital in the hydrogen atom.

The purpose of the present study is to answer the question could the nearest neighboring proton impact cosmological recombination at such distances  $R$  between protons? For this, a scheme of calculation based on the QMR was elaborated and applied to the calculation of probabilities of free-bound transitions into a highly excited attractive state of  $H_2^+$ . For large  $R$  the transition probability is expressible as

$$W_{i \rightarrow f}(R) = W_{i \rightarrow f}^{(0)} + \frac{1}{R} W_{i \rightarrow f}^{(1)} + O(R^{-2}), \quad (1)$$

in which  $W_{i,f}^{(0)}$  determines the transition probability on an isolated proton, and  $W_{i,f}^{(1)}$  accounts for a correction caused by the participation of another proton in recombination. Calculations revealed that compared with the first term the contribution of the second term in (1) increases from 0.001 at  $n=100$  to 0.05 at  $n=400$ . This means that for highly excited states the impact of the QMR on cosmological recombination was perceptible.

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\*email: [tamaz.kereselidze@tsu.ge](mailto:tamaz.kereselidze@tsu.ge)

## AN ATOMIC DATA OPTIMIZATION METHOD FOR IMPROVED KILONOVA OPACITY MODELING

**R. Ferreira da Silva**<sup>\*a</sup>, A. Flörs<sup>b</sup>, G. Leck<sup>b,c</sup>, J. M. Sampaio<sup>a</sup>, G. Martínez-Pinedo<sup>b,c,d</sup>, P. Amaro<sup>e</sup>, J. P. Marques<sup>a</sup>, L. Leitão<sup>a</sup>, L. Shingles<sup>b</sup>

<sup>a</sup>Laboratório de Instrumentação e Física Experimental de Partículas (LIP) and Faculdade de Ciências, Universidade de Lisboa (FCUL), Portugal

<sup>b</sup>GSI Helmholtzzentrum für Schwerionenforschung, Planckstraße 1, 64291 Darmstadt, Germany

<sup>c</sup>Institut für Kernphysik (Theoriezentrum), Fachbereich Physik, Technische Universität Darmstadt, Schlossgartenstraße 2, 64289 Darmstadt, Germany

<sup>d</sup>Helmholtz Forschungsakademie Hessen für FAIR, GSI Helmholtzzentrum für Schwerionenforschung, Planckstraße 1, 64291 Darmstadt, Germany

<sup>e</sup>Laboratory for Instrumentation, Biomedical Engineering and Radiation Physics (LIBPhys-UNL), Department of Physics, NOVA School of Science and Technology, NOVA University Lisbon, 2829-516 Caparica, Portugal

In 2017, the identification of an electromagnetic counterpart to the gravitational wave signal GW170817 constituted direct evidence for the production of r-process elements during the collision of neutron stars [1]. One of the principal sources of uncertainty for modeling the resulting kilonova, essential to probe and characterize the ejecta, comes from the atomic data used. Small relative errors (e.g. few percent) in the transition wavelengths, or larger errors in the oscillation strengths (tens of percent), can make interpretation of the spectra or the identification of features of specific elements [2,3] difficult or even impossible to achieve. The high degree of complexity of open f-shell elements, expected to be present in the ejecta, in combination with the necessity for large datasets to comprehensively capture opacity behavior across both the optical and infrared ranges, makes the use of full *ab initio* codes impractical in most instances due to their intensive computational demands [4]

Using the publicly available Flexible Atomic Code software package [5], we have developed an optimization procedure to provide atomic data (energy levels and oscillator strengths) which attempts to improve consistency with available experimental or *ab initio* data while retaining efficiency in the calculations. In this work we analyze the sensitivity of the data to the optimization method and how it allows for a controlled and systematic improvement of accuracy when compared to other methods [6,7]. Furthermore we investigate how this optimization technique affects our calculations as well its impact on line-by-line and gray opacity data.

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\*email: rfsilva@lip.pt

## Exploring ab-initio and semi-empirical small-scale atomic structure models of neutron-capture elements

S. Caliskan<sup>a,\*</sup>, J. Grumer<sup>a</sup>

<sup>a</sup>Theoretical Astrophysics, Department of Physics and Astronomy, Uppsala University, Sweden

Recent advancements in astrophysics, such as the James Webb space telescope (JWST) and the LIGO/Virgo gravitational wave detectors, have introduced new demands on atomic physics. With the JWST operating in the infrared spectral regime, and the LIGO/Virgo leading to the ground-breaking discovery of the first neutron-star-merger event accompanied by a kilonova transient (arguably a dominant production site for neutron capture elements) [1], have highlighted the need for reliable atomic data for the heavier elements, in particular in the infrared.

However, the current databases are both incomplete and poor in quality when it comes to heavy elements. This lack of information on atomic energy levels and processes is partly due to the complexities involved in carrying out atomic structure calculations for many of these elements, notably the lanthanides.

A significant challenge posed by lanthanides is the presence of multiple configurations with many levels and overlapping energies, giving rise to perturbing states. These elements often have orbitals that are closely aligned energetically so that different occupations lead to configurations of similar energies. Current state-of-the-art atomic structure codes assume an orthonormal orbital basis set. However, separate calculations of two competing configurations reveal significant non-orthonormalities between the orbitals of each configuration. This can lead to inaccurate expectation values if not taken into account properly.

In this contribution, we present methods for performing atomic structure calculations that address this critical issue while also ensuring that the wavefunctions remain compact enough for efficient computations of collisional-radiative properties across a wide range of atomic systems needed, for instance, in kilonova spectral modeling. Taking neutral gold as a representative system and using the relativistic atomic structure code GRASP2018 [2], we explore targeted optimization techniques to treat the orbital non-orthonormalities. Moreover, we investigate semi-empirical rescalings of diagonal matrix elements to further improve the quality of the wavefunction, as recently discussed in the context of the GRASP code by Li et al. [3].

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\*email: sema.caliskan@physics.uu.se

## A VARIATIONAL ATOMIC MODEL OF PLASMA ACCOUNTING FOR ION RADIAL CORRELATIONS AND ELECTRONIC STRUCTURE OF IONS

T. Blenski <sup>a</sup>, **R. Piron** <sup>\*,b,c</sup>

<sup>a</sup>Laboratoire “Interactions, Dynamiques et Lasers”, UMR 9222, CEA-CNRS-Université Paris-Saclay, Centre d’Études de Saclay, F-91191 Gif-sur-Yvette Cedex, France.

<sup>b</sup>CEA, DAM, DIF, F-91297 Arpajon, France.

<sup>c</sup>Université Paris-Saclay, CEA, Laboratoire Matière en Conditions Extrêmes, F-91680 Bruyères-le-Châtel, France.

We report on a new model of ion-electron plasma (or nucleus-electron plasma) that accounts for the electronic structure around nuclei (i.e. ion structure) as well as for ion-ion correlations [1]. The model equations are obtained through the minimization of an approximate free-energy functional, and it is shown that the model fulfills the virial theorem.

The main hypotheses of this model are 1) nuclei are treated as classical indistinguishable particles 2) electronic density is seen as a superposition of a uniform background and spherically-symmetric distributions around each nucleus (system of ions in a plasma) 3) free energy is approached using a cluster expansion 4) resulting ion fluid is modeled through an approximate integral equation.

In this poster we describe the set of hypotheses of this model, sketch the derivation of the model equations and comment on them. We show how this model fulfills the virial theorem, allowing a sound definition of the related thermodynamic quantities. Then, we show some preliminary numerical results regarding the equation of state, as well as quantities related to radiative properties, such as the oscillator strengths. These results are compared with results from other models such as VAAQP or INFERNO. Finally we discuss some limitations of the model.

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\*email: robin.piron@cea.fr



## STELLAR OPACITIES IN LAB USING A HIGH INTENSITY LASER

Hanna Lahmar <sup>a</sup>, Franck Delahaye <sup>b</sup>, Sebastien Le Pape <sup>a</sup>, Frédéric Pérez <sup>a</sup>, Patrick Audebert <sup>a</sup>, Sophie Baton <sup>a</sup>, Patrick Renaudin <sup>c</sup>, Ludovic Lecherbourg <sup>c</sup>, Christophe Blancard <sup>c</sup>, Laurent Jacquet <sup>c</sup>, Annaïg Chaleil <sup>b</sup>,

<sup>a</sup> LULI, Sorbonne Université and Ecole Polytechnique de Paris, Palaiseau, 91128 Palaiseau, France

<sup>b</sup> Observatoire de Paris - LERMA, Sorbonne Université and Paris Observatory, Meudon Campus, 92190 Meudon, France

<sup>c</sup> CEA, DAM, DIF, F-91297 Arpajon, France

The opacity of the Sun radiative zone is a key to understanding energy flux in the Sun interior as well as its structure. The opacity of the radiative zone is mostly governed by oxygen, iron and neon absorption [1], but most of the questioning lies on the iron opacity.

In 2015, experiments carried out on the Z-machine exhibited large discrepancies between experimental results and modeling [2]. Ever since, only a handful of experiments challenge to create in laboratory solar-relevant conditions. In this poster, I will present the results obtained on a new opacity platform at LULI laboratory, based on isochoric heating of iron by an ultra-intense laser. These results will be compared to state-of-the-art atomic simulations.

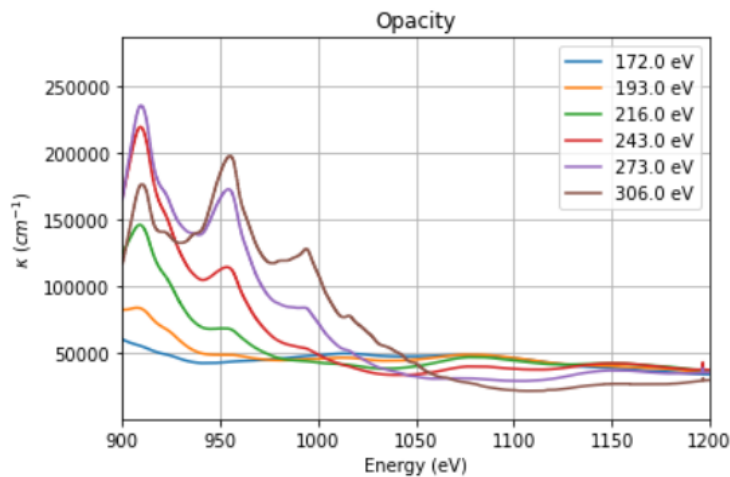


Figure 1: Simulated opacity of the heated iron at different temperature using OP.

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\*email: [hanna.lahmar@polytechnique.edu](mailto:hanna.lahmar@polytechnique.edu)

## Erbium Optical Spectra from Pellet Ablation Cloud in the Large Helical Device for Laboratory Assessment of Atomic Data

Priti<sup>1\*</sup>, Hiroyuki A. Sakaue<sup>1</sup>, Gediminas Gaigalas<sup>2</sup>, Motoshi Goto<sup>1,3</sup>, Izumi Murakami<sup>1,3</sup>,  
Tetsutaro Oishi<sup>4</sup>, Masaomi Tanaka<sup>5,6</sup>, Nobuyuki Nakamura<sup>7,1</sup>, Daiji Kato<sup>1,8</sup>

<sup>1</sup>National Institute for Fusion Science, National Institutes of Natural Sciences, Toki, Gi509-5292, Japan

<sup>2</sup>Institute of Theoretical Physics and Astronomy, Vilnius University, Vilnius LT-10257, Lithuania

<sup>3</sup>Department of Fusion Science, SOKENDAI, Toki, Gifu 509-5292, Japan

<sup>4</sup>Department of Quantum Science and Energy Engineering, Graduate School of Engineering, Tohoku University, Sendai, Miyagi 980-8579, Japan

<sup>5</sup>Astronomical Institute, Tohoku University, Sendai 980-8578, Japan

<sup>6</sup>Division for the Establishment of Frontier Sciences, Organization for Advanced Studies, Tohoku University, Sendai 980-8577, Japan

<sup>7</sup>Institute for Laser Science, The University of Electro-Communications, Tokyo 182-8585, Japan

<sup>8</sup>Interdisciplinary Graduate School of Engineering Sciences, Kyushu University, Fukuoka 816-8580, Japan

The atomic data of heavy elements, especially rare-earth metals, plays a crucial role in enhancing our understanding and interpreting the kilonova spectra and the underlying astrophysical processes. Among these elements, Erbium (Er) is particularly intriguing to look for in kilonova spectra [1]. In order to assess the atomic data emission spectra from Er are measured in the optical region. In the present experiment, Er was injected into the core plasma of the Large Helical Device (LHD) through carbon pellets containing Er powders. As soon as the pellet entered in the plasma, the intense heat flux generated by the plasma caused immediate ablation on its surface, forming an ablation cloud temporarily in its vicinity. The radiation spectra from this ablation cloud were measured in the 380- 400 nm region. Most of the observed lines in the spectra belonged to CII and ErII ions. To analyze the observed emission line spectra, a line shape analysis incorporating Doppler and Stark broadening was employed. As the current plasma is in a magnetic field (~2.75T), a contribution to line broadening due to several Zeeman components was also considered. From the stark width, the electron density of the plasma was evaluated. Since the electron density of the ablation cloud was high, we could assume local thermal equilibrium (LTE) for the ablation cloud plasma. Additionally, the transition probability of the Er II line observed at 393.863 nm was obtained through Boltzmann plot analysis [2].

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\*[priti.priti@nifs.ac.jp](mailto:priti.priti@nifs.ac.jp)

## STUDY OF B-LIKE IONS X-RAY EMISSION SPECTRA IN AN ELECTRON-CYCLOTRON RESONANCE ION SOURCE PLASMA

Louis Duval <sup>a,b,\*</sup>, Emily Lamour <sup>b</sup>, Stéphane Macé <sup>b</sup>, Jorge Machado <sup>c</sup>, Nancy Paul <sup>a</sup>,  
Christophe Prigent <sup>b</sup>, Martino Trassinelli <sup>b</sup>, Paul Indelicato <sup>a</sup>.

<sup>a</sup> *Laboratoire Kastler-Brossel, Sorbonne Université, CNRS, ENS-PSL Research University, Collège de France, Case 74; 4, place Jussieu, F-75005 Paris, France*

<sup>b</sup> *Institut des NanoSciences de Paris, CNRS, Sorbonne Université, 4 Place Jussieu, 75005 Paris, France*

<sup>c</sup> *Universidade Nova de Lisboa Laboratório de Instrumentação Engenharia Biomédica e Física da Radiação, Departamento de Física, Faculdade Ciências e Tecnologia, Universidade Nova de Lisboa, 2829-516 Caparica, Portugal*

Chandra and XMM-Newton brought astrophysical x-ray spectroscopy to a new era by providing the first high-resolution (0.5% in the X-ray band) measurements. These improvements have led to a need for more precise atomic data to interpret the astrophysical measurements. Later measurements, showing unknown x-ray contributions, drew the question of new physics [1], which was finally resolved by new measurements using ion sources [2]. The extensive usage of microcalorimeters in recent (Hitomi) and future (Athena/XFU and XRISM) missions give new perspectives for x-ray measurements of astrophysical objects [3]. Concurrently, thanks to modern intense ion sources [4], in-lab precise measurements of transitions in highly-charged ions, like in sulfur, allow to improve the modelling of the measurements [5]. We present here new reference-free high-precision measurements of x-ray transitions in boron-like argon and sulfur. The measurements were performed with an Electron Cyclotron Resonance Ion Source and a double-crystal spectrometer installed in Paris at Sorbonne Université [6]. These spectra show multiple transitions, which required the use of Bayesian model selection methods to determine the number of spectral components and their characteristic profile. This is performed using the nested sampling method implemented in the nested fit code [7] which will be also introduced.

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\*email: [louis.duval@lkb.upmc.fr](mailto:louis.duval@lkb.upmc.fr)

# TRANSITION PROBABILITY MEASUREMENTS FOR LANTHANIDE ELEMENTS USING LASER-INDUCED BREAKDOWN SPECTROSCOPY

Kodangil Supriya<sup>a</sup>, Masayuki Iwata<sup>a</sup>, Daiji Kato<sup>b</sup>, Masaomi Tanaka<sup>c</sup>, Hajime Tanuma<sup>d</sup>, Nobuyuki Nakamura<sup>a\*</sup>

<sup>a</sup> Institute of Laser Science, The University of Electro-Communications, Tokyo, Japan

<sup>b</sup> National Institute for Fusion Science, Gifu, Japan

<sup>c</sup> Astronomical Institute, Tohoku University, Sendai, Japan

<sup>d</sup> Department of Physics, Tokyo Metropolitan University, Tokyo, Japan

Atomic data of rare-earth elements are having great importance in many fields, especially in astrophysics. Recently, the study of kilonovae emissions led scientists to consider neutron star mergers as a source of heavy elements, such as lanthanides. Thus, the necessity of highly accurate and precise spectroscopic data, especially the transition probability, increased drastically for the radiative transfer simulation of kilonovae [1]. In this poster, we present transition probability measurements for some lanthanide elements using laser-induced breakdown spectroscopy (LIBS).

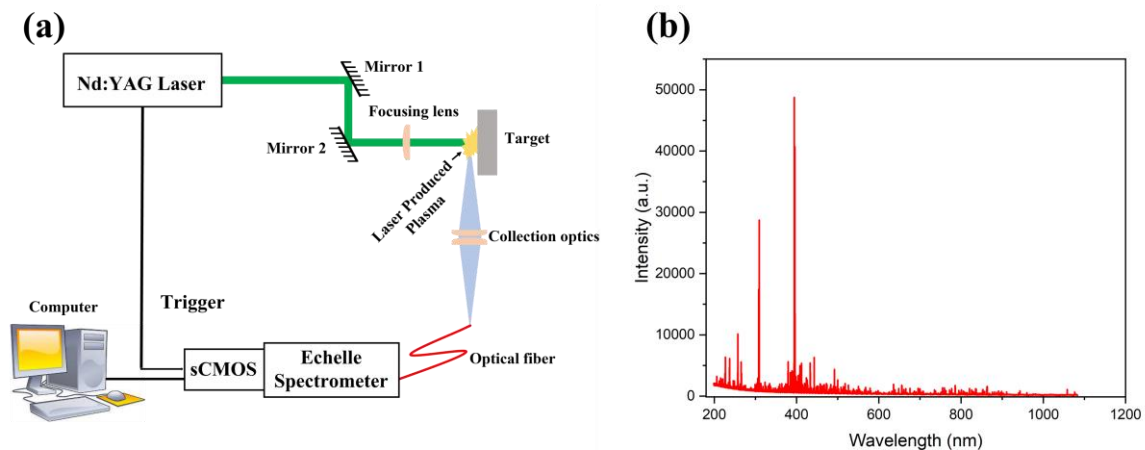


Figure 1: (a) Schematic of the experimental setup. (b) LIBS spectrum of an Al-La alloy.

LIBS is an atomic emission spectroscopic technique generally used for elemental analysis [2]. Figure 1(a) shows a schematic diagram of the LIBS setup. For evaluating the transition probabilities, an alloy of aluminum containing 5% lanthanoid elements (La, Ce, and Er) is used as a target placed in a chamber filled with Ar gas ( $\sim 200$  Pa). A typical LIBS spectrum of Al-La alloy is shown in figure 1(b). Considering the LTE condition of the plasma, the Boltzmann plot method is used for deducing the transition probabilities of emission lines which are not reported in the NIST atomic spectra database [3].

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## HIGH-RESOLUTION TALIF SPECTROSCOPY FOR OPTICAL DIAGNOSTICS IN COLD PLASMAS

Cyril Drag<sup>a,\*</sup>, Christophe Blondel<sup>a</sup>, Pascal Chabert<sup>a</sup>, Benjamin Esteves<sup>a</sup>

<sup>a</sup>LPP, CNRS, Sorbonne Université, Université Paris-Saclay, Observatoire de Paris,  
Ecole polytechnique, Institut polytechnique de Paris, F-91128 Palaiseau cedex, France

Two-photon absorption laser induced fluorescence (TALIF) method is commonly used to measure atomic densities and temperatures in gaseous media, especially for plasma diagnostics. TALIF consists in recording the fluorescence following the two-photon excitation of an atomic species. For oxygen density measurements, a widespread protocol is to compare the fluorescence yield to that measured in Xe vapor, the density of which can be known straightforwardly, when illuminated by the same optical system. However, quantitative analysis relies on knowledge of the ratio of both two-photon cross-sections  $\sigma^{(2)}$  involved. Direct measurement of the integrated cross-section  $\sigma^{(2)}(\text{Xe})$  can be done by non-linear absorption spectroscopy [1]. We determined the integrated cross-section for the  $6p'[3/2]_2$  level, and find a value that is more than a factor of 2 smaller than the admitted one.

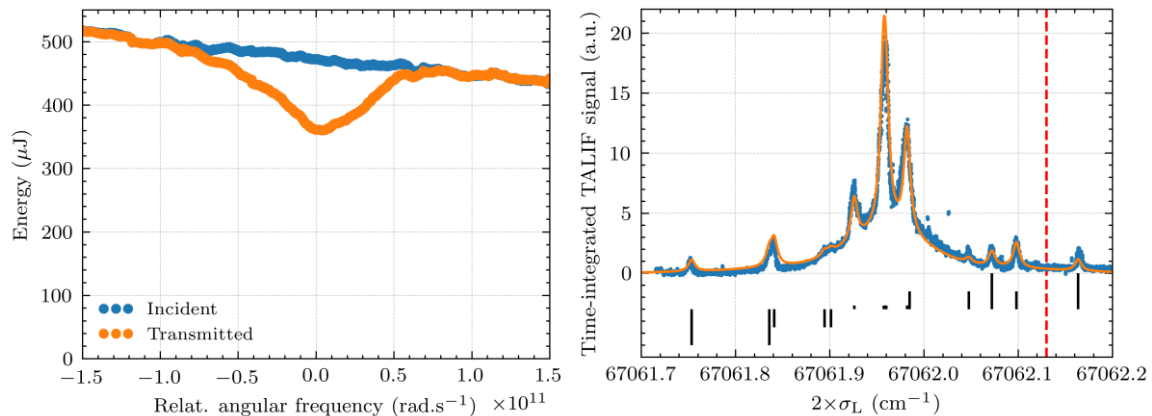


Figure 1: Left: Two-photon absorption spectra of the  $6p'[3/2]_2$  resonance of Xe. ( $n = 1.63 \times 10^{24}$   $\text{at}\cdot\text{m}^{-3}$ ,  $L = 51$  cm,  $w_x \sim w_y \sim 310$   $\mu\text{m}$  and pulse duration of 6.4 ns). Right: Doppler-free fluorescence spectra, following excitation of the ( $^3\text{P}_2$ )  $6p^2[1]_0^3_{3/2}$  of I.

TALIF spectroscopy also leads to the determination of the temperature of atomic species in the plasma, via Doppler broadening, provided that a sufficiently narrow-line laser is used. For this purpose, we have specially built [2] a pulsed single-mode ns-laser. Furthermore, for atoms with a non-zero nuclear spin, hyperfine structures can underlie the Doppler profile. These structures have been determined for iodine and xenon by Doppler-free spectroscopy [3,4]. For noble gases, we have established a relation that makes a rough estimation of the hyperfine structure possible as a function of atomic quantum numbers [4].

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\*email: cyril.drag@lpp.polytechnique.fr

## **Development and Commissioning of the UNIST Electron Beam Ion Trap for X-Ray Spectroscopy of the Highly Charged Ions at PAL-XFEL**

**SungNam Park<sup>a</sup>, Bokkyun Shin<sup>b</sup>, Emre Cosgun<sup>a</sup>, Moses Chung<sup>a\*</sup>**

<sup>a</sup>Ulsan National Institute of Science and Technology, 50, UNIST-gil Ulsan 44919, Republic of Korea

<sup>b</sup>Pohang Accelerator Laboratory, Jigokro-127-beongil, Nam-gu, Pohang, Gyongbuk 37673, Republic of Korea

An electron beam ion trap (EBIT) is a device that creates and studies highly charged ions (HCIs). To maximize its portability to move in and away from the accelerator beamlines, we adopt permanent magnets to reduce the size and maintenance cost. A 0.84 T magnetic field at the trap center gives a trap capacity of  $10^7$ . By sweeping the electron beam energy from 2.4 to 3.3 keV at 10 mA, the silicon drift detector successfully measures KLL lines of the highly charged states of argon and confirms the existence of up to He-like argon. Before the highly charged iron measurement for astrophysics purposes, we conducted preliminary experiments on connecting the EBIT with the PAL-XFEL (Pohang Accelerator Laboratory X-ray Free Electron Laser) hard X-ray beamline over two R&D beam times. We report our first operation at the XFEL facility, demonstrating the x-ray fluorescence measurement using the highly charged argon.

\*email: [ilk\\_simon@unist.ac.kr](mailto:ilk_simon@unist.ac.kr) / [mchung@unist.ac.kr](mailto:mchung@unist.ac.kr)

## EXPERIMENTAL METASTABLE LIFETIMES AT DESIREE STORAGE RING – FIRST STOP : BARIUM

Uldis Berzins<sup>a</sup>, Jose Navarette<sup>b</sup>, Paul Martini<sup>b</sup>, Arturs Ciniņš<sup>a</sup>, Dag Hanstorp<sup>c</sup>, Henning Schmidt<sup>b</sup>, **Henrik Hartman**<sup>d,\*</sup>

<sup>a</sup>University of Latvia, Institute of Atomic Physics and Spectroscopy, Latvia

<sup>b</sup>Stockholm University, AlbaNova University Centre, SE-10691 Stockholm, Sweden

<sup>c</sup>Gothenburg University, Department of Physics, SE-10691 Gothenburg, Sweden

<sup>d</sup>Malmö University, Faculty of Technology, SE-20506 Malmö, Sweden

We are developing a laser probing technique at the Double Electrostatic Cryogenic Storage Ring DESIREE at Stockholm university, Sweden [1]. The excellent vacuum and temperature conditions allows to store the barium ions  $\text{Ba}^+$  with a beam lifetime of 500s. We present our first measurements of the  $5d\ ^2D_{3/2}$  metastable state of Ba II with a lifetime around 80 s with a 1% uncertainty.

We apply a pump and probe technique utilizing two lasers. One red laser emptying the metastable state and probing the population, and a blue laser repopulating the state by transferring all the population from the ground state  $6s\ ^2S_{1/2}$  to the  $5d\ ^2D_{3/2}$  state investigated. By varying the time delay between pump and probe, the lifetime curve is built up.

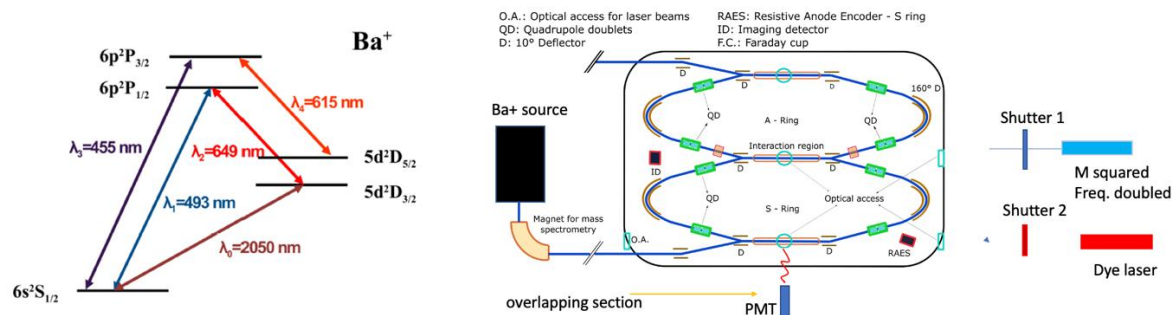


Figure 1: *left*: Energy level diagram of Ba II, with metastable  $5d\ ^2D_{3/2}$ . *Right*: The DESIREE storage ring and the experimental setup

Thanks to the excellent storage conditions, we see only very small systematic effects such as repopulation and collisional quenching. Future studies will include more complex spectra such as Fe II.

A consortium consisting of Stockholm University (SU), the University of Gothenburg (UGOT) and Malmö University (MaU) operate DESIREE as a national infrastructure since January 2018 with support from the Swedish research Council VR. Authors from UL were supported by ERDF project No. 1.1.1.5/19/A/003: and ERDF project No. 1.1.1.1/19/A/144.

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\*email: Henrik.Hartman@mau.se

# ATOMIC DATA AND OPACITY CALCULATIONS IN MODERATELY CHARGED LANTHANIDE IONS IN THE CONTEXT OF KILONOVA EMISSION MODELING

Helena Carvajal Gallego<sup>a</sup>, Jérôme Deprince<sup>a,b</sup>, Patrick Palmeri<sup>a</sup>, Pascal Quinet<sup>a,c</sup>

<sup>a</sup>Physique Atomique et Astrophysique, Université de Mons – UMONS, B-7000, Mons, Belgium

<sup>b</sup>Institut d'Astronomie et d'Astrophysique, Université Libre de Bruxelles, B-1050 Brussels, Belgium

<sup>c</sup>IPNAS, Université de Liège, B-4000 Liège, Belgium

The LIGO-VIRGO collaboration observed a neutron star merger (GW170817 event) thanks to the first detection of gravitational waves. They also detected the electromagnetic emission of the gigantic explosion called kilonova which is a hot and radioactive matter ejected in the space [1]. In the latter, nuclear reactions take place and form heavy nuclei such as lanthanides ( $Z = 57 - 71$ ) which contribute strongly to the luminosity and spectra of the kilonova. Such elements produce millions of lines due to their complex configurations characterized by an unfilled 4f subshell [2].

To interpret the spectrum of a kilonova, it is therefore crucial to precisely know the radiative parameters characterizing these elements. In recent years, several studies have been carried out (e.g. [3-4]), for the first degrees of ionisation (up to 3+) but almost all these investigations were limited to the analysis of kilonovae in a temperature range below 20000 K. In order to extend the study to early phases of kilonovae (i.e.  $T > 20000$  K), it is essential to know the radiative parameters of lanthanide ions in higher charge stages (see e.g. [5-8]).

The present work focusses on atomic data and opacity calculations for lanthanides from the fourth to the ninth degree of ionization, for typical ejecta conditions such as the density  $\rho = 10^{-10}$  g cm<sup>-3</sup>, the time after the merger  $t = 0.1$  day and temperatures  $T > 20000$  K. In order to do that, we used the pseudo-relativistic Hartree-Fock (HFR) method as implemented in Cowan's codes [9] to calculate the radiative parameters. The expansion formalism [10-12] was then used in order to compute the opacity, at 25000 K, 35000 K and 40000 K, which are extremely important for astrophysicists [13].

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- \*email: helena.carvajalgallego@umons.ac.be



# ATOMIC DATA AND OPACITY CALCULATIONS IN Nb, Ag, Hf, Os AND Au IONS FOR KILONOVA SPECTRAL ANALYSES

Sirine Ben Nasr<sup>a,\*</sup>, Helena Carvajal Gallego<sup>a</sup>, Jérôme Deprince<sup>a,b</sup>, Patrick Palmeri<sup>a</sup>, Pascal Quinet<sup>a,c</sup>

<sup>a</sup>Atomic Physics and Astrophysics, University of Mons, B-7000 Mons, Belgium

<sup>b</sup>Institute of Astronomy and Astrophysics, University Libre of Brussels, CP 226, B-1050 Brussels, Belgium

<sup>c</sup>IPNAS, University of Liège, Sart Tilman, B-4000 Liège, Belgium

Neutron star (NS) mergers are at the origin of gravitational waves (GW) detected by LIGO/Virgo interferometers [1]. Such events produce a large amount of elements heavier than iron by a rapid neutron capture (r-process) nucleosynthesis. Among these elements, those belonging to the fifth and sixth rows of the periodic table, are the greatest contributors to the opacity affecting the kilonova spectra, after the lanthanides and actinides. In the present work, new calculations of atomic structures and radiative parameters (wavelengths and oscillator strengths) are reported for a large number of spectral lines in some representative elements belonging to the fifth row, namely Nb ( $Z = 41$ ) and Ag ( $Z = 47$ ), and belonging to the sixth row, namely Hf ( $Z = 72$ ), Os ( $Z = 76$ ) and Au ( $Z = 79$ ) from neutral to triply ionized states. The results obtained were used to calculate the expansion opacities characterizing the kilonova signal observed resulting from the collision of two NS, for typical conditions corresponding to time after the merger  $t = 1$  day, the temperature in the ejecta  $T \leq 15000$  K, and a density of  $\rho = 10^{-13}$  g.cm<sup>-3</sup> [2]. The results presented in this work are the most complete currently available and are useful for astrophysicists to interpret kilonova spectra.

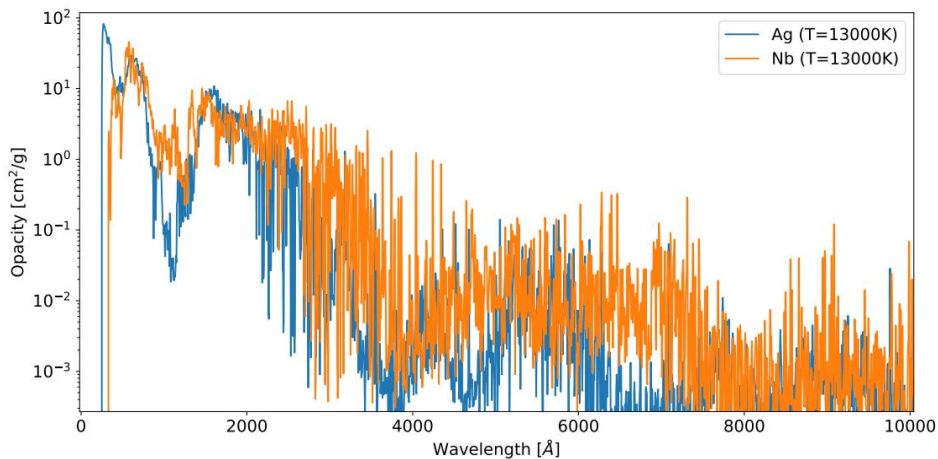


Figure 1: Expansion opacity for Nb and Ag, calculated with  $T = 13\,000$  K, with  $\rho = 10^{-13}$  g.cm<sup>-3</sup>,  $t = 1$  d and  $\Delta\lambda = 10$  Å.

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\*email: sirine.bennasr@umons.ac.be

## Atomic calculations for V – XI ionized $r$ -process elements for early kilonova

Smaranika Banerjee<sup>a\*</sup>, Masaomi Tanaka<sup>b,c</sup>, Daiji Kato<sup>d,e</sup>, Gediminas Gaigalas<sup>f</sup>

<sup>a</sup>Stockholm University, Roslagstullsbacken 21, Stockholm 106 91

<sup>b</sup>Astronomical Institute, Tohoku University, Sendai 980-8578, Japan

<sup>c</sup>Division for the Establishment of Frontier Sciences, Organization for Advanced Studies, Tohoku University, Sendai 980-8577, Japan

<sup>d</sup>National Institute for Fusion Science, Toki 519-5292, Japan

<sup>e</sup>Interdisciplinary Graduate School of Engineering Sciences, Kyushu University, Kasuga 816- 8580, Japan

<sup>f</sup>Institute of Theoretical Physics and Astronomy, Vilnius University, Vilnius LT-10257, Lithuania

We perform the atomic structure calculations by using Hebrew University Lawrence Livermore Atomic Code or HULLAC [1] to construct the data for the energy levels and transition probabilities for all  $r$ -process elements from Ca - Ra ( $Z = 20-88$ ) ionized to the states V – XI [2, 3, 5]. Using the atomic data, we calculate the bound-bound opacities for the elements ionized to different states (see Fig. 1 for variation of mean opacities for different ionization at density  $10^{-10}$  g cm<sup>-3</sup>). Such opacities are suitable to calculate the light curves at an early time ( $t < 1$  day) of the astronomical transient kilonova from neutron star merger. Understanding the light curves of kilonova from early time provides the hint to understand the origin of heavy  $r$ -process elements and hence, is of extreme importance.

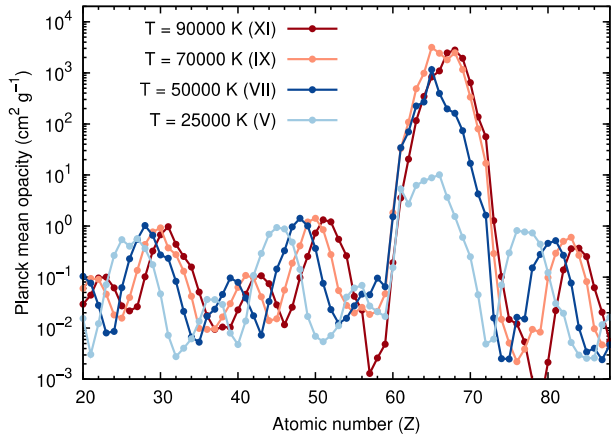


Figure 1: The mean opacities for different elements suitable to calculate early kilonova ( $t < 1$  day) from the binary neutron star merger (Banerjee et al, 2023, submitted to ApJ).

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\*email: smaranika.banerjee@astro.su.se

## **DETAILED NLTE ABUNDANCE ANALYSIS OF 20 NUCLEAR STELLAR CLUSTER/DISK STARS**

**Brian Thorsbro<sup>a,\*</sup>, Anish Amarsi<sup>b</sup>, Govind Nandakumar<sup>\*</sup>**

<sup>a</sup>Observatoire de la Côte d'Azur, CNRS UMR 7293, BP4229, Laboratoire Lagrange, F-06304  
Nice Cedex 4, France

<sup>b</sup>Theoretical Astrophysics, Department of Physics and Astronomy, Uppsala University, Box  
516, SE-751 20 Uppsala, Sweden

<sup>c</sup>Lund Observatory, Department of Physics, Lund University, Box 43, 221 00 Lund, Sweden

Nuclear star clusters are near ubiquitous in galaxies: they are present in ~70% of early- and late-type galaxies with stellar masses above  $10^8$ - $10^{10}$  solar masses. Further, the masses of nuclear star clusters show scaling relationships with the masses of their host galaxies, which suggests the idea that the nuclei of galaxies may have co-evolved with their hosts. Also supported by simulations, the very inner parts of galaxies are thought to provide clues to processes that shape galaxy formation and evolution.

We present a detailed NLTE abundance analysis of 20 stars in the Nuclear Star Cluster and the Nuclear Stellar Disk using recently calculated NLTE departure coefficients. We compare the results with an equivalent analysis of stars located in the disk further out in the Galaxy. Like previously analysed and published silicon abundances for the same set of stars, we show that even for elements such as calcium there is a significant difference between stars located in the Nuclear Stellar Cluster/Disk and stars located further out in the Milky Way disk.



## Japan-Lithuania Opacity Database for Kilonova

Daiji Kato<sup>a,b,\*</sup>, Izumi Murakami<sup>a,c</sup>, Masaomi Tanaka<sup>d,e</sup>, Smaranika Banerjee<sup>f</sup>,  
Gediminas Gaigalas<sup>g</sup>, Laima Kitovienė<sup>g</sup>, and Pavel Rynkun<sup>g</sup>

<sup>a</sup>National Institute for Fusion Science, Toki 519-5292, Japan

<sup>b</sup>Interdisciplinary Graduate School of Engineering Sciences, Kyushu University, Kasuga 816-8580, Japan

<sup>c</sup>Fusion Science Program, SOKENDAI, Toki 519-5292, Japan

<sup>d</sup>Astronomical Institute, Tohoku University, Sendai 980-8578, Japan

<sup>e</sup>Division for the Establishment of Frontier Sciences, Organization for Advanced Studies,  
Tohoku University, Sendai 980-8577, Japan

<sup>f</sup>Stockholm University, Stockholm 114 21, Sweden

<sup>g</sup>Institute of Theoretical Physics and Astronomy, Vilnius University, Vilnius LT-10257,  
Lithuania

We have recently constructed optical absorption data of r-process element ions [1], which are in high demand for the analysis of kilonova observation associated with neutron star mergers. The data were developed by theoretical calculations using HULLAC code [2], and made a database available at NIFS [3] in cooperation of Japan and Lithuanian experts. The database contains energy level and oscillator strength data of neutral through triply charged ions for most of the r-process elements ( $Z = 26 - 88$ ). In the database, bound-bound Plank mean opacities calculated with those atomic data for abundance distributions at given electron fractions ( $Ye$ ) are also available at temperature and density grids for 1,000 – 25,500 K and  $10^{-19.5} - 10^{-5} \text{ g/cm}^3$ , respectively.

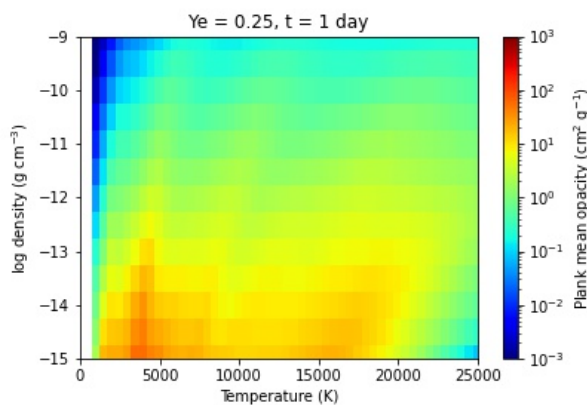


Fig 1. Plank mean opacity for  $Ye = 0.25$  and 1 day after the merger.

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\*email: kato.daiji@nifs.ac.jp

# Zeeman Spectroscopy of Tellurium

Shikha Rathi<sup>a\*</sup>, Ł. M. Sobolewski<sup>b</sup>, L. Sharma<sup>a</sup>, J. Kwela<sup>b</sup>

<sup>a</sup>Indian Institute of Technology Roorkee, Roorkee, India

<sup>b</sup>Institute of Experimental Physics, Faculty of Mathematics, Physics and Information,  
University of Gdansk, 80-308, Poland

Tellurium spectroscopic studies have received a lot of interest recently as a result of the use of Te-like systems in highly accurate optical clocks [1]. However, Te's complicated multielectron spectra, which contain several  $p^k n^l$  electronic configurations, present a challenge for both theoretical and experimental spectroscopic studies. The last experimental work on the structure of Te I was published in 1982-1983. Previous theoretical work on Te are mostly limited to ground and low excited states. Therefore, in this work, Zeeman structure of eight lines of  $^{130}\text{Te}$  are studied using high-resolution emission spectroscopy in the range 640-990 nm (see Figure 1). Landé  $g_J$  factors for seven levels were determined for the first time. The validity of present experimental data is proved by performing theoretical calculations using the multiconfiguration Dirac-Hatree-Fock (MCDHF) method incorporated in GRASP2018 [2] package. The calculations were performed for 53 levels belonging to the  $5p^4$ ,  $5p^3 6s$ ,  $5p^3 5d$ ,  $5p^3 6p$ ,  $5p^3 8s$ ,  $5p^3 8d$  and  $5p^3 9d$  configurations. Moreover, theoretical Landé  $g_J$  factors of 19 levels are new, and no experimental values are available for comparison.

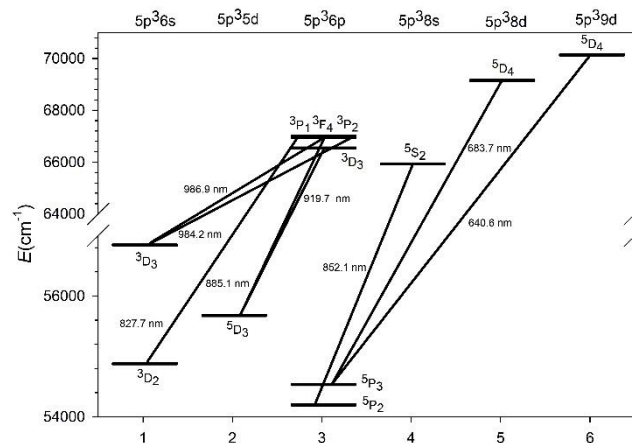


Figure 1: Energy-level diagram of Te I with investigated transitions.

The average level of agreement between the current theoretical and experimental findings is 2.4%, with individual data pair levels ranging from 0.6% to 4.8. The percentage average discrepancy between the theoretical energy predicted in this work and the NIST values is only 1.4%. The agreement between the calculated and NIST values of the Landé factors is, on average less than 2.5 %. We believe the present studies extends the existing data on Landé factors.

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\*email: srathi@ph.iitr.ac.in

## SIMULATION OF Pm-LIKE BISMUTH SPECTRA IN AN EBIT

**J. P. Marques**<sup>\*a,b</sup>, M. C. Martins<sup>c</sup>, J. M. Sampaio<sup>a,b</sup>, P. Amaro<sup>c</sup>, J. P. Santos<sup>c</sup>, P. Indelicato<sup>d</sup>,  
and F. Parente<sup>c</sup>

<sup>a</sup>LIP – Laboratório de Instrumentação e Física Experimental de Partículas,  
Av. Prof. Gama Pinto 2, 1649-003 Lisboa, Portugal

<sup>b</sup>Faculdade de Ciências, Universidade de Lisboa, 1749-016 Lisboa, Portugal

<sup>c</sup>Laboratory of Instrumentation, Biomedical Engineering and Radiation Physics (LIBPhys-  
UNL), Department of Physics, NOVA School of Science and Technology,  
NOVA University Lisbon, 2829-516 Caparica, Portugal

<sup>d</sup>Laboratoire Kastler Brossel, Sorbonne Université, CNRS, ENS-PSL Research University,  
Collège de France, Case 74, 4 Place Jussieu, 75005 Paris, France

We use a multiconfiguration Dirac-Fock code [1,2] to calculate electronic excitation cross sections and radiative decay transition probabilities for a large number of atomic levels in Pm-like bismuth. By numerically solving a set of equilibrium equations we were able to obtain the level populations of the  $4f^{14}5s$ ,  $4f^{13}5s5f$ ,  $4f^{13}5s5d$ ,  $4f^{13}5s5p$ , and  $4f^{13}5s^2$  configurations and synthesized spectra for a number of electronic density values in an EBIT for 640 keV incident electron energy.

The synthesized spectrum we obtained for  $10^{10} \text{ cm}^{-3}$  electronic density agrees qualitatively with the experimental data of Kobayashi et al. [3]. We found significant differences between our simulations and Kobayashi's for several electronic density values.

The emission lines position and relative intensity can also be compared with laser produced plasma spectra, to improve the identification of the Pm-like ions and provide experimental values of electron density at those plasma conditions.

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\*email: [jmmarques@fc.ul.pt](mailto:jmmarques@fc.ul.pt)

# Measurement of Charge Exchange Cross Sections for Highly Charged Ions Collision with He

B Ren<sup>a</sup>, Z Xia<sup>a</sup>, T Meng<sup>a</sup>, M Ma<sup>a</sup>, J Xiao<sup>a</sup>, and B Wei<sup>a\*</sup>

<sup>a</sup>Institute of Modern Physics, Key Laboratory of Nuclear Physics and Ion-Beam Application (MOE), Fudan University, Shanghai 200433, China

The charge exchange (CX) process between ions and the neutral target is of great significance in explaining the X-ray emission spectrum of the solar system. To investigate the CX process in the lab, an experimental instrument setup based on the 150 kV high-voltage platform with an electron cyclotron resonance (ECR) ion source at Fudan University was built to measure the absolute single- and double-electron capture cross sections and  $nl$ -resolved state-selective charge exchange cross sections between low-energy highly charged ions and neutral targets. The  $nl$  state-selective charge exchange cross-section of  $\text{Ar}^{8+}$  colliding with He, and the absolute and state-selective cross sections between  $\text{O}^{6+}$  and He were obtained [1-2].

As shown in Fig. 1, a series of measurements on the charge exchange of  $\text{Ar}^{8+}$  ion with He were performed in the collision energy range from 1.4 to 20 keV/u. It was found electrons were mainly captured in the  $n = 4$  state of  $\text{Ar}^{7+}$  ions compared to the  $n = 3, 5,$  and  $6$  captures, which was in agreement with the scaling law prediction for dominant capture. And the relative cross sections were also reported for  $4s$ -,  $4p$ -,  $4d$ -, and  $4f$ -resolved state-selective capture [1].

To further extend the research, the investigation of the singlet charge exchange process of  $\text{O}^{6+}$  and He was performed both experimentally and theoretically. The total and state-selective ( $n = 3, 4, 5$  and partially  $3s$ ) cross sections for the singlet electron capture have been measured in the energy range of 2.63-37.5 keV/u. The state-selective cross section of  $n = 5$  above 4.5 keV/u was reported experimentally for the first time. Total and state-selective cross sections were also calculated in the energy range of 0.3-100 keV/u, performing a good agreement with the experiment result. And the importance of electronic correlation was found compared with the previous methods [2].

Furthermore, the total electron-capture cross section between  $\text{O}^{6+}$  with  $\text{CO}_2$ ,  $\text{CH}_4$ ,  $\text{H}_2$ , and  $\text{N}_2$  has been measured [3].

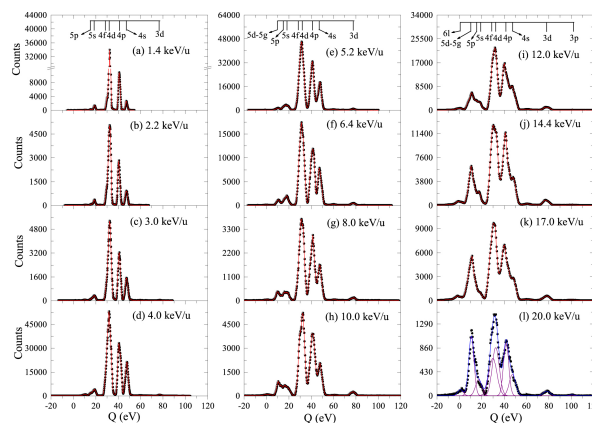


Figure 1: The measured Q spectra of CX between  $\text{Ar}^{8+}$  and He.

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- \*email: brwei@fudan.edu.cn



# The role of the $3 \rightarrow 5$ excitation channels in the dielectronic recombination of M-shell Fe ions: the Na and Mg isoelectronic sequences

G. Visentin<sup>a,b\*</sup> and S. Fritzsche<sup>a,b,c</sup>

<sup>a</sup> Helmholtz-Institut Jena, Jena, 07743, Germany

<sup>b</sup> GSI Helmholtzzentrum für Schwerionenforschung, Darmstadt, 64291, Germany

<sup>c</sup> Friedrich-Schiller -Universität Jena, Jena, 07743, Germany

The important role played by dielectronic recombination (DR) of M-shell Fe ions in the observed absorption X-ray spectra of Seyfert galaxies [1,2] have encouraged a thorough investigation of the related plasma DR rate coefficients in support of astrophysical observations. So far, theoretical modeling of such processes has accounted for the sole contributions due to  $\Delta n = 0,1$  excitation channels (see, for instance, [1]). However, it was pointed out that at reasonably high temperatures even the neglected  $\Delta n = 2$  channels may remarkably contribute to the total temperature-dependent DR rates [3]. This has spurred us to investigating the contribution of the  $\Delta n = 2$  excitation channels for the  $3 \rightarrow 5$  electron excitations to the plasma rate coefficients of initially Na-like and Mg-like Fe ions in the  $10^5 - 10^9$  K temperature range, by means of the Multi-Configurational Dirac-Hartree-Fock method. As a result, the contribution to the total plasma DR rates due to this excitation channel was found to be relevant and comparable to the  $\Delta n = 0,1$  analogs.

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