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ADAS-EU
ADAS for fusion in Europe

Grant: 224607

Hugh Summers, Martin O'Mullane, Francisco Guzman and Luis Menchero

ADAS-EU setup report 1

22 June 2010

Workpackages : 22-1-1, 23-1-1, 25-1-1, 25-2-1, 26-3-1
Category : PP

ADAS-EU setup report 1

Hugh Summers, Martin O'Mullane, Francisco Guzman and Luis Menchero

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Abstract: *The report reviews setup task completion for project months 1-9*

Contents

Preface

This set-up report is the first of a series of three such reports, deliverable under the ADAS-EU project, which summarise the setting-up activities.

H P Summers
22 June 2010

Chapter 1

Overview and milestone STP1

The milestone STP1 concerns 'Training and placement of PDRA1 complete at FZ Juelich, report of local on-site support targets available; first sub-contracts (S5, S7) negotiated and active. Decisions on work package extensions' and was scheduled for completion by month 7 and the associated report SETUP1 to be available at month 7. The scheduling of completion has been moved to month 10 for the reasons summarised below.

PDRA1, Dr. Francisco Guzman, is appointed and was in post at 1 Jul. 2009 - a delay of three months. The training schedule was adjusted to accomodate this. Additionally, the failure to achieve appointment of PDRA2 at the first attempt necessitated some re-ordering of the implementation of the various sub-contracts. It was possible to accelerate two of these moving them into this extended first setup period. Four sub-contracts (S2, S4, S5, S8) are now successfully in place. Planned training of Dr. Guzman has been achieved apart from a final portion to take place in July 2010.

Engagement with the scientific programme at FZ Juelich has principally concerned implementing molecular hydrogen data in the ADAS framework, following the draft monograph of Janev, Reiter and Samm ('Collisional and radiative processes in hydrogen plasmas'). Strong dialogue has taken place with Professor Reiter at FZ Juelich. The planned early interaction with Professor Janev was not fulfilled in 2009 since the Guzman start date moved outside the Janev period at FZ Juelich. This will be caught back in 2010. Other interests included a wish for photon efficiency updates for light neutral element influx. There was a strong wish for inputs to the ERO code, especially neutral tungsten. This was not immediately satisfiable, but was contributory to accelerating planned ADAS-EU sub-contracts relating to neutral and near neutral complex heavy elements. The special knowledge and capability of Dr. Guzman for computing state selective charge exchange cross-sections and associated ion impact excitation cross-sections was valuable. It was decided to extend these calculation and compilations for light element bare nuclei receivers - particularly Be^{+4} and B^{+5} while Dr. Guzman is at FZ Juelich.

It is noted that the re-location of Dr. Guzman to CEA Cadarache/ITER has been resheduled to month 25. This is to ensure fair balance of time between FZ Jeulich and CEA Cadarache/ITER in light of his delayed starting date. The associated milestone STP3 and report SETUP_3 are in consequence rescheduled to month 25.

In summary STP1 has been reached and part of milestone STP2 within this first nine month timeframe.

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Chapter 2

Work package reports

2.1 Work package 25-1-1

Preparation of the two ADAS-EU Research Fellow position descriptions (RPDRA1, PDRA2) were completed and issued for advertisement on 4 Feb 2009. This was somewhat later than anticipated because of human resources administrative procedure issues. In the light of this delay, it was decided to advertise both PDRA positions at the same time. The descriptors are attached in Appendix A [1,2]. The positions were displayed on the principal academic appointments web sites, including that of Strathclyde University and circulated very extensively to fusion laboatories, astrophysical laboratories and University departments interested in atomic/plasma physics throughout the world.

The Interviews were scheduled for 23/24 April 2009 at Culham Science Centre.

Candidates were short listed by Professor Hugh Summers, Dr. Martin O'Mullane and Dr. Allan Whiteford. Summaries were prepared and these together with references were circulated to the ADAS-EU Governance Committee members for comment and ranking.

The interview board comprised Professor Hugh Summers (Chair) ADAS-EU Director, Physics, University of Strathclyde; Dr. William Morris, Head of Experiments, UKAEA Culham Laboratory; Dr. Remy Guirlet, Director of Spectroscopy, CEA Cadarache, France; Dr. Dmitri Borodin (via tele-conf.), ADAS Steering Committee, IEF-Plasmaphysics, FZ Juelich, Germany; Dr. Allan Whiteford, ADAS-EU Manager,Physics, University of Strathclyde.

Six candidates were short-listed and references taken up. All candidates expressed a wish to be considered for both the PDRA1 and PDRA2 positions. One candidate was interviewed via teleconferencing facilities, the remaining five were interviewed in person. Four candidates were deemed appointable.

Position PDRA1 (placement Forschunszentrum Juelich in Germany and thereafter at CEA Cadarache, France) was offered to Dr. Francisco Guzman and was accepted. The agreed starting date for Dr. Guzman was 1 July 2009. The appointment commencement was therefore four months later than scheduled.

Position PDRA2 (placement Max-Planck-Institut fuer Plasmaphysik, Garching-bei-Muenchen, Germany) was offered to a second candidate. After ten days delay to consider the offer, this candidate declined the post.

By this stage, other appointable candidates were no longer available, so the PDRA2 position remained unfilled.

It was agreed that immediate reissue of the PDRA2 advertisement should not be done. Instead it was agreed to wait a few months for a fresh cohort of PhD students to complete.

Interview assessment forms, supplementary interview assessment forms and interview decision forms are archived at Human Resources, University of Strathclyde.

2.2 Work packages 23-1-1 and 22-1-1

In the view of the successful appointment of only PDRA1 at this stage and its delayed start, induction training scheduling was adjusted. It is noted that Dr. Guzman is an ion-atom collision theorist with substantial computational experience. He was inexperienced in atomic population and ionisation state modelling for the plasma environment and in general plasma physics. Professor Summers visited FZ Juelich from 13-17 Jul. 2009 and from 3-7 Aug. 2009 for first discussions with Dr. Guzman and with scientific staff at FZ Juelich. Reports are attached in appendix B [1,2]. Dr. Guzman visited UKAEA/JET for discussions, further orientation and initial ADAS practice from 17-21 Aug. 2009. Then from 21-25 Sep. 2009 Dr Guzman visited Dr. Whiteford and Dr. O'Mullane at the Department of Physics, University of Strathclyde to collect an ADAS-EU laptop and train further on ADAS usage. It was decided that in view of the proximity of the first ADAS-EU course, 8-16 Oct. 2009 at IPP Garching, that Dr. Guzman would attend as a participating student to receive lectures on background atomic physics and practical exercising in interactive ADAS. Finally it was decided that Dr. Guzman would attend the 17th Culham Plasma Physics Summer Schoool 12-23 Jul. 2010 to fill in background on plasma physics. This will complete his induction and background training amounting to approximately eight weeks of close engagement with ADAS-EU and training staff. This is to be compared with an anticipated maximum of nine weeks.

2.3 Work packages 22-2-1 and 23-2-1

These items will appear in report SETUP2.

2.4 Work package 25-2-1: Sub-contract technical specification

2.4.1 Atomic structure and electron data for heavy element ions

For sub-contract work package WP-S2 (" Neutral and near neutral structure data"), a potential European single source was identified which could provide the ADAS-EU requirements. This was the Department of Physics, University Mons-Hainaut, Belgium, led by Professor Emile Biemont. A preliminary visit was made by Professor Hugh Summers from 25-26 Feb. 2009 to assess the capabilities of the group and engage in discussions at to whether and how the objectives could be achieved. The report of the visit is attached in appendix C[1.1]. It formed the basis for the setting up of the scientific specification for the sub-contract which is attached in appendix C[1.2]. The sub-contract was specified to have a duration of 18 months since the programme included external experimental measurements for which machine time had to be negotiated.

2.4.2 Positive ion impact data for fusion applications

For sub-contract work package WP-S8 ("CTMC and CCAO cross-section update"), a potential European single source was identified which could provide the ADAS-EU requirements. This was the University of Groningen, Netherlands led by Professor Ronnie Hoekstra. A preliminary visit was made by Professor Hugh Summers from 19-20 Mar. 2009 to assess the capabilities of the group and engage in discussions at to whether and how the objectives could be achieved. The report of the visit is attached in appendix C[2.1]. It formed the basis for the setting up of the scientific specification for the sub-contract which is attached in appendix C[2.2]. The sub-contract was specified to have a duration of 12 months. x

2.4.3 Electron impact cross-section data for fusion applications

For sub-contract work package WP-S4 ("Ionisation and dielectronic measurements"), a potential European single source was identified which could provide the ADAS-EU requirements. This was the Institut fuer Atom- und Molekulphysik, Justus-Liebig Universitt, Giessen, Germany led by Professor Alfred Mueller. A preliminary visit was made by Professor Hugh Summers from 3-4 Jun. 2009 to assess the capabilities of the group and engage in discussions at to whether and how the objectives could be achieved. The report of the visit is attached in appendix C[3.1]. It formed the basis for the setting up of the scientific specification for the sub-contract which is attached in appendix C[3.2]. The sub-contract was specified to have a duration of 12 months. The sub-contract was specified to have a duration of 18 months since the programme included external experimental measurements for which machine time had to be negotiated.

2.4.4 Charge exchange and ion impact data for fusion plasma spectroscopy

For sub-contract work package WP-S5 ("Improved CTMC and CCMO crodss-sections"), a potential European single source was identified which could provide the ADAS-EU requirements. This was the Departamento de Quimica, Universidad Autonoma de Madrid, Spain led by Professor Luis Mendez and Professor Luis Errea. A preliminary visit was made by Professor Hugh Summers from 9-10 Jun. 2009 to assess the capabilities of the group and engage in discussions at to whether and how the objectives could be achieved. The report of the visit is attached in appendix C[4.1]. It formed the basis for the setting up of the scientific specification for the sub-contract which is attached in appendix C[4.2].

2.5 Work package 26-3-1

The work package task comprises the preparation of this report.

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Appendix A

ADAS-EU postdoctoral fellowship advertisements

[1] adas-EU_pdra1_post_HR_details
[2] adas-EU_pdra2_post_HR_details

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Ref: xx/xxxx/2009

Principal: Professor Andrew Hamnett

Research Fellow (1)
(Fixed-term post until 31 Dec 2012)

Department of Physics

1. NATURE OF APPOINTMENT

You will participate in a Euratom Framework 7 Support Action on atomic physics for magnetic confinement fusion research in Europe, called ADAS-EU. You will bring to bear special expertise in atomic data, atomic models, spectroscopic diagnostic methods and the plasma environment at Associated Laboratories of the European Fusion Programme and at the up-coming international fusion project ITER.

You will join a team of experts, linked to the ADAS Project, who have for many years engaged in furthering world fusion research and in sustaining forefront atomic physics inputs to it.

This ~ 45 month position will be based for the first ~ 18 months at the IEF-Plasmaphysics, Forschungszentrum Jülich in Germany, and thereafter at CEA Cadarache and the ITER Organization, located together at St Paul lez Durance in the South of France. This is an exciting and challenging position for an ambitious and dedicated candidate committed to European collaboration and long-term fusion objectives.

More information about ADAS-EU and ADAS may be found at http://www.adas-fusion.eu/ and at http://www.adas.ac.uk .

2. THE UNIVERSITY AND THE CITY

The University is situated in the heart of the City of Glasgow, between the medieval cathedral and the commercial centre. Transport, shops and entertainment are close at hand. Glasgow is the industrial and commercial capital of Scotland and the various groups that have contributed to its population over the centuries have given it a cosmopolitan outlook. It has a lively cultural life as home of the national orchestra, opera and ballet and several theatre companies and it possesses a number of fine art galleries; it is the headquarters of the national press and broadcasting media. Glasgow's numerous higher education establishments have made it a major educational centre.

The Scottish countryside and its splendid recreational and sporting facilities are easily reached from Glasgow.

In addition to the staff club on campus the University owns a historic country house set in a fifty acre estate on the shores of Loch Lomond which is run as an educational and recreational centre for staff and their families.

3. THE UNIVERSITY OF STRATHCLYDE

The University of Strathclyde was formed from the Royal College of Science and Technology and the Scottish College of Commerce and received its Charter in 1964. Both these institutions had long traditions of involvement in higher education, in the case of the Royal College dating back to 1796.

The University merged with the former Jordanhill College on 1 April 1993 — staff and students of the former Jordanhill College becoming the University's fifth Faculty, the Faculty of Education.

The total number of students actively associated with the University is over 14,000. The full-time students are broadly distributed over disciplines as follows: Engineering including Architecture – 2,450; Science and Applied Sciences – 3,000; Arts and Social Sciences – 2,050; Business Management and Professional Studies – 3,050; Education – 3,100. A high proportion of students are aged 21 or over. The University has over 3,700 employees including some 1,600 academic and academic-related staff.

Further information on the University, including its Library and computing provision is available by visiting the University's web site on http://www.strath.ac.uk/

The University of Strathclyde operates a strict, No-Smoking policy.

4. DEPARTMENT OF PHYSICS

For further information on the Department, see http://www.phys.strath.ac.uk/.

5. ADAS and ADAS-EU

The Atomic Data and Analysis Structure, ADAS, evolved from an initial structure created at the JET Joint Undertaking in the period 1984-1993. The first objective of the Project, namely the creation of a common software and data package under UNIX was achieved between 1994 and 1996 with the enthusiastic support and funding of leading European fusion and astrophysical laboratories and the agreement and active participation of JET. ADAS has been in a continuing maintenance and extended development phase from 1996 to the present and the Project has expanded to include most of the leading fusion laboratories in the world. The Project is managed by the Department of Physics, University of Strathclyde under the guidance of a Steering Committee.

ADAS for Fusion in Europe, hereafter called ADAS-EU, is a Framework 7 CSA support activity of four years duration (Jan 2009- Dec 2012) for efficient implementation of atomic data in plasma diagnostics and plasma modelling at fusion laboratories throughout Europe, for promotion of validation experiments, for management of extended databases of relevant fundamental and applied data and for promotion of key fundamental atomic data calculation and measurement in European Institutions. It will enable improved effectiveness and completeness of analysis of existing fusion experiments and lay all necessary groundwork for ITER and beyond.

6. JOB DESCRIPTION

You will play a key role in delivering the primary scientific objectives of ADAS-EU, that is, the provision of analysis tools and necessary atomic and molecular data for atomic and molecular spectroscopy and broadband radiation detection at all wavelengths and in all plasma regions and for plasma models. All these aspects to be in the context of European-wide unified/shared methodologies, databases and maintenance.

There are five main themes: (1) heavy element spectroscopy and models; (2) charge exchange spectroscopy; (3) beam emission spectroscopy; (4) special features; (5) diatomic spectra and collisional-radiative models. You will acquire the ability to support all these areas. You will share leadership in the development of themes 2, 4 and 5. For the first ~18 months you will specialize in themes 2 (part) and 5 (part) and will be based at the Institut für Energieforschung – Plasmaphysik, Forschungszentrum Jülich, Jülich in Germany. For the rest of the project you will be based at Commissariat a L'Energie Atomique, CE De Cadarache, and at the ITER Organization, both at St Paul lez Durance in France and will specialise in themes 2 (part) and 4.

You will receive special training at EFDA-JET in the United Kingdom on ADAS and relating atomic physics to fusion experiments and studies and then you will have the on-site support of an ADAS-EU manager in integrating your activities with the local fusion activities at your placement. In later years you will participate as a tutor in the annual ADAS-EU course for fusion research scientists. You will share in the ADAS-EU series of visits and support to other Associated Laboratories of the European fusion programme.

7. PERSON SPECIFICATION/SELECTION CRITERIA

See attached FORM GR5

8. CONDITIONS OF SERVICE AND SALARY

This appointment to the end of 2012 will be made in terms of the enclosed conditions of service, with the exception of the hours of work and annual leave entitlement which will relate to those of equivalent status staff at the laboratory at which the post is based. The appointment will be at Research and Associated Staff grade 7 (current salary in the range €30,000- €45,000 per annum). Salary will be paid in Euro. Annual and/or merit increments will be adjusted to compensate for Sterling/Euro currency movements. Appointees will be subject to the taxation regime of their country of placement.

9. APPLICATION PROCEDURE

A full curriculum vitae should be attached to the application form. The names and addresses of three referees should be given on the application form. The referees may be contacted by the University without further permission from the candidate. You should also provide a covering letter specifying why you believe yourself suitable for this post.

The University operates a normal retirement age of 65 or the September following 65^{th} birthday. Applications will only be accepted from people up to the age of 64 years and 6 months at the date of their application unless otherwise stated. This is in line with the Employment Equality (Age) Regulations 2006.

Applications should be lodged with Human Resources, University of Strathclyde, McCance Building, 16 Richmond Street, Glasgow, G1 1XQ by Friday 27 February 2009.

We value diversity and welcome applications from all sections of the community

Person Specification/Selection Criteria

FORM GR5

Post Title: ADAS-EU Research Fellow **Department: Physics**

CRITERIA	**STANDARD**	***E/D**	**MEASURED BY**	
			CV	**Interview**
1 Educational and/or Professional Qualifications	PhD in physics, theoretical physics or theoretical chemistry in one of the areas - radiating properties of plasmas, plasma modelling, diagnostic spectroscopic analysis of plasmas, calculation or measurement of electron-ion or atom-ion collisions.	E	X	
2 Experience/ Training	Experience of working and collaborating in a large experimental environment - magnetic or inertial confinement devices, astrophysical spacecraft or similar.	D	X	
	Experience of the computational and data flow infrastructure of large scale experiments.	D	X	
3 Job Related Skills and Achievements	Ability and confidence to use computational tools in support of objectives.	E	X	X
	Ability to organise, plan and use time efficiently	E		X
	Ability to analyse and then think creatively	E		X
	Relating to the full scope of a problem - fundamental to applied, theoretical to experimental	D		X
	Excellent written and verbal communication skills	E	X	X
	Ability to engage with theorists and experimentalists	D		X
4. Personal Attributes	Strong interpersonal skills, friendly and outgoing	E		X
	Willingness to keep learning and adapting	E		X
	Team orientated	E	X	X
	Willingness to travel	E		X
5. Other Relevant Factors	Preparedness to participate in training – self and others	E		X
	Required to publish scientific papers and present at conferences.	E		X

E=Essential/D=Desirable

CONDITIONS OF EMPLOYMENT
RESEARCH STAFF

1. GENERAL CONDITIONS

Members of staff are subject to the Charter and Statutes and the Ordinances and Regulations of the University, published in the Calendar, and to any amendments or additions thereto approved by the University Court and, in the case of the Charter and Statutes, Privy Council.

The University Court recognises the Strathclyde University and Colleges Union (SUCU) as the sole body with which it will negotiate and consult on all collective issues concerned with the terms and conditions of employment of Research staff. Such terms and conditions may be varied by the University Court after negotiation and consultation with SUCU.

Further information on the terms and conditions specified in this document is contained in the Staff Handbook, which also includes further details of such conditions as provision for sick/injury leave and pay, leave of absence, holidays and holiday pay, individual grievance procedures, review and disciplinary procedures and collective agreements. Should you not receive a copy of the handbook on appointment a reference copy is accessible by visiting Human Resources.

2. CONTINUOUS SERVICE

In the case of new appointments, unless otherwise stated in the letter of appointment, the date of continuous employment for the purposes of statutory employment rights will be taken to be the date of appointment contained therein. In the case of promotions, regradings or transfers, previous service is continuous.

3. ALLOCATION OF POST

The post to which each member of staff is appointed is allocated to the department or other area named in member's letter of appointment and any accompanying papers. Should the University Court deem it necessary, in the furtherance of the objectives of the University specified in its Charter, it shall, having consulted with the parties concerned and having received the advice of the Senate, re-allocate the post and/or the duties pertaining partially or wholly to it to another department or area. Any such re-allocation will be without prejudice to the other conditions of employment of the holder.

If the need arises during the course of employment for members of staff to work outside the U.K. for a period (or periods) of more than one month then such arrangements will be subject to mutual agreement. Members of staff would then be provided with a statement in advance setting out the terms covering such periods of employment.

4. RESPONSIBILITY AND SERVICE

Each member of staff is responsible for the proper performance of allocated duties to the person or persons specified in the member's letter and any accompanying papers. Unless otherwise indicated members of staff are appointed for full time service. Members of staff may not accept outside paid employment, including personal consultancies without the permission of Court, which will not be unreasonably withheld.

5. WORKING TIME

Working time is that required to fulfil the duties of the post. The University Court recognises that research Staff carry out these duties in a variety of ways appropriate to the nature of the research activity, but expects regular contact to take place between the research staff employee and the supervisor/grantholder (where these positions are occupied by different individuals) during normal working hours on week days. There are exceptions to this pattern which may involve contact at other locations or in the evenings, or at weekends, but these arrangements will be made with the agreement of the member of staff concerned.

Duties may, by arrangement with Head of Department, include some teaching associated with the post (up to a maximum of 40 hours per semester) for which no additional payment will be made.

Additional work which does not fall within the scope of that described above may by arrangement attract payment which must be authorised and processed through the payroll.

6. HOLIDAYS

Research staff have an entitlement to accrue days of paid annual holiday at the rate of 2.5 days per calendar month; this equates, for staff employed throughout the leave year, to an annual leave entitlement of thirty one days per year. The University leave year begins on 1st October. Research staff will normally be expected to take holidays accrued within the leave year. In exceptional circumstances, accrued leave days may be carried forward into the next leave year. Holidays accrued must be taken by arrangement with the Head of Department within the contract period. There are eleven days of public holiday to which research staff are also entitled if these days fall within the contract period. In addition to the eleven public days of holiday the University presently closes on four additional days over the Christmas and New Year period. **These four days count against the accrued annual holiday entitlement.**

7. SICK LEAVE

During any period of absence through illness or injury provided the appropriate medical certificates are received the University will pay a member of staff (having taken account of the aggregate of all periods of absence due to illness during the twelve months immediately preceding the first day of the current absence) as follows:

Period of Continuous Employment at commencement of absence from work	Full Pay	Half Pay
Less than 1 year	1 month	1 month
1 year but less than 2 years	2 months	2 months
2 years but less than 3 years	4 months	4 months
3 years but less than 5 years	5 months	5 months
5 years or more	6 months	6 months

In order to manage the University's sick pay scheme the University requires to maintain sickness absence records on individual members of staff. When making payments after the expiry of statutory sick pay the University will deduct an amount equivalent to any benefit normally payable by the Department of Health and Social Security. For this and other details see staff handbook.

8. SALARY AND SUPERANNUATION

Appointments are made within an appropriate grade of the University's grading structure for Research staff, which is linked to that for academic staff; any nationally awarded enhancements of the grade will be paid. Placing on grade is according to qualifications and experience, and where the post derives from externally provided financial support, to the nature of support. Salaries are payable monthly by means of a credit transfer to a specified bank account.

New members of staff, under age 60, will be admitted to membership of the Universities' Superannuation Scheme on taking up appointment unless they notify the University in advance that they do not wish to be admitted to membership of USS. USS requires a contribution from the member (currently 6.35 per cent of salary), to which a contribution of salary is added by the University as required by USS. New members of staff over age 60 are not admitted automatically as special terms, and a higher contribution rate (7.35 per cent), apply. Such staff should contact the Pensions Section if they wish to join the scheme.

New members of staff may opt out of USS within three months of taking up appointment when they will be treated as if they had never been members. After three months members of Staff who wish to withdraw from USS during their employment will be required to give a minimum of 28 days' notice in writing to the University. Any member of staff who wishes to opt out should contact the Pensions Section in the first instance.

Full details of the Scheme are available for reference purposes at the Pensions Section of Finance Office, John Anderson Campus and from Human Resources, Jordanhill Campus.

9. PLACE OF RESIDENCE

The University does not normally place specific restrictions upon the place of residence of members of staff. They are, however, expected to reside in a location which is compatible with the satisfactory fulfilment of all the duties associated with their appointment and with membership of the academic community.

10. PERIOD OF EMPLOYMENT

Members of staff are employed on the conditions indicated in individual letters of appointment and any accompanying papers. The University is not obliged to give notice of termination or continue any employment beyond the end of that period. Where the period of the contract of employment is for one year or less it may be terminated short of the fixed term period by 1 month's notice on either side. Where the period of the contract of employment is for more than one year, or where there have been a further contract or series of contracts immediately consecutive, the employment may be terminated short of the fixed term period by 3 months' notice on either side.

If the appointment is for a fixed term it will expire at the end of the period without the necessity for notice.

Revised November 2006

Service Commitment to

Applicants for Employment

Our commitment to you as the applicant is:

- Your application will be acknowledged *unless stated otherwise in the advertisement* within five working days of receipt. To enable us to meet this, acknowledgement postcards, where enclosed with further particulars, should be completed and returned with your application. Unless otherwise stated in the advertisement, you will also be informed of the outcome of your application as soon as possible.

- If called for interview you will be advised promptly and clearly of the interview arrangements. Your interview will be conducted in a businesslike and friendly manner and will comply with recognised good employment practice. To assist us in meeting our standards we ask that you promptly confirm your attendance (or otherwise) at interview and advise us of any change in your address or Curriculum Vitae.

- You will also be advised of any major delays in the appointment procedure. We will only approach referees nominated by you.

- You will be informed of the outcome of interview as soon as possible. If you are being offered a post you will be written to within 2 working days of the decision being taken. The offer will normally include a duplicate copy which you are required to sign and return to conclude the contract. **Payment of an appropriate salary is dependent on this.**

- We are committed to achieving the standards we have set and to receiving and acting upon constructive feedback from our clients.

- If you are not satisfied with the service you have received, please raise the matter in the first instance with the person with whom you have been dealing. This person will either deal with the complaint to your satisfaction or else advise you how to proceed next. If you feel that dealing with the matter in this way is inappropriate, then write to me at Human Resources, University of Strathclyde, McCance Building, 16 Richmond Street, Glasgow G1 1XQ, and I will respond.

Bill Sutherland
Director

Human Resources
University of Strathclyde
John Anderson Campus
McCance Building
Glasgow G1 1XQ

Ref: xx/xxxx/2009

Principal: Professor Andrew Hamnett

Research Fellow (2)
(Fixed-term post until 31 Dec 2012)

Department of Physics

1. NATURE OF APPOINTMENT

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ADAS for Fusion in Europe, hereafter called ADAS-EU,I s a Framework 7 CSA support activity of four years duration (2009-2012) for efficient implementation of atomic data in plasma diagnostics and plasma modelling at fusion laboratories throughout Europe, for promotion of validation experiments, for management of extended databases of relevant fundamental and applied data and for promotion of key fundamental atomic data calculation and measurement in European Institutions. It will enable improved effectiveness and completeness of analysis of existing fusion experiments and lay all necessary groundwork for ITER and beyond.

6. JOB DESCRIPTION

You will play a key role in delivering the primary scientific objectives of ADAS-EU, that is, the provision of analysis tools and necessary atomic and molecular data for atomic and molecular spectroscopy and broadband radiation detection at all wavelengths and in all plasma regions and for plasma models. All these aspects to be in the context of European-wide unified/shared methodologies, databases and maintenance.

There are five main themes: (1) heavy element spectroscopy and models; (2) charge exchange spectroscopy; (3) beam emission spectroscopy; (4) special features; (5) diatomic spectra and collisional-radiative models. You will acquire the ability to support all these areas. You will share leadership in the development of themes 1, 2, 3 and 5. You will be based at the Max-Planck Institut fur Plasmaphysik Garching-bei-München in Germany.

You will receive special training at EFDA-JET in the United Kingdom on ADAS and relating atomic physics to fusion experiments and studies and then you will have the on-site support of an ADAS-EU manager in integrating your activities with the local fusion activities at your placement. In later years you will participate as a tutor in the annual ADAS-EU course for fusion research scientists. You will share in the ADAS-EU series of visits and support to other Associated Laboratories of the European fusion programme.

7. PERSON SPECIFICATION/SELECTION CRITERIA

See attached FORM GR5

8. CONDITIONS OF SERVICE AND SALARY

This appointment to the end of 2012 will be made in terms of the enclosed conditions of service, with the exception of the hours of work and annual leave entitlement which will relate to those of equivalent status staff at the laboratory at which the post is based. The appointment will be at Research and Associated Staff grade 7 (current salary in the range €30,000- €45,000 per annum). Salary will be paid in Euros. Annual and/or merit increments will be adjusted to compensate for Sterling/Euro currency movements. Appointees will be subject to the taxation regime of their country of placement.

9. APPLICATION PROCEDURE

A full curriculum vitae should be attached to the application form. The names and addresses of three referees should be given on the application form. The referees may be contacted by the University without further permission from the candidate. You should also provide a covering letter specifying why you believe yourself suitable for this post.

The University operates a normal retirement age of 65 or the September following 65th birthday. Applications will only be accepted from people up to the age of 64 years and 6 months at the date of their application unless otherwise stated. This is in line with the Employment Equality (Age) Regulations 2006.

Applications should be lodged with Human Resources, University of Strathclyde, McCance Building, 16 Richmond Street, Glasgow, G1 1XQ by Friday 27 February 2009.

We value diversity and welcome applications from all sections of the community

Person Specification/Selection Criteria

FORM GR5

Post Title: ADAS-EU Research Fellow **Department: Physics**

CRITERIA	**STANDARD**	***E/D**	**MEASURED BY**	
			CV	**Interview**
1 Educational and/or Professional Qualifications	PhD in physics, theoretical physics or theoretical chemistry in one of the areas - radiating properties of plasmas, plasma modelling, diagnostic spectroscopic analysis of plasmas, calculation or measurement of electron-ion or atom-ion collisions.	E	X	
2 Experience/ Training	Experience of working and collaborating in a large experimental environment - magnetic or inertial confinement devices, astrophysical spacecraft or similar.	D	X	
	Experience of the computational and data flow infrastructure of large scale experiments.	D	X	
3 Job Related Skills and Achievements	Ability and confidence to use computational tools in support of objectives.	E	X	X
	Ability to organise, plan and use time efficiently	E		X
	Ability to analyse and then think creatively	E		X
	Relating to the full scope of a problem - fundamental to applied, theoretical to experimental	D		X
	Excellent written and verbal communication skills	E	X	X
	Ability to engage with theorists and experimentalists	D		X
4. Personal Attributes	Strong interpersonal skills, friendly and outgoing	E		X
	Willingness to keep learning and adapting	E		X
	Team orientated	E	X	X
	Willingness to travel	E		X
5. Other Relevant Factors	Preparedness to participate in training – self and others	E		X
	Required to publish scientific papers and present at conferences.	E		X

E=Essential/D=Desirable

CONDITIONS OF EMPLOYMENT
RESEARCH STAFF

1. GENERAL CONDITIONS

Members of staff are subject to the Charter and Statutes and the Ordinances and Regulations of the University, published in the Calendar, and to any amendments or additions thereto approved by the University Court and, in the case of the Charter and Statutes, Privy Council.

The University Court recognises the Strathclyde University and Colleges Union (SUCU) as the sole body with which it will negotiate and consult on all collective issues concerned with the terms and conditions of employment of Research staff. Such terms and conditions may be varied by the University Court after negotiation and consultation with SUCU.

Further information on the terms and conditions specified in this document is contained in the Staff Handbook, which also includes further details of such conditions as provision for sick/injury leave and pay, leave of absence, holidays and holiday pay, individual grievance procedures, review and disciplinary procedures and collective agreements. Should you not receive a copy of the handbook on appointment a reference copy is accessible by visiting Human Resources.

2. CONTINUOUS SERVICE

In the case of new appointments, unless otherwise stated in the letter of appointment, the date of continuous employment for the purposes of statutory employment rights will be taken to be the date of appointment contained therein. In the case of promotions, regradings or transfers, previous service is continuous.

3. ALLOCATION OF POST

The post to which each member of staff is appointed is allocated to the department or other area named in member's letter of appointment and any accompanying papers. Should the University Court deem it necessary, in the furtherance of the objectives of the University specified in its Charter, it shall, having consulted with the parties concerned and having received the advice of the Senate, re-allocate the post and/or the duties pertaining partially or wholly to it to another department or area. Any such re-allocation will be without prejudice to the other conditions of employment of the holder.

If the need arises during the course of employment for members of staff to work outside the U.K. for a period (or periods) of more than one month then such arrangements will be subject to mutual agreement. Members of staff would then be provided with a statement in advance setting out the terms covering such periods of employment.

4. RESPONSIBILITY AND SERVICE

Each member of staff is responsible for the proper performance of allocated duties to the person or persons specified in the member's letter and any accompanying papers. Unless otherwise indicated members of staff are appointed for full time service. Members of staff may not accept outside paid employment, including personal consultancies without the permission of Court, which will not be unreasonably withheld.

5. WORKING TIME

Working time is that required to fulfil the duties of the post. The University Court recognises that research Staff carry out these duties in a variety of ways appropriate to the nature of the research activity, but expects regular contact to take place between the research staff employee and the supervisor/grantholder (where these positions are occupied by different individuals) during normal working hours on week days. There are exceptions to this pattern which may involve contact at other locations or in the evenings, or at weekends, but these arrangements will be made with the agreement of the member of staff concerned.

Duties may, by arrangement with Head of Department, include some teaching associated with the post (up to a maximum of 40 hours per semester) for which no additional payment will be made.

Additional work which does not fall within the scope of that described above may by arrangement attract payment which must be authorised and processed through the payroll.

6. HOLIDAYS

Research staff have an entitlement to accrue days of paid annual holiday at the rate of 2.5 days per calendar month; this equates, for staff employed throughout the leave year, to an annual leave entitlement of thirty one days per year. The University leave year begins on 1st October. Research staff will normally be expected to take holidays accrued within the leave year. In exceptional circumstances, accrued leave days may be carried forward into the next leave year. Holidays accrued must be taken by arrangement with the Head of Department within the contract period. There are eleven days of public holiday to which research staff are also entitled if these days fall within the contract period. In addition to the eleven public days of holiday the University presently closes on four additional days over the Christmas and New Year period. **These four days count against the accrued annual holiday entitlement.**

7. SICK LEAVE

During any period of absence through illness or injury provided the appropriate medical certificates are received the University will pay a member of staff (having taken account of the aggregate of all periods of absence due to illness during the twelve months immediately preceding the first day of the current absence) as follows:

Period of Continuous Employment at commencement of absence from work	Full Pay	Half Pay
Less than 1 year	1 month	1 month
1 year but less than 2 years	2 months	2 months
2 years but less than 3 years	4 months	4 months
3 years but less than 5 years	5 months	5 months
5 years or more	6 months	6 months

In order to manage the University's sick pay scheme the University requires to maintain sickness absence records on individual members of staff. When making payments after the expiry of statutory sick pay the University will deduct an amount equivalent to any benefit normally payable by the Department of Health and Social Security. For this and other details see staff handbook.

8. SALARY AND SUPERANNUATION

Appointments are made within an appropriate grade of the University's grading structure for Research staff, which is linked to that for academic staff; any nationally awarded enhancements of the grade will be paid. Placing on grade is according to qualifications and experience, and where the post derives from externally provided financial support, to the nature of support. Salaries are payable monthly by means of a credit transfer to a specified bank account.

New members of staff, under age 60, will be admitted to membership of the Universities' Superannuation Scheme on taking up appointment unless they notify the University in advance that they do not wish to be admitted to membership of USS. USS requires a contribution from the member (currently 6.35 per cent of salary), to which a contribution of salary is added by the University as required by USS. New members of staff over age 60 are not admitted automatically as special terms, and a higher contribution rate (7.35 per cent), apply. Such staff should contact the Pensions Section if they wish to join the scheme.

New members of staff may opt out of USS within three months of taking up appointment when they will be treated as if they had never been members. After three months members of Staff who wish to withdraw from USS during their employment will be required to give a minimum of 28 days' notice in writing to the University. Any member of staff who wishes to opt out should contact the Pensions Section in the first instance.

Full details of the Scheme are available for reference purposes at the Pensions Section of Finance Office, John Anderson Campus and from Human Resources, Jordanhill Campus.

9. PLACE OF RESIDENCE

The University does not normally place specific restrictions upon the place of residence of members of staff. They are, however, expected to reside in a location which is compatible with the satisfactory fulfilment of all the duties associated with their appointment and with membership of the academic community.

10. PERIOD OF EMPLOYMENT

Members of staff are employed on the conditions indicated in individual letters of appointment and any accompanying papers. The University is not obliged to give notice of termination or continue any employment beyond the end of that period. Where the period of the contract of employment is for one year or less it may be terminated short of the fixed term period by 1 month's notice on either side. Where the period of the contract of employment is for more than one year, or where there have been a further contract or series of contracts immediately consecutive, the employment may be terminated short of the fixed term period by 3 months' notice on either side.

If the appointment is for a fixed term it will expire at the end of the period without the necessity for notice.

Revised November 2006

Service Commitment to

Applicants for Employment

Our commitment to you as the applicant is:

- Your application will be acknowledged *unless stated otherwise in the advertisement* within five working days of receipt. To enable us to meet this, acknowledgement postcards, where enclosed with further particulars, should be completed and returned with your application. Unless otherwise stated in the advertisement, you will also be informed of the outcome of your application as soon as possible.

- If called for interview you will be advised promptly and clearly of the interview arrangements. Your interview will be conducted in a businesslike and friendly manner and will comply with recognised good employment practice. To assist us in meeting our standards we ask that you promptly confirm your attendance (or otherwise) at interview and advise us of any change in your address or Curriculum Vitae.

- You will also be advised of any major delays in the appointment procedure. We will only approach referees nominated by you.

- You will be informed of the outcome of interview as soon as possible. If you are being offered a post you will be written to within 2 working days of the decision being taken. The offer will normally include a duplicate copy which you are required to sign and return to conclude the contract. **Payment of an appropriate salary is dependent on this.**

- We are committed to achieving the standards we have set and to receiving and acting upon constructive feedback from our clients.

- If you are not satisfied with the service you have received, please raise the matter in the first instance with the person with whom you have been dealing. This person will either deal with the complaint to your satisfaction or else advise you how to proceed next. If you feel that dealing with the matter in this way is inappropriate, then write to me at Human Resources, University of Strathclyde, McCance Building, 16 Richmond Street, Glasgow G1 1XQ, and I will respond.

Bill Sutherland
Director

Human Resources
University of Strathclyde
John Anderson Campus
McCance Building
Glasgow G1 1XQ

Appendix B

Travel reports linked to Dr Guzman induction

[1] summary_juelich_13-17jul09
[2] summary_juelich_3-7aug09

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ADAS-EU Travel Report

Location: Institute for Plasma Physics, Forschungzentrum Jeulich, Germany.
Date: 13-17 Jul 2009.
ADAS-EU staff: Hugh Summers.
Persons visited: Ratko Janev, Francisco Guzman, Dmitri Borodin

Items:

(1) Preliminary discussions with Dmitri Borodin and Francisco Guzman centred on the expected tasks and points of participation of Francisco at Juelich and with Juelich staff. A number of areas were identified: molecular data, combined scenarios of atomic data/development/application – especially edge modelling codes, CXS and BES.

(2) Discussions were held with Francisco Guzman on aspects of establishing an ADAS data format for diatomic molecules (only H_2 at this stage) equivalent to a specific ion file. This included level indexing, separation of electron and ion collision data into distinct datasets, transition indexing, fit parameters and numerical cross-sections, ion collision types.

(3) Discussions were held with Ratko Janev and Francisco Guzman on the specific H_2 and associated data to be implemented in ADAS formats. The primary material is in a draft document by Janev, Reiter and Samm to be published by Springer. All the data is in the form of parametric fits to preferred data – essentially selected by Janev. The preferred curves were established by hand plotting, construction of a preferred hand drawn curve and then empirical adjustment of a fitting form and its parameters. Original hand plots for extraction and tabulation of the preferred curve are not all available, although a substantial, but unsorted, body of them are at Juelich.

(4) The draft book is still undergoing amendments. Not all chapters were immediately available to Francisco Guzman and myself.

(5) First discussions with Dmitri Borodin centred on tungsten and particularly data to help with the interpretation of W^0 and W^{+1} spectral emission in the visible from WF_6 injection at PISCES-B. Line ratios are observed in W^0 but there is more idea of absolute intensities in W^{+1}. Interpretation requires ADAS PECs and SXBs.

(6) Discussion with Dmitri Borodin continued into support of the ERO 3-D particle tracking code. Dmitri promoted collaboration with Vainshtein on atomic data resources, some of whose data on ground state ionization is in ERO.

(7) Dmitri provided a list of currently observed tungsten lines for consideration and response from the ADAS team.

(8) Hugh Summers pointed out the ADAS/ADAS-EU plans for lifting the database for the neutral and near neutral heavy elements. Dimtri encouraged rapid progress in this which he considered a priority.

(9) Further discussions with Francisco Guzman and Dmitri Borodin were concerned with ADAS-EU sub-contracting with UAM Madrid and with the 2009 ADAS-EU course – for which Dmitri will act as a special tutor on Monte Carlo transport modelling.

HPS
22 Jul 09

ADAS-EU Travel Report

Location: Institute for Plasma Physics, Forschungzentrum Jeulich, Germany.
Date: 3-7 Aug 2009.
ADAS-EU staff: Hugh Summers.
Persons visited: Detlev Reiter, Francisco Guzman, Dmitri Borodin, Alexander Marchuk

Items:

(1) Discussions were held with Detlev Reiter, Francisco Guzman and myself on the H_2 database conversion for ADAS. It was Detlev's view that unification of the data for fusion plasma application was very desirable. It was clear from him that the purely fit forms as available has some anxieties. Erratic behaviour in asymptotic regions, lack of attribution of the fits and incomplete records of the preferred originating data in some cases gave pause for anxiety. Detlev pointed out that in some cases he had tried to go back to original sources to reform the preferred cross-section curve, but that he and associates did not have the time to revisit everything. He supported the inclusion of preferred numerical data in the molecular ADAS data formats as well as the fits. Detlev also supported strongly the preparation of appropriate ADAS $H_2/H/H_2^+/H^+/H_3^+$ collisional-radiative codes for the validation and verification of the assembled ADAS data.

(2) Discussions with Alexander Marchuk and Francisco Guzman took place on linkage of ADAS beam emission modelling and ADAS soft X-ray feature models with local FZ Juelich models in this area developed by Alexander. The physics of the two scenarios was discussed in depth. It was clear that the ADAS codes and the direction of their future development did not marry well with the FZ Juelich work. The latter did not match the generality sought for the ADAS codes. Also, restrictions in the handling of some of the processes such as dielectronic recombination, choices of cross-section etc. at FZ Juelich were not compatible with ADAS objectives. The FZ Juelich work had a short term experimental comparison objective. It was agreed that the streams of work would continue in parallel without attempt at unification at least at this stage.

(3) I and Francisco Guzman worked intensively on the Janev, Reiter, Samm H_2 data, revealing and making decisions on many issues as they appeared. Although the task is of much larger magnitiude than expected, a pattern for ADAS molecular data formats is gradually evolving. It is agreed that the whole ADAS-EU team will discuss the recommendation stemming from Francisco and my efforts when Francisco visits UKAEA/JET 17-21 Aug.

(4) A query arose from Volker Philipps about influx of beryllium with back reference to photon efficiencies provided by Mike Stamp some years ago. Francisco Guzman participated in this discussion. I explained the evolution of beryllium data in ADAS since the Stamp reference and the issues concerning the 2 ^{3}P metastable. In fact the question had already been settled to Volker Philipps satisfaction. Francisco Guzman and I discussed the physics of influx determination via spectroscopy and the how the ADAS models and data are used to assist this. Francisco will be in a position to deal with queries of this character in the future.

HPS
12 Aug 09

Appendix C

Sub-contracting set-up visit reports and sub-contracts

[1.1] summary_mons_25-26feb09
[1.2] contract_mons_30jul09
[2.1] summary_groningen_19-20mar09
[2.2] contract_groningen_27sept09
[3.1] summary_giessen_03-04jun09
[3.2] contract_giessen_30jul09
[4.1] summary_madrid_09-10jun09
[4.2] contract_madrid_30jul09

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ADAS-EU Travel Report

Location: Department of Physics and Astrophysics, University of Mons-Hainaut, Mons, Belgium.
Date: 25-26 February 2009.
ADAS-EU staff: Hugh Summers.
Persons visited: Emile Biémont, Patrick Palmeri, Pascal Quinet.

Items:

(1) Discussion centred on establishing an ADAS-EU subcontract with the Department of Physics and Astrophysics, University of Mons-Hainau to improve the quality of atomic physics modelling and data for fusion in the area of neutral and near neutral heavy species.

(2) Hugh Summers outlined the general context of the planned contribution, that is, its relationship to the baseline of ADAS modelling for heavy species, the current inadequacy of the baseline for neutral and near neutral atoms and ions and the wish to lift this baseline selectively for heavy species of direct relevance to fusion.

(3) Emile Biémont outlined the work of the group. He describing the theoretical calculations of complex heavy atom/ion structure and transition probabilities carried out at Mons-Hainaut using adaptations of the Cowan methodology – especially the inclusion of core polarization in the model potentials and the use of large scale configuration interaction. Their optimisation of Slater integral scaling factors is based on dedicated experimental wavelength and lifetime measurements (laser spectroscopy, LIF) made on the targetted species in a long-term collaboration with the University of Lund, Sweden. They have substantial experience on a range of heavy element ions, including WII, WIII, TaI , TaIII, Cd-isoelectronic sequence. Current work extends to TcI and RuI of recent stellar astrophysical interest. Their focus is generally on the 5^{th} and 6^{th} period elements and they have experience of most outer shell configurations (4d, 4f etc.) from a iso-electronic point of view.

(4) Hugh Summers said that there was particular interest in WI and deduction of its influx via visible spectroscopy. He pointed out that there is one commonly used visible line observed, but in an alternate spin system from the ground. He said that in addition to W, there were other species such as Ta and Re linked to W, heavy rare gases, Kr and Xe and then a range of possible marker species (for erosion) spanning 5^{th} and 6^{th} periods. Although we sought to identify these marker species from XUV/EUV spectroscopy of the core in highly ionized states, there would also be merit in identifying them at source from neutral visible lines if possible. Hf, Sn, Ag, Au, Lu and La were mentioned. Hugh Summers also stressed that the fusion objectives would be identified lines for influx inference and then calculated photon efficiencies for the diagnostic deduction. This would require an extension beyond the transition probability calculation to collision strengths and ionization coefficients. However, he pointed out that significant progess would be made with plane wave Born cross-sections, based on a good structure, due to the relatively high plasma electron temperature at the sputtering source.

(5) Parick Palmeri pointed out that at Mons- Hainaut they had no experience of evaluating the Bessel function integrals and would need some help on this. Also they would need guidance and/or code support in outputting results in ADAS formats. Hugh Summers said data would be needed in ADAS adf04 format, but that on both points the ADAS_EU managers Martin O'Mullane and Allan Whiteford had a lot of experience and codes and support would be provided.

(6) The possible influx in metastable states was discussed. Hugh Summers said that in principle, with identified lines in both ground and metastable spin systems, the fluxes in ground and metastable could be treated as independent measurements. Failing that a coupling between the spin systems would need to be assumed or calculated. Hugh Summers though this might be a potential RMatrix calculation just including the ground/metastable system – challenging but feasible, and a long way short of the extreme difficulty of a full RMatrix calculation of the whole heavy atom which paralleled the Mons-Hainaut structure calculations. This was felt to be somewhat down the line – perhaps to be considered following a successful first step.

(7) It was agreed to focus on the neutral stages of three or four elements, that these should be new species from the Lund experimental point of view. Hugh Summers should identify the preferred atoms speedily including and where possible the prospective diagnostic lines in the visible. Mons-Hainaut would then put in the experiment time proposal to Lund.

(8) It was agreed that a timescale of about one year was reasonable, but that there should be good contact (visits both ways) during the period. The objective should be a close collaboration of mutual benefit – not an ADAS-EU contract issue and then forget until completion.

(9) ADAS-EU would expect to get early delivery of results and data into the ADAS databases from the contract. There would be no barrier to free open publication. It was thought that there might be mutual benefit in joint publication(s) which explored the fusion implementation dimension and purposes.

(10) It was assumed that the contract would spell out in detail the species, study and deliverables for which the sub-contract price would be a fair payment on the basis of staff time. It was felt/hoped that finer financial breakdown would not be required, and need not be of concern to ADAS-EU management or auditors.

(11) A new issue of polarisabilities, their calculation and use arose. Mons_Hainaut progress has depended on the inclusion of core polarisability in the model potentials and then polarisation corrections in the evaluation of the dipole radial integrals for the CI wave functions. Hugh Summers felt that this might answer a need for the accelerated bbgp dielectronic calculations of the ADAS heavy species baseline. He hoped to use static dipole polarisabilities (of the excited parent ion from a dielectronic point of view) to establish the fine energy separations of high spectator nl (nlj) sub-states – a crucial point for doubly excited state redistribution. It was speculated that the average polarisability used in the model potential might be combined with (or corrected by) the valence electron exact polarisability contribution via the Mons-Hainaut dipole corrections. It was agreed to think further on this possibility.

HPS
27Feb.09

ADAS-EU CONTRACT

ATOMIC STRUCTURE AND ELECTRON DATA FOR HEAVY ELEMENT IONS

THE TUNGSTEN IONS W^{+0} TO W^{+4}AND ADJACENT ELEMENT SYSTEMS

H. P. Summers

30 July 2009

1. Summary

It is proposed to commission a set of atomic structure calculations and measurements from Prof. Emile Biémont, Department of Physics, University Mons-Hainaut, Belgium. This reference quality sixth-period fundamental data will benchmark iso-nuclear and iso-electronic sequence data available in the ADAS database and guide further large scale production. It will extend the scope of collisional-radiative data and model support provided under the ADAS-EU Project to the European magnetic confinement fusion community. The data, which supports influx studies and spectral measurements on low ionisation states of heavy species, will be interfaced to spectral measurements on fusion devices at EURATOM Associated laboratories through tailored spectral line 'scripts' within the Atomic Data and Analysis Structure, ADAS.

The work will make extensive use of the methods and codes developed by Prof. Biémont, Dr. Palmeri, Dr. Quinet and co-workers. The calculations will be performed at University Mons-Hainaut and LIF lifetime measurements at Lund and at CRYRING, Stockholm, Sweden. The data will be organised and relayed from Mons to ADAS in established specific ion data formats with the assistance of ADAS-EU staff. Conversion to spectrum line photon efficiencies and similar derived data will take place at UKAEA/JET Facility and University of Strathclyde. The fundamental and derived data in appropriate ADAS data format collections will be released after assessment and validation to the public domain via OPEN-ADAS [1].

The duration of the project will be eighteen months (Sept. 2009 - Jan. 2011) at a fixed price of €10,000.

2. Background

The strategy, originated at the JET Facility and now followed by fusion laboratories throughout the world participating in the ADAS Project, for the description of the radiation emission of impurity ions has been the establishment of an integrated atomic data and analysis structure (ADAS). ADAS seeks to provide at appropriate quality, all the derived data required for global modelling and quantitative spectroscopic diagnosis and analysis [2]. The system is based on the initial preparation of collections of fundamental atomic transition probability and excitation rate data for specific ions called *specific ion files*. Various ADAS computer codes then prepare all the derived data such as net power loss coefficients, spectral line contribution functions etc. in a form directly usable in experimental analysis and in plasma models. The fundamental and derived databases are centrally maintained and accessible by standard routines for modelling and diagnostic applications (eg. edge studies, VUV and XUV spectroscopy). The effectiveness and precision in the applications depends on the quality and availability of fundamental data. In this context a specific need is enhanced provision for low ionisation stages of heavy elements up to and including tungsten. Such enhancement is a central theme of the ADAS-EU Euratom/Framework 7 Support Action. Recognizing the complexity of some of the fusion relevant heavy element ions and current bounds on atomic reaction computability, ADAS-EU policy falls into two parts. Firstly a modest number of high precision reference calculations and/or measurements at the front edge of current capability are sought. Secondly, as well as direct embedding of the associated precise data in the databases, the data should be exploited as fiducials which can suggest adjustments or global/regional scalings to the large scale semi-automated mass production calculations of the ADAS heavy element baseline. This 'lift of the baseline' is the central objective and the primary delivery.

One of the main sources of spectroscopic properties of atoms and low ionisation stage ions of heavy elements is the group of Prof. Biémont. This group has steadily developed and systematised their methods which use underpinning atomic structure calculations to analyse observed LIF spectra at the Lund Laser Centre (LLC) (Lund, Sweden) and possibly at CRYRING (Stockholm, Sweden). The adjustment and optimising of theory to observations provides identified reference energy levels and transition probabilities, along with insight into the controlling configuration interactions and orbital characteristics [3]. The group has worked on many systems, specialising in lanthanides, but including ions touching [4] and adjacent to the present fusion interest [5]. Additionally the group developed and maintains the DREAM database [6] of energy levels and parameters for lanthanides and also the DESIRE database (database for sixth row elements) [7]. The approach of Prof. Biemont is ideally suited for matching to and strengthening the ADAS atomic modelling system along the manner described in the first paragraph of this section. The group's theoretical structure calculations are principally based on the Cowan code - exploiting the semi-relativistic Hartree-Fock (HFR) variant, but exploiting also multi-configuration Dirac-Fock (MCDF) [8]. It is noted that baseline mass production in ADAS principally uses the Cowan code. However the extended special techniques used by the group – such as model potentials for core polarisation and correction factors for core-penetration - along with optimising to experimental spectra, lift the analysis and description to reference level.

In the fusion domain, the neutral and near neutral ions of elements are inflowing from inner wall surfaces contacted by the plasma. They ionise rapidly as they enter the relatively high (albeit divertor or edge) temperature plasma dispersing from their source as the ions become entrained in parallel transport along the magnetic field lines. Detection of the species and deduction of its influx is the main diagnostic and this is ideally inferred from spectrum lines in the visible. For heavy elements, the deduction is difficult due to the lack of strong identified lines and the presence of metastables. Thus for example, the only useful line at this time for WI is the transition $5d^5(^6S)\ 6s\ ^7S_3$ - $5d^5(^6S)\ 6p\ ^7P_4$ (ΔE=24938.39 cm-1) which is not in the ground state spin system. Fully validated influx requires matching of influx in two successive ionisation stages, summed over the various metastable contributors [9]. This is demanding in spectroscopy and in the theoretical provisions of identifications, generalised collisional-radiative modelling and photon efficiencies - especially for heavy species. The proposal directly targets the fundamental specialist atomic data critical points in enabling this diagnostic capability for the ITER scenario. In doing so it is recognised that the highest precision methods for electron impact excitation cross-sections are not yet computationally feasible for the systems W^{+0}-W^{+4}. But the plasma regime is highly ionising with principal cross-sections in the Born-Bethe regime. Availability of high-grade theoretical atomic structure allows evaluation of the Born-Bessel integrals. Also the lowest intersystem transitions, omitted in Born approximation, may be accessible to restricted R-matrix study.

The block of ions, W^{+5}- W^{+15}, occurring in the tokamak divertor, have individually narrow shells and small emission measures, but collectively influence the local radiated power balance. Comprising partially filled d- and f-shell systems, these rare-earth-like configurations have been extensively analysed by the group of Prof. Biémont. This sub-contract provides an opportunity, through guided mapping of data across databases, to lift the quality of ADAS radiated power modelling of such intermediate heavy ions.

3. The proposed work

The work falls into four parts, namely lifetime measurement and transition probability analysis, Born-Bessel integral incorporation and re-calculation, inter-database mapping of selected ion parameters, guided adoption of structure parameters in ADAS baseline modelling - including static dipole polarisabilities.

(1) Extension of analysed 6^{th} period ions by selective studies from the ions Ta^{+0}-Ta^{+3}, W^{+0}-W^{+3}, Re^{+0}-Re^{+3}

(2) Implementation of Born-Bessel integral and Born cross-section evaluation using Mons-Hainaut wavefunctions generated from energy level and oscillator strength analyses.

(3) Production of ADAS adf04 data sets mapped from Mons-Hainaut analyses and databases, spanning the ion group of (1) and selections from the lanthanide systems.

(4) Establishment of preferred parameters for Cowan code calculations, in the 6^{th} period ion region, as an extrapolation and interpolation of Mons-Hainaut analyses. Generation of dipole polarisabilities for ground and excited states of the above systems at configuration average resolution or beyond as feasible.

Integration of data into ADAS will be executed by staff of ADAS-EU, including the conversion to the key derived data format adf11, adf13, and adf15. ADAS-EU staff will pay working visits to Mons-Hainaut to assist with execution of the above tasks as appropriate. A copy of ADAS software will be made available on a workstation at the Department of Physics, University of Mons-Hainaut at no charge for local use.

4. The Financial Provision

The operations and calculations outlined in the previous section will be carried out over a period of eighteen months (Sept. 2009 - Jan. 2011). Financial provision is made as a contribution to the time allocated to the investigation by the senior investigators (Prof. Biémont, Dr. Palmeri, Dr. Quinet) and their research staff. No travel funds or computation costs are sought.

Item		€
Univ. Mons-Hainaut (fixed price)		10,000
	total	10,000

References

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ADAS-EU Travel Report

Location: Kernversneller Institute, Groningen, Netherlands.
Date: 19-20 March 2009.
ADAS-EU staff: Hugh Summers.
Persons visited: Ronnie Hoekstra.

Items:

(1) Discussion centred on establishing an ADAS-EU subcontract with the University of Groningen to improve the quality of atomic physics modelling and data for fusion in the area of ion impact ionisation, charge exchange and excitation.

(2) Ronnie reviewed the current character of experimental work in atomic physics at KVI/Groningen. It was noted that the high energy KVI ion beam line as used for earlier JET collaborative studies on the spectroscopic methods for state selective charge transfer was no longer in use. Recent work uses recoil ion momentum spectroscopy in so-called COLTRIMS and MOTRIMS systems. Ion beam sources include the KVI ECR source delivering ion charge states up to 25-times ionised as well as the Heidelberg EBIT. Typical results include single electron capture by Ar^{+15} - Ar^{+18} at energies up to 14keV q^{-1} from He donor and capture by Xe^{+18} and Xe^{+24} from Na donor at energies 0-5-4.5keV/amu. For Xe, n-shell selective capture is into shells n=13-20 and n=19-24 for the two studied ions respectively.

(3) Ronnie pointed out that the magneto-optical trap was limited in the species which could be used since suitable lines for laser light absorption were required. Much of the KVI recent KVI work is with Na. It was noted that the KVI had a history of study with Na including capture from Na(2s) and Na(2p) and with aligned Na(2p) states. Also capture from longitudinally and tangentially aligned Na(2p) states did not match expectations in the low energy region.

(4) The KVI group has an interest in astrophysical applications of charge transfer at relatively low energies. These include capture from ebullient atoms and molecules from comets by solar wind ions and by capture reactions in the solar system halo. Research on the interaction of ions with surfaces continues, but the largest thrust at the moment is ion on collisional interaction with biological molecules in the pursuit of cancer therapies. Methods have been developed for introduction and electrostatic guiding of such molecules into the ion beam collisional reaction chamber.

(5) Ronnie retains his interest in the magnetic confinement fusion area, in the ion-atom, ion-molecule reactions which occur and in the quality and completeness of the data available.

(6) Hugh reviewed the ion collision issues he wished addressed and developed in ADAS-EU. CXS was moving to higher z with a need most importantly for state selective capture data to high sub-dominant n-shells from H(n=1) and H(n=2) to receiver charge states $10 < z <\sim 36$. The intermediate energy range ~40keV/amu remained the most challenging. Hugh was concerned that review and maintenance of ion impact excitation and ionisation of the beam atoms (H(n=1-4) and He) was not keeping pace. Much of the data in use was in format adf02 and a number of the entries there are old scaling expressions in need of revision or replacement. An expert assessment of the data status, of the scope and value of more recent experimental and theoretical results and programme of revision was needed. In particular an assessment as to whether data is now adequate to support more adf04-like specific ion collections of data rather than simple reaction lists (adf02). In this respect the paradigm is the old collaboration with JET Joint Undertaking.

(7) Hugh explained the planned direction of ADAS-EU studies of differential (in angle) collisions with beam atoms and the Stark manifold characteristics of the beam (H) target. He was concerned not only about primary ion excitation from the ground, but also the redistributive collisions, the distinguishability of m and k mixing (in the nkm Stark quantisation) and differential effects between impacting ions of different mass and therefore thermal speed. Hugh felt that KVI experimental experience and guidance with oriented atoms and angular differential cross-sections would greatly help this development.

(8) Hugh explained the limited hydrogen molecular extension planned for ADAS-EU and the new data formats to be introduced and supported. KVI studies with H_2 were germaine to this.

(9) Hugh outlined how he though an ADAS-EU sub-contract should function. Since it was required to be for support, it should principally provide a channel for the effective passage of KVI/Groningen experimental cross-sections, experience and guidance into ADAS and

thence on to impact and support diagnostics and fusion. Effective use of funds would be for the time of KVI/Groningen staff to work with ADAS-EU staff to make this interface work. It was realized that of course the on-going research and production mattered, but that ADAS-EU monies were insufficient and not so appropriate for that. Rather an effective ADAS-EU engagement would give leverage in application for national research grants. It was also felt that ADAS and ADAS-EU could help to foster interest in diploma students at Groningen by arranging working visits to the fusion laboratories and so on.

(10) Target ADAS data formats for upgrade and maintenance in the collaboration would be adf01 (CX and target excitation versions), general z adf49, adf02 (including replacement with a format for specific ions), adf24 and molecular extensions adf50. Rationalisation would be required.

(11) Generally there was excellent enthusiasm from University of Groningen/KVI for sub-contracting reflecting the above interests and Hugh was mandated to work-up the actual contract and its scientific content in interchange with Ronnie.

HPS
17 June 2009

ADAS-EU CONTRACT

POSITIVE ION IMPACT DATA FOR FUSION APPLICATIONS

DATA FOR HYDROGEN AND HELIUM BEAM STOPPING AND EMISSION

H. P. Summers

27 September 2009

1. Summary

It is proposed to commission a data review, evaluation of selective database restructuring and initial data filling of new ADAS data formats from Prof. Ronnie Hoekstra, KVI, University of Groningen, Netherlands. These actions centre on the current provisions of ion impact data for neutral hydrogen and helium isotope beam stopping and emission in the range 5keV/amu to ~200keV/amu in the ADAS databases. It will extend the scope of collisional-radiative data and model support provided under the ADAS-EU Project to the European magnetic confinement fusion community The data, which supports hydrogen beam stopping and emission due to ion colliders, will be interfaced to spectral measurements and beam and beam-sourced ion transport models for fusion devices at EURATOM Associated laboratories and ITER through tailored data formats within the Atomic Data and Analysis Structure, ADAS.

The work will make use of the methods and experience developed by Prof. Hoekstra and co-workers in support of the JET experiment and new experimental capabilities at KVI. Experiments clarifying orientation/alignment and angular differential cross-sections will be performed with the MOTRIMS/COLTRIMS capability at KVI in conjunction with the KVI ECR source and the Heidelberg EBIT. Restructured data formats and new data formats for angular differential cross-sections and dressed ion impact reactions will be designed, organised and initially filled at KVI in engagement with ADAS-EU staff. Conversion to derived data formats through collisional-radiative modelling, especially beam stopping, effective emissivities and appropriate 'driver/receiver reaction resolved' data will take place at UKAEA/JET Facility and University of Strathclyde. The fundamental and derived data in appropriate ADAS data format collections will be released after assessment and validation to the public domain via OPEN-ADAS [1].

The duration of the project will be one and a half year (Oct. 2009 - Apr. 2011) at a fixed price of €10,000.

2. Background

The strategy, originated at the JET Facility and now followed by fusion laboratories throughout the world participating in the ADAS Project, for the description of the radiation emission of impurity ions has been the establishment of an integrated atomic data and analysis structure (ADAS). ADAS seeks to provide at appropriate quality, all the derived data required for global modelling and quantitative spectroscopic diagnosis and analysis [2]. The fundamental and derived databases are centrally maintained and accessible by standard routines for modelling and diagnostic applications (eg. edge studies, VUV and XUV spectroscopy). The effectiveness and precision in the applications depends on the quality and availability of fundamental data. In this context a specific need is enhanced provision for neutral beam stopping and emission with both hydrogen and helium isotope beam species and plasma ion colliders. Such enhancement is a central theme of the ADAS-EU Euratom/Framework 7 Support Action. Recognizing the importance of diagnostic spectral observations of beam emission for ITER, the use of negative ion-sourced beams and the consolidation of beam and slowing down particle transport models, ADAS-EU policy falls into two parts. Firstly a modest number of related fundamental measurements at the front edge of current capability will be made. Of necessity some of these fundamental measurements are indicative rather than direct since exact matching of reactants to the fusion case is not possible. Secondly, the measurements will be used to guide model and data enhancements as outlined below - an area of considerable experience and success in the earlier collaboration between JET and KVI. The associated upgrade of ADAS beam stopping and emission is the central objective and the primary delivery.

One of the main sources of experimental cross-sections for highly charge ion colliders on neutral targets is the group of Prof. Hoekstra. Focussing in the early nineties on spatially resolved spectroscopic measurements along the ion collider beam line downstream from the target, the work provided benchmark state resolved charge transfer data for fusion neutral beam scenarios, underpinning associated calculations [3]. The group maintained strong engagement with the JET Joint Undertaking and the fusion community throughout the nineties, extending the ADAS charge exchange databases and modelling capability to include helium donors (ground and metastable) and excited hydrogen donors [4] as well as adding beam excitation cross-section data [5]. In recent years, the group has introduced recoil ion momentum spectroscopy and cold atom traps, working extensively with helium and sodium with ion colliders from in-house ECR sources and from external EBIT sources. The studies span from Ar^{+15} – Ar^{+18} state selective single electron capture from helium [6] through to ionisation and capture in He^{+2} /Na collisions [7]. Such latter studies which can include differential cross-section measurement and target (Na 3p) alignment are specially noted for this proposal. The group has strong contacts with theoretical groups and has maintained a strong interest in review and assessment of ion/atom collision data. It has participated in many International Atomic Energy Agency sponsored data reviews and collaborative research programs.

For magnetic confinement fusion devices penetrated by fast neutral beams for heating or diagnostic purposes, the atomic reactions of the beam and plasma ions are a central issue. They moderate the deposition of energy by the beams into the plasma and initiate the charge transfer and beam excitation reactions which lead to charge exchange spectroscopy (CXS) and beam emission spectroscopy (BES). In the advance towards ITER, ions of heavier species such as argon and beyond become significant for beam stopping. Also the key motional Stark effect (MSE) internal field measurement will become dependent on beam emission spectroscopy rather than polarization. There are then some atomic physics issues for attention. Plasma ion impact dominates electron for excitation of beam atoms and all impurity ion species in the plasma contribute, broadly in proportion to their share of z_{eff}. The primary excitation cross-section data is currently insufficiently precise at all energies to sustain the hoped-for precision of the BES diagnostic, relying in many cases on z-scaled values. Also, along with a required extension to heavier species, it is noted that partially stripped impurity ions may be present in the confined plasma. The collision of an impurity ion with a beam atom state, because of the fast beam speed is essentially directional, the effective cross-sections being only partial angularly integrated cross-sections over a solid angle depending on the beam to thermal speed ratio – larger for light thermal nuclei (such as deuterons) and fast ions. The target atom, usually a hydrogen isotope, in an excited shell has Stark alignment and distortion orthogonal to the beam direction. Collisions, from a collisional-radiative modelling perspective may be seen as potentially differentiating in their influence on n, k or m mixing (in Stark quantisation) where the n=2, 3 and 4 shells are the most important. All these effects have not yet been included in beam emission/beam stopping. Attention to the above considerations is the key to increasing the scope of the BES diagnostic and to 'lifting' the ADAS database and modelling to the level of precision sought for ITER.

3. The proposed work

The work falls into four parts:

(1) Assessment, extension and re-specification of ADAS data format adf02. Data sets will be for specific target neutral, will follow the broad pattern of adf04 files and will include excitation, net CX and ionisation data. The data for the light elements colliders He^{+2}, Be^{+4}, B^{+5}, C^{+6}, O^{+8} and Ne^{+10} will be considered and updated. The format will remain as a total cross-section type.

(2) Assessment of angular differential excitation and ionisation cross-sections for selected ion colliders with $He(1s^2)$ target from MOTRIMS/COLTRIMS measurement. Investigate with ADAS-EU staff the structure for a new ADAS data format for ion impact angular differential data for He $(1s^2)$ & H(1s) and the possibilities of initial filling with a transfer algorithm from the total cross-section database of (1) and the study above.

(3) Assessment of angular differential excitation, ionisation and charge transfer cross-sections for selected ion colliders with Na(3s) and aligned Na(3p) targets from MOTRIMS measurement. Investigate with ADAS-EU staff the possibilities of initial filling the new angular differential cross-section ADAS format for H(n=2) & H(n=3) Stark states with a transfer algorithm from the total cross-section database of (1) and the study above.

(4) Investigatation with ADAS-EU staff of the character of Stark nkm mixing for neutral hydrogen beams in the energy range 5-200 keV/amu beam emission studies.

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Integration of data into ADAS will be executed by staff of the ADAS-EU, including the conversion to the key derived data format adf12, adf21, and adf22. ADAS-EU staff will pay working visits to Groningen to assist with execution of the above tasks as appropriate. A copy of ADAS software will be made available on a workstation at the KVI, University of Groningen at no charge for local use.

4. The Financial Provision

The operations and calculations outlined in the previous section will be carried out over a period of eighteen months (Oct. 2009 – Apr. 2011). Financial provision is made as a contribution to the time allocated to the investigation by the senior investigator (Prof. Hoekstra) and his research staff. No travel funds or computation costs are sought.

Item		€
KVI, University of Groningen (fixed price)		10,000
	total	10,000

References

[1] http://www.adas.ac.uk/openadas.php

[2] http://www.adas.ac.uk

[3] R Hoekstra, H Anderson, F W Bliek et al. (1998) Atomic and Molecular Data & their Applications (ed. Mohr, AIP Press) pp37-56

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ADAS-EU Travel Report

Location: Institut für Atom- und Molekülphysik, Justus-Liebig Universität, Giessen, Germany.
Date: 03-04 June 2009.
ADAS-EU staff: Hugh Summers.
Persons visited: Alfred Müller, Stefan Schippers.

Items:

(1) Discussion centred on establishing an ADAS-EU subcontract with the Institut für Atom- und Molekülphysik to improve the quality of atomic physics modelling and data for fusion in the area of electron impact ionisation and dielectronic recombination with emphasis on highly ionised ions of heavy elements.

(2) Alfred described the experimental capabilities of his laboratory. In-house principal measurements to-date are performed on a cross-beam apparatus with a high current high precision, spatially scanning, electron beam implementing the animated beams method for absolute cross-section measurement. A high-resolution energy scan technique reveals the fine detail in the relative cross-sections which are then normalized to the absolute values. Typically 4k energy steps may be obtained in a 200eV sweep. The compact ECR, all permanent magnet, ion source can provide charge states of appropriate species up to <~ 25. The system is used for single and multiple ionization of a wide range of target ions. A second apparatus is in place which incorporates a gas cell and an exciting electron beam. This will give access to selected ion atom reactions as well as allowing some exploration of metastable fractions from the ECR source. The second main strand of experiments exploits merged electron and ion beams in the Heidelberg heavy ion storage ring cooler for radiative and dielectronic recombination cross-section measurements. Collaborative experiments in the past have also used Cryo-ring in Sweden, but this device is now no longer maintained.

(3) Alfred described some recent and current measurements. On ionization, recent results include ionization of Li^+, both ground and metastable, with very good agreement with CCC calculations. Also single ionization of highly ionized ions (uncertain which cases ~ $Ni^{+17?}$ or such like) which show disagreement with Pindzola/Loch CADW. The experimental results are ~ factor 2 larger, with the experimental data showing many resonance features below the excitation/autoionisation thresholds (REDA features probably) not included in CADW. Also new ionization cross-sections (including multiple ionization) of xenon and tin ions were described. Alfred notes stronger resonances sometimes in double ionization than in single ionization. Probably double ionization remains <~ 10% of single ionization, but he is unsure of picture with inner filled d- and f-shells. Many measurements of singly ionized ions (eg Sc^+, Mg^+). Many DR studies have been made, including some very detailed comparisons with precise theory (Lindroth) (eg Na^{+8}) with very good agreement. Alfred notes the well delineated DR resonances in most of the cases studied, but has some experience of dense (quasi-continuum) DR resonances in complex systems with quantitative measurement possible (cf Au^{+25} study in 1998). DR analysis requires consideration of field ionization in the cooler region. Alfred has participated in detailed studies of such high n-shell suppression which are essential for precise quantifying of DR cross-section measurements. Alfred has experience of the effect of crossed electric and magnetic fields on high n-shell resonance mixing, including the enhancement and suppression effects, which appear as only modest(<~10%) corrections for highly ionized systems.

(4) Hugh focussed discussion on four aspects of electron-ion collisions which are important for the on-going fusion program and for ITER as summarised and discussed in the following sections.

(5) A concern is the establishment of benchmark DR measurements for tungsten ions W^0 – W^{+25} and iso-electronically similar systems where discrepancies of the ADAS modelled ionisation state with fusion spectral observations are largest. High temperature DR is the concern, not the so-called low-temperature DR. It was noted that Autostructure calculations, as used now to produce adf09 files up to the M-shell, could not be continued in the same manner up to such tungsten ions. Rather ADAS would expect to use BBGP approximation and would seek to add parametric adjustment factors to low partial wave behaviour to match measurement benchmarks. Successful parametrisation would be endorsed by both Giessen staff and ADAS-EU staff and show regularity along iso-electronic sequences and between similar iso-nuclear systems. Mixing (and losses) by both fields and collisions of the doubly excited DR states could be addressed by ADAS

population models and the field effect comparison with observation would be a valuable check.

(6) On ionisation, Hugh pointed out that current and near future baseline impact ionisation data in the ADAS database (adf23 and adf07) would come from a scripted mass production variant of the Loch/Pindzola CADW approximation, based on promotion rules. Benchmarks for tungsten ions W^0 – W^{+25} and iso-electronically similar systems would again be essential for the lifting of the baseline. The demonstrated capability at Giessen would be very valuable for this. The REDA resonance issue and the discrepancies mentioned in (3) above were noted. Hugh felt that simple threshold adjustments of Burgess Cases 1 and 2 type for excitation/autoionisation had some relevance to the REDA issue. Again an agreed parametric prescription/adjustment of some universal applicability, satisfying both Giessen and ADAS-EU staff, would be a desirable outcome and a method of utilising the experimental benchmarks.

(7) The third item on the fusion agenda is multiple ionisation. Earlier remarks in Vienna by Alfred suggested that double ionisation could exceed single ionisation, reinforcing an anxiety from Hugh that multiple ionisation/shake-off/shake-down for complex, shallow filled, inner d- and f-shell systems should be examined. Contemplating the preliminary Giessen results for tin ions suggested that although resonances for two electron ionisation were sometimes larger than the single ionisation resonances, probably the total double ionisation cross-section remained <~15% of the single electron cross-section. The Giessen experimental set-up is well placed to check this for tungsten ions – which would be a worst possible case. Hugh pointed out that he expected to get some Auger/cascade calculations from Vilnius as part or ADAS-EU sub-contracting, but that experimental benchmarks would be most important.

(8) The final topic was field ionisation. Hugh noted the use of Stark mapping models for n-shell field ionisation in the DR measurements and expressed an interest in adapting some of this type of modelling to the hydrogen beam stopping case. Alfred directed attention to a Giessen review of this although others (such as Nikolic) had carried out the main computations for the DR work. Also Hugh noted the possibility of redistribution (by collisions or fields) in the BBGP DR computations. These points would be followed up at some stage, but were less critical than the principal cross-section measurements.

(9) Hugh outlined how he though an ADAS-EU sub-contract should function. Since it was required to be for support, it should principally provide a channel for the effective passage of Giessen experimental cross-sections and research into ADAS and thence on to impact and support diagnostics and fusion. Effective use of funds would be for the time of Giessen staff to work with ADAS-EU staff to make this interface work. It was realized that of course the on-going research and production mattered, but that ADAS-EU monies were insufficient and not so appropriate for that. Rather an effective ADAS-EU engagement would give leverage in application for DFG grants for beam time on the Heidelberg heavy ion storage ring. It was also felt that ADAS and ADAS-EU could help to foster interest in diploma students at Giessen by arranging working visits to the fusion laboratories and so on.

(10) Target ADAS data formats for upgrade and maintenance in the collaboration would be adf07, adf09 and adf23 with attention also to consequences for the derived data format adf11.

(11) Generally there was excellent enthusiasm from the Institut für Atom- und Molekülphysik for sub-contracting reflecting the above interests and Hugh was mandated to work-up the actual contract and its scientific content in interchange with Alfred.

HPS
12 June 2009

ADAS-EU CONTRACT

ELECTRON IMPACT CROSS-SECTION DATA FOR FUSION APPLICATIONS

IONISATION AND RECOMBINATION OF HEAVY ELEMENT IONS

H. P. Summers

1 July 2009

1. Summary
It is proposed to commission selected ionisation and recombination measurements and associated evaluations from Prof. Alfred Müller, University of Giessen, Germany. This reference quality sixth-period fundamental data will benchmark iso-nuclear and iso-electronic sequence data available in the ADAS database and guide further large scale production. It will extend the scope of collisional-radiative data and model support provided under the ADAS-EU Project to the European magnetic confinement fusion community The data, which supports deduction of the ionisation state of heavy species, will be interfaced to plasma transport models and to diagnostic spectral measurements on fusion devices at EURATOM Associated laboratories and ITER through tailored data formats within the Atomic Data and Analysis Structure, ADAS.

The work will make extensive use of the methods and measurement techniques developed by Prof. Müller, Prof. Schippers and co-workers. The ionisation cross-section measurements will be from the crossed-beams apparatus and ECR source at Giessen, combining animated-beams and high resolution energy-scan methods. The recombination cross-section measurements will focus on dielectronic recombination exploiting the merged beam method in the electron cooler of the Heidelberg heavy ion storage ring. The data will be organised and relayed from Giessen to ADAS with the assistance of ADAS-EU staff. Conversion to derived data formats through collisional-radiative modelling data will take place at UKAEA/JET Facility and University of Strathclyde. The fundamental and derived data in appropriate ADAS data format collections will be released after assessment and validation to the public domain via OPEN-ADAS [1].

The duration of the project will be eighteen months (Sept. 2009 - Jan. 2011) at a fixed price of €10,000.

2. Background
The strategy, originated at the JET Facility and now followed by fusion laboratories throughout the world participating in the ADAS Project, for the description of the radiation emission of impurity ions has been the establishment of an integrated atomic data and analysis structure (ADAS). ADAS seeks to provide at appropriate quality, all the derived data required for global modelling and quantitative spectroscopic diagnosis and analysis [2]. The fundamental and derived databases are centrally maintained and accessible by standard routines for modelling and diagnostic applications (eg. edge studies, core plasma, XUV spectroscopy). The effectiveness and precision in the applications depends on the quality and availability of fundamental data. In this context a specific need is enhanced provision for low ionisation stages of heavy elements up to and including tungsten. Such enhancement is a central theme of the ADAS-EU Euratom/Framework 7 Support Action. Recognizing the complexity of some of the fusion relevant heavy element ions and current bounds on atomic reaction computability, ADAS-EU policy falls into two parts. Firstly a modest number of high precision reference calculations and/or measurements at the front edge of current capability are sought. Secondly, as well as direct embedding of the associated precise data in the databases, the data should be exploited as fiducials which can suggest adjustments or global/regional scalings to the large scale semi-automated mass production calculations of the ADAS heavy element baseline. This 'lift of the baseline' is the central objective and the primary delivery.

One of the main sources of ionisation and recombination cross-section measurements of both low and high ionisation stage ions of heavy elements is the group of Prof. Müller. The group has focussed on ionisation and recombination (both radiative and dielectronic) cross-sections with special attention to the delineation of resonant structures and to absolute measurements [3]. The group has established and maintained very strong collaborations with theoretical groups who calculate electron impact ionisation and recombination [4]. This engagement has led to important clarifications, to calculation extensions and has pointed the way forward, for example in 'low temperature DR' [5], excitation-autoionisation, REDA [6] etc. The group has worked on many systems, including ions touching and adjacent to the present fusion interest [7, 8]. The approach of Prof. Müller is ideally suited for matching to and strengthening the ADAS atomic modelling system along the manner described in the first paragraph of this section. On dielectronic recombination, *inter alia*, the theoretical point of comparison includes the AUTOSTRUCTURE code (IPIR approximation) [9] and developments there from. It is noted that the large scale production of dielectronic recombination in ADAS uses the AUTOSTRUCTURE code. Similarly on ionisation, *inter alia*, the theoretical point of comparison includes the CADW code (configuration average distorted wave approximation) [10] as used by ADAS.

In the fusion domain, a principal concern is the behaviour of heavy element impurities – in particular tungsten – in the plasma environment. Tungsten inner wall components will be present at the locations of high thermal load in the divertor/strike-zones of ITER and so will be the subject of intensive study at current machines, such as JET and AUG in the preparations for ITER. From an atomic physics perspective, tungsten is particularly challenging for lower ionisation stages W^{+0} - W^{+25} with active inner and outer *d*- and *f*-shells. For dielectronic recombination, it is expected that the many resonant series will produce an unresolved quasi-continuum in the cross-section, a complexity compounded by possibly several metastable initial capturing ion states. State selective dielectronic coefficient calculations, such as those generated by AUTOSTRUCTURE (currently up to about Mg-like systems) must be abbreviated for the very complex systems above and experimental fiducials are required for this new territory. For electron impact ionisation of W^{+0} - W^{+25}, it is anticipated that excitation-auto-ionisation will dominate direct ionisation, however the completeness of the current CADW approach and its convergence towards experimental values as z increases is not yet demonstrated. There are experimental indications that REDA resonances may be substantial. Semi–empirical adjustments to ADAS baseline, large coverage, theoretical methods for such effects do need benchmarking. Also, in the relatively highly ionising plasma environment for an inflowing near neutral tungsten ion, multiple ionisation (as a correction to successive single ionisations) needs to be quantified.

The group of Prof. Müller has a demonstrated capability for experimental measurements which bear on the above issues and experience with similar systems to those of direct concern for fusion. This sub-contract provides an opportunity for benchmark measurements, choice of broad-coverage computational methods and guided use of global parametric scaling adjustments of data, to lift the quality of ADAS ionisation state modelling for such low to intermediate charge state heavy ions.

3. The proposed work

The work falls into four parts, namely dielectronic recombination cross-section measurements and analysis, ionisation cross-section measurements and analysis, assessment of calculations and definition of global/zonal, parametric (generally z-scaled) adjustments for recombination and ionisation.

(1) Selective dielectronic recombination cross-section measurements of 6th period element ions from ions W^{+0}-W^{+25} or isoelectronically equivalent adjacent element ions focussing on d- and f-shell (as inner and outer shells) parent transition contributions.

(2) Assessment and comparison of results in terms of Burgess-Bethe (BBGP) approximations. Identification/recommendation of global/zonal parametric adjustments.

(3) Selective ionisation cross-section measurements of 6th period element ions from ions W^{+0}-W^{+25} or isoelectronically equivalent adjacent element ions focussing on excitation-autoionisation and REDA resonances for active inner d- and f-shells. Measurements will include multiple ionisation cross-sections.

(4) Assessment and comparison of results in terms of distorted wave approximations and BBGP type adjustments for REDA. Identification/recommendation of global/zonal parametric adjustments.

Integration of data into ADAS will be executed by staff of the ADAS-EU, including incorporation of fiducials and adjustments into the key fundamental data formats adf09 and adf23 and re-processing for the derived data formats adf07 and adf11. ADAS-EU staff will pay working visits to Giessen to assist with execution of the above tasks as appropriate. A copy of ADAS software will be made available on a workstation at the Department of Physics, University of Giessen at no charge for local use.

4. The Financial Provision

The operations and calculations outlined in the previous section will be carried out over a period of eighteen months (Sept. 2009 - Jan. 2011). Financial provision is made as a contribution to the time allocated to the investigation by the senior investigators (Prof. Prof. Müller, Prof. Schippers) and their research staff. No travel funds or computation costs are sought.

Item		€
Univ. Giessen (fixed price)		10,000
	total	10,000

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ADAS-EU Travel Report

Location: Department of Chemistry, University Autonoma, Madrid, Spain.
Date: 09-10 June 2009.
ADAS-EU staff: Hugh Summers.
Persons visited: Luis Mendez, Luis Riera, Clara Illescas, Francesco Guzman

Items:

(1) Discussion centred on establishing an ADAS-EU subcontract with the Department of Chemistry to improve the quality of atomic physics modelling and data for fusion in the area of state selective charge transfer and ion impact collision processes for neutral hydrogen beams and thermal plasma.

(2) Luis Mendez gave an overview presentation of recent calculations and results relating to magnetic confinement fusion. This included studies targetting species of importance for charge exchange spectroscopy with fast (~40-80keV/amu) neutral hydrogen isotope beams. Classical (CTMC improved) and semi-classical (CCMO) calculations have been completed for H(1s) donor with Li^{+3} , B^{+5}, Ne^{+10} and Ar^{+18} receiver with preferred linking between energy ranges. This provides a comprehensive total, n- and nl- resolved data for CXS emission modelling. CTMC results were also described for H(2s) donor (B^{+5} and Ne^{+10}) and for Ar^{+16} receivers from H(1s). Quantal calculations involving partial stripped oxygen (O^{+2}) and nitrogen (N^{+2}) ions at lower near thermal energies and reactions between protons and Be^{+0} were summarised. Work is also in progress for ion collisions with light molecules and in extension of classical CTMC modelling to bi-electronic processes - especially neutral helium.

(3) Francesco Guzman presented first results of CXS analysis carried out at IPP Garching over the last four months with Costanza Maggi. The analysis considered CXS visible transitions in Ne^{+9}, Ar^{+17}, Ar^{+16} and Ar^{+15}. Also a B^{+4} CXS line was included. The recent data from UAM was incorporated in ADAS adf01 data sets and converted to adf12 effective emission coefficients. These were used in CHEAP analysis and contrasted with using the older ADAS data - especially the influence of unimproved CTMC. First preliminary results, supported by quantitative soft X-ray argon concentration determination are encouraging for the correctness of the revised, improved CTMC work. This is a different conclusion from the findings of Carine Giroud at JET. These developments are important steps in establishing and building confidence in CXS data in ADAS for heavier receiving ions and a strong encouragement for continuing close collaboration with UAM under ADAS-EU.

(4) Hugh Summers focussed discussion on four aspects of ions/atom collisions which are important for the on-going fusion program and for ITER as summarised and discussed in the following sections.

(5) Fast neutral beam CXS spectroscopy of individual impurity lines in the visible will continue to be a key diagnostic methodology. Hugh Summers pointed out the expectation that such methods would probably not extend much above residual- charge-state ions >~ 25, but that the many, low-intensity CXS emission, probably unidentified quasi-continuum would remain of concern as a background - confusing determination of weak signals such as slowing alpha particle CXS. He felt that interpolation and extrapolation of CTMC (improved for sub-dominant levels and single-microcanonical for dominant levels) based on scaled z-scaled quantities, normalized n-shell parametrisation and l-shell functional forms would probably be sufficient, but that that further results for example for z~25 and z~25 would add confidence and strengthen such handling. Francesco expressed anxiety about whether n-shell behaviour exhibited sufficient regularity, although Clara felt such scalability was already evident. Also Clara had already some CTMC data for Kr^{+36}. Z-scaling (of total cross-sections) has received recent attention at UAM and it was felt that optimising and choice of scaling form were appropriately part of the effective utilisation of additional individual calculations (such as Kr^{+36}) . Confidence was expressed in the high precision of the recent B^{+5} data and the desirability of revisiting the other light elements such as Be^{+4}, C^{+6} and O^{+8}. It was agreed that such on-going checking and lifting of the precision of the ADAS database was very desirable.

(6) Hugh Summers drew attention to the importance of beam hydrogen atom excitation and ionization data due to plasma impurity ion impact and pointed out that quantitative beam emission spectral analysis would be a key diagnostic approach in ITER. He also noted the complementarity to the charge exchange data, the preference to have both from the same calculations and the weakness of the ADAS databases for ion impact excitation. Luis

Mendez said that the UAM methods such as CTMC did equally well provide both charge exchange and target excitation, but that the latter were usually not tabulated. Some repetition of older calculations might be required to fill in but there was no problem in principle. Hugh Summers described also the finer detail of beam emission, the role of Stark states, directionality and nkm mixing and observed that although availability of isotropic total excitation cross-sections would be helpful, the more sophisticated approach was ultimately desirable and should be within the scope of reasonable extension of current (especially classical trajectory) methods. Luis Riera saw parallels with other calculations at UAM and this was felt an interesting topic for further thought.

(7) Hugh Summers described the handling of total charge transfer at thermal energies for transport modelling, adf11 datasets and the simplifications introduced by superstages. Luis Mendez was concerned about the low energy endothermic or exothermic character of the total CX cross-sections. Hugh Summers felt that at higher residual- charge-state ions, the capture to high n-shells, their high availability and the weak influence of the core meant that cross-sections would essentially be flat to all relevant lower energies. Attention should be focused on the shell boundary ions and to the near neutral heavy element ions. All agreed that the latter were problematic, but Luis Mendez felt that some simpler methods had relevance and that some input from UAM was possible.

(8) The last area was high quality charge exchange at thermal energies involving partially stripped light impurity ions in the edge/divertor for spectroscopy. It was noted that Costanze Maggi had worked on this for the carbon ions in the past and had made use of UAM data – incorporating them in the key adf04 files. Hugh Summers felt that although the direct influence of state selective charge exchange on the impurity line emission tended to be overwhelmed by electron collisions in the Maggi studies, it still affected the ionization state. Also, the current tendency to very low temperatures and higher densities in the divertor mean that CX and the hydrogen spatial shell overlaps with the emitting ion spatial shells become more favourable. It was felt that this area should not be neglected and that UAM had special strength in cross-section provision for it through their close-coupling molecular methods.

(9) Although lithium and sodium edge diagnostic beams were noted, it was felt that, at least for the present, this was in the special sphere of interest Ratko Janev, Josef Schweinzer and the Vienna group.

(10) Hugh Summers outlined how he though an ADAS-EU sub-contract should function. Since it was required to be for support, it should principally provide a channel for the effective passage of UAM cross-sections and research into ADAS and thence on to impact and support diagnostics and fusion. Effective use of funds would be for the time of UAM staff to work with ADAS-EU staff to make this interface work. It was realized that of course the on-going research and production mattered, but that ADAS-EU monies were insufficient and not so appropriate for that. Rather an effective ADAS-EU engagement would give leverage in application for national research grants. It was also felt that ADAS and ADAS-EU could help to foster interest in students at UAM by arranging working visits to the fusion laboratories and so on. The fact of Francesco joining the ADAS-EU staff meant that excellent engagement with UAM would be excellent.

(11) Target ADAS data formats for upgrade and maintenance in the collaboration would be adf01, adf02 and adf04 with attention also to consequences for the derived data formats adf11, adf12 and adf15.

(12) Generally there was excellent enthusiasm by UAM for sub-contracting reflecting the above interests and Hugh Summers was mandated to work-up the actual contract and its scientific content in interchange with Luis Mendez.

HPS
11 June 2009

ADAS-EU CONTRACT

CHARGE EXCHANGE AND ION IMPACT DATA FOR FUSION PLASMA SPECTROSCOPY

STATE-SELECTIVE CHARGE TRANSFER AND EXCITATION FOR LOW/MEDIUM CHARGE PROJECTILES AND NEUTRAL HYDROGEN TARGETS

H. P. Summers

30 July 2009

1. Summary

It is proposed to commission a set of charge transfer and associated target excitation and ionisation cross-section calculations from TCAM group [1] (Prof. Luis Méndez, Prof. Luis Errea, Dr. Clara Illescas, Dr. Ismanuel Rabadán and coworkers, Departamento de Química, Universidad Autónoma de Madrid, Spain). These high quality, fundamental state selective data for neutral hydrogen isotope targets and representative low - high mass, highly ionised projectiles will benchmark iso-nuclear and iso-electronic sequence interpolated and extrapolated data available in the ADAS database and guide further large scale production. It will extend the scope of collisional-radiative data and model support provided under the ADAS-EU Project to the European magnetic confinement fusion community The data, which supports charge exchange studies and spectral measurements with hydrogen, both in neutral beams and in thermal plasma, will be interfaced to spectral measurements on fusion devices at EURATOM Associated laboratories through tailored spectral line 'scripts' within the Atomic Data and Analysis Structure, ADAS.

The work will make extensive use of the methods and codes developed by Prof. Riera, Prof. Méndez, Prof. Errea and co-workers. The calculations will be performed at Universidad Autónoma de Madrid. The data will be organised and relayed from Madrid to ADAS in established ADAS data formats with the assistance of ADAS-EU staff. Conversion to spectrum line effective emission coefficients, stopping coefficients and similar derived data will take place at UKAEA/JET Facility and University of Strathclyde. The fundamental and derived data in appropriate ADAS data format collections will be released after assessment and validation to the public domain via OPEN-ADAS [2].

The duration of the project will be eighteen months (Sept. 2009 - Jan. 2011) at a fixed price of €10,000.

2. Background

The strategy, originated at the JET Facility and now followed by fusion laboratories throughout the world participating in the ADAS Project, for the description of the radiation emission of impurity ions has been the establishment of an integrated atomic data and analysis structure (ADAS). ADAS seeks to provide at appropriate quality, all the derived data required for global modelling and quantitative spectroscopic diagnosis and analysis [3]. The system is based on the initial preparation of collections of fundamental atomic data for specific ions typically including energy levels, transition probabilities and ion and/or electron impact coefficients. Various ADAS computer codes then prepare all the derived data such as net power loss coefficients, spectral line contribution functions etc. in a form directly usable in experimental analysis and in plasma models. The fundamental and derived databases are centrally maintained and accessible by standard routines for modelling and diagnostic applications (eg. edge studies, beam-penetrated plasma studies, visible and VUV spectroscopy). The effectiveness and precision in the applications depends on the quality and availability of fundamental data. In this context a specific need is enhanced provision of state selective charge transfer and excitation data for neutral hydrogen, present both in fast beams and in thermal plasma, in interaction with selected impurity species. Such enhancement is a central theme of the ADAS-EU Euratom/Framework 7 Support Action. Recognizing the complexity of handling some of the fusion relevant heavier element ions and current bounds on atomic reaction computability, ADAS-EU policy falls into two parts. Firstly a modest number of high precision reference calculations and/or measurements at the front edge of current capability are sought. Secondly, as well as direct embedding of the associated precise data in the databases, the data should be exploited as fiducials which can suggest adjustments or global/regional scalings to the large scale semi-automated mass production calculations of the ADAS medium-heavy element baseline. This 'lift of the baseline' is the central objective and the primary delivery.

One of the main sources of calculations of state selective ion impact cross-sections with neutral hydrogen targets is the group established by Prof. Riera. This group has steadily developed and systematised their methods which span from the low energy to high energy regimes and encompass a wide range of both fully ionised and partially ionised colliders. For the low energy regime, the group is a principal exponent of the close-coupled molecular orbital method capable of delivering benchmark quality calculations [4]. These benchmarks can include state-selective charge transfer cross-sections from neutral hydrogen to partially stripped ions of fusion relevant light elements such as carbon or oxygen [5] in the near edge thermal environment as well as total charge transfer. The group has also an wide experience in ion-molecule collisions; in particular, H^+ + H_2 collisions have been studied in several works (see [6] and references therein). The TCAM group has also applied the method at higher energies towards the range of neutral hydrogen heating beams for detailed comparisons with simpler high-energy-specific methods [7]. The group has special interest in developing and exploiting classical trajectory Monte Carlo methods, primarily applying to the high energy regime but extending towards lower energies through sophisticated microcanonical superpositions [8]. The group has worked on many systems, but has specialised recently on the requirements of charge exchange spectroscopy in magnetic confinement fusion. In particular, they have focussed on extended precision calculations for the light elements beryllium and boron as the fully stripped receivers Be^{+4} [9] and B^{+5} [10] as well as the important medium weight rare gas argon as a fully stripped Ar^{+18} and the partially stripped Ar^{+16} receivers [11]. The group has also extended the calculations to include the excited hydrogen, H(2s), as a donor to B^{+5} and Ne^{+10} [12]. The approach of the TCAM group is ideally suited for matching to and strengthening the ADAS atomic modelling system along the manner described in the first paragraph of this section.

In the fusion domain, charge transfer from neutral hydrogen isotopes is of importance near the plasma edge where ebullient thermal neutral hydrogen from the walls interacts with low ionisation stages of impurity elements. State selective charge transfer directly modifies the excited populations which emit observed spectrum lines as well as modifying the balance of ionisation state. Then in fast neutral beam penetrated plasma, plasma and impurity ion impact is the dominant process determining the beam stopping and the state of excitation of the beam atoms. Beam emission spectroscopy, that is analysis of the emission by the excited neutral beam atoms is a key diagnostic closely linked to and influenced by the motional Stark effect in magnetic confinement fusion. The charge transfer part of beam stopping to the plasma impurity ion colliders is the initiating mechanism of charge exchange spectroscopy - another central diagnostic. Neutral beams are usually of neutral hydrogen isotopes for plasma heating but may be specifically diagnostic beams and on occasions may be of neutral helium isotopes or of hydrogen with helium admixture. Both positive ion and negative ion beam sources are relevant to fusion and ITER. The ion-atom collision cross-section data (excitation, ionisation and charge transfer) requirements for these two diagnostic approaches are large since each requires sophisticated collisional-radiative population modelling and the characteristic energy ranges of each beam type in interaction with thermal plasma ion colliders must be spanned. In the experimental spectroscopic diagnostic analysis of the beams/plasma interaction zone, multichord visible spectroscopy is used – principally Stark resolved Balmer alpha for the beam emission and high transitions between sub-dominant levels for the charge exchange spectroscopy. The polarisation/directional characteristics of the beam emission is a key part of the beam emission diagnostic application.

The planning for ITER has focussed attention on heavier impurity elements such as argon and above as charge exchange spectroscopy emitters. This development has potentially important implications for transport studies since CXS from an ion succession such as Ar^{+18}, Ar^{+17} and Ar^{+16} may be observed spatially resolved along the beam-line. Although elements substantially heavier than argon produce a more grass-like CXS spectrum, weak and unsuited to conventional spectrum-line CXS, it has an implications for other planned measurements such as detection of slowing alpha particle emission against the (apparent) Bremsstrahlung continuum. Also it is noted that the cross-section database for impurity ion impact excitation of beam atoms is less complete and assured than that of charge exchange. These issues may be directly addressed by the particular capabilities of the TCAM group. In this respect, the use of both CTMC and one-centre close-coupling expansions is specially suited to be applied in collaboration with Prof. Bernard Pons (CELIA, Université de Bordeaux I, France). This sub-contract provides an opportunity, through selected ion studies, to lift the quality of ADAS ion impact cross-section database and thereby increase the precision and completeness of the charge exchange and beam emission application support.

3. The proposed work

The work addresses ion impact collision cross-section data in both in the higher energy fast neutral beam regime and in the low energy thermal plasma regime and falls into four parts, namely, improved CTMC calculations of nl-resolved CX data from fast hydrogen isotope beams and associated hydrogen target excitation data, examination and recommendation of global parametric forms for nl-resolved data interpolation and extrapolation, studies of low energy transfer from neutral hydrogen to partially stripped ionisation stages of light elements and recommendation of total charge exchange cross-sections for collisional-radiative modelling of ionisation state in thermal edge plasma.

(1) Extension of existing CTMC and improved CTMC calculations to include complete nl-selective charge exchange cross-section data from H(1s) targets and associated H(1s) target excitation to l-resolved levels with n≤4 in interaction with selected fully stripped projectiles up to Kr^{+36} at energies above 10keV/amu. The collision data will be assembled in ADAS adf01 format.

(2) Extension of CTMC calculations to evaluate nl-resolved charge exchange cross sections for collisions of selected ions with H(n=2).

(3) Assessment of global parametric fitting forms for total, n- and nl-resolved charge exchange data as a function of z for interpolation and extrapolation. Parametric forms will be optimised by fitting to the selected data of (1) above and used to provide an adf01 baseline for arbitrary charged projectiles for the fast hydrogen beam target and energy range.

(4) Incorporation of selected bench mark CCMO calculations for partially stripped light impurity ion in interaction with thermal neutral hydrogen in ADAS specific ion files of format adf04.

(5) Review and recommend total charge transfer approximations and rate coefficients for thermal neutral hydrogen donors in interaction with arbitrary low charge state (principally residual charge <4) thermal impurity ion receivers. The thermal ranges will correspond with the electron temperature range of significant fractional abundance of the impurity ions in fusion plasma. The data will be incorporated as CCD and PRC category data in the ADAS data format adf11 baseline.

Integration of data into ADAS will be executed by staff of the ADAS-EU, including the conversion to the key derived data format adf11, adf12, adf21 and adf22. ADAS-EU staff will pay working visits to Universidad Autónoma de Madrid to assist with execution of the above tasks as appropriate. A copy of ADAS software will be made available on a workstation at the Departamento de Química, Universidad Autónoma de Madrid at no charge for local use.

4. The Financial Provision

The operations and calculations outlined in the previous section will be carried out over a period of eighteen months (Sept. 2009 - Jan. 2011). Financial provision is made as a contribution to the time allocated to the investigation by the senior investigators (Luis Errea, Clara Illescas, Luis Méndez, and Ismanuel Rabadán) and their research staff. No travel funds or computation costs are sought.

Item		€
Universidad Autónoma de Madrid (fixed price)		10,000
	total	10,000

References

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