INDC International Nuclear Data Committee

Uncertainty Assessment and Benchmark Experiments for Atomic and Molecular Data for Fusion Applications

Summary Report of an IAEA Technical Meeting

IAEA Headquarters, Vienna, Austria

19-21 December 2016

Prepared by

Hyun-Kyung Chung and Bastiaan J. Braams,

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Abstract

The Technical Meeting on Uncertainty Assessment and Benchmark Experiments for Atomic and Molecular Data for Fusion Applications was held on 19 to 21 of December 2016 with 54 participants and IAEA staff from 20 countries and 1 international organization. The meeting with 41 presentations and 16 posters along with 3 technical discussion sessions was by far one of the largest meetings that the atomic and molecular data unit organized. The purpose of the meeting was to prioritize data needs for fusion applications, discuss experimental benchmarks and uncertainty quantification methods for atomic and molecular data, and promote a network of atomic and molecular physicists doing benchmark experiments and computations. Technical discussions led to proposals of benchmarking measurements taking into account the most recent developments in the experimental as well as theoretical areas and networking activities to reinvigorate experimental work to support atomic and molecular databases for plasma applications.

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1. Introduction

Computer simulations play a critical role in understanding physical and chemical systems. In the last decade verification, validation and uncertainty quantification (VVUQ) of computer simulations has become an important research topic in the physical and chemical sciences and engineering. In support of optimization-based design of a fusion reactor and high precision diagnostics of plasmas in fusion devices the IAEA Atomic and Molecular (A+M) Data Unit has been pursuing VVUQ activities for theoretical A+M data. Our objective is to encourage and support the data development community to provide data users with reasonable uncertainty estimates for calculated A+M data and especially for calculated cross sections. After a series of meetings and discussions with theoretical atomic physicists organized by the Unit it has become clear that the VVUQ methods for theoretical data should develop in collaboration with experimental physicists and benchmark experiments.

A Technical Meeting on "Uncertainty Assessment and Benchmark Experiments for Atomic and Molecular Data for Fusion Applications" was held on 19 to 21 of December 2016 with 54 participants and IAEA staff from 20 countries and an international organization ITER. Participating member states are Australia (1), Brazil (1), Canada (2), China (5), Czech Republic (1), France (2), Germany (4), Hungary (1), India (4), Japan (7), Jordan (1), South Korea (4), Poland (1), Portugal (1), Romania (1), Russia Federation (2), Spain (2), Sweden (1), UK (3), USA (7) and ITER (1). There were 41 scheduled presentations and 16 posters along with 3 technical discussion sessions.

The scientific advisory committee (SAC) of this meeting was formed to advise the Unit on the scope of meetings, recommendations of invited speakers and selection of contributed presentations. The SAC members are H.-K. Chung of IAEA (Scientific Secretary) and B. J. Braams of IAEA, K. R. Bartschat of Drake University, Des Moines, IA, USA, S. Buckman of Australian National University, Canberra, Australia, I. Murakami of National Institute for Fusion Science, Toki-City, Japan, D. R. Schultz of University of North Texas, TX, USA, J. Tennyson of University College London, UK, D. Reiter of Forschungszentrum Jülich, Germany and A. Wolf, Max Planck Institute for Nuclear Physics, Heidelberg, Germany. S. Buckman and D. R. Schultz could not attend the meeting due to schedule conflict. They recommended more than 55 possible speakers and finally 32 speakers were invited. There were 22 applications for contributed presentations and 2 applications with irrelevant topics were rejected.

The meeting was meant to advance data-oriented research on A+M processes and properties that are important for plasma simulations and plasma diagnostics for fusion energy development and other plasma applications. Leading theoretical and experimental A+M physicists were invited along with plasma physicists using A+M data to discuss uncertainty assessments and benchmark experiments for A+M data for fusion and other plasma applications. The discussion topics were as follows:

- Prioritization of A+M data needs for fusion applications.
- Experimental methods and systems to benchmark theoretical A+M collision data.
- Target uncertainties of A+M collision data for fusion applications.
- Uncertainty quantification methods for theoretical A+M data.
- Network of A+M physicists doing benchmark experiments and computations.

The meeting participants discussed the most important data needs for fusion applications, decided what can be done to benchmark those data and formulated a plan of action among experimental and theoretical A+M physicists to carry out this benchmarking and perform the associated uncertainty assessment. The discussions led to specific proposals for measurements to set new benchmarks for prioritized data. Along with the discussions about new benchmark experiments there were discussions and proposals about suitable theoretical methods to compute these data, and how and by whom this can be done.

This report contains the proceedings of the meeting, conclusions and future work. The list of participants is provided in Appendix 1 and the meeting agenda in Appendix 2. The abstracts of all presentations are also provided in Appendix 3.

2. Proceedings of the Meeting

Meera Venkatesh, the Director of the Division of Physical and Chemical Sciences (NAPC) and Arjan Koning, the Head of the Nuclear Data Section (NDS) welcomed participants and emphasized the role of the IAEA Nuclear Data Section and the A+M Data Unit in the field of fusion and data research. Particularly the area of nuclear data has actively developed the area of uncertainty quantification (UQ) of nuclear data and an interaction between the nuclear data community and the atomic and molecular data community will be synergistic in advancing UQ technology. Bas Braams, the outgoing Unit Head of the Atomic and Molecular Data Unit (AMU) described the meeting objectives.

The three day meeting proceeded with presentations of 20 minutes each organized in 10 sessions, one poster session on Monday afternoon and three technical discussion sessions.

There were 7 presentations in the first session chaired by B. Braams on the topic of **Atomic and Molecular Data Needs for Fusion Applications** by R. Barnsley of ITER on "Atomic and molecular data at ITER- status and prospects", D. Reiter of Forschungszentrum Juelich, Germany on "Molecular And PMI Database In Current Edge Plasma Transport Codes, And Forward Sensitivity Analysis", D. P. Stotler of Princeton Plasma Physics Laboratory, Princeton, NJ, USA on "Sensitivity of Tokamak Transport Modeling to Atomic Physics Data: Some Examples", T. Nakano of Naka Fusion Institute, National Institutes for Quantum and Radiological Science and Technology (QST), Japan on "Contribution of Quantitative Spectroscopy to Fusion Plasma Research", U. von Toussaint of Max Planck Institute for Plasma Physics, Garching, Germany on "Bayesian Approaches to Uncertainty Quantification in Plasma-wall Interaction Modelling", K. Fujii of Kyoto University, Kyoto, Japan on "Bayesian Inference for the LHD Experiment Data" and I. Zhang of Chinese Academy of Science, Hefei, China on "Application of Atomic Data to W Spectra on EAST Tokamak"

The second session chaired by C. Ballance on the topic of **Theoretical Molecular Collision Data** proceeded with 3 presentations by J. Tennyson from University College London, UK on "Uncertainty Quantification in Calculations of Molecular Processes", by B. K. Antony from Indian Institute of Technology (ISM), Dhanbad, India on "A Stepwise Procedure to Explore Uncertainty and Reliability in Theoretical Cross Section Data for Electron and Positron Scattering" and V. Kokoouline from University of Central Florida, Orlando, FL, USA on "Uncertainty Evaluation in Theoretical Calculations of Cross Sections for Electron-molecule Collisions".

The third session chaired by A. Müller on the topic of **Experimental Molecular Collision Data** proceeded with 3 presentations by G. García from Spanish National Research Council, Madrid, Spain on "Evaluated Electron and Positron-molecule Scattering Data for Modelling Particle Transport in the Energy Range 0-10000 eV", J. Fedor from Heyrovsky Institute, Czech Republic on "Dissociative Electron Attachment Cross Section in H_2 and D_2 at the 4 eV Resonance" and E. Krishnakumar from Tata Institute of Fundamental Research, Mumbai, India on "Recent Developments in Absolute Cross Section Measurements for Dissociative Electron Ionization of and Attachment to Molecules".

After three oral sessions, the first day finished with a technical discussion on "**Priorities of A&M Data for Fusion Applications**" chaired by D. Reiter and I. Murakami and a poster Session of 16 posters followed by a reception hosted by IAEA.

Posters were presented by A. A. Buchachenko from Skolkovo Institute of Technology Moscow, Russia on "Ab Initio Studies of the Collisions Involving Lanthanide Atoms and Ions", K.-B. Chai from Korea Atomic Energy Research Institute, Daejeon, Republic of Korea on "Plasma Emission Spectroscopy When There Is Magnetic Reconnection Associated with Rayleigh-Taylor Instability in

the Caltech Spheromak Jet Experiment", D. Darby-Lewis from University College London, UK on "R-Matrix Calculations of Electron Impact Electronic Excitation of BeH", J. Kaur from Indian School of Mines, Dhanbad, JH, India on "Electron Interactions With Plasma Reactive Carbon Tetrachloride Molecule: An Extensive Cross Section Study", J. Liu from Chinese Academy of Sciences, Hefei, China on "A+M Data Application in EAST Tokamak Edge Simulation of Impurity Seeding Plasma", I. F. Schneider from CNRS, Université du Havre, France on "Resonant Electron-Molecular Cation Collisions in the Edge Plasmas of Fusion Devices: New State-to-State Cross Sections and Rate Coefficients", J. M. Seminario from Texas A&M University, USA on "Towards the Simulation of Plasma Chemistries from Atomistic and Molecular First Principles Methods", S. Singh from Indian School of Mines, Dhanbad, JH, India on "Positron Scattering Cross Sections For Plasma Relevant Hydrocarbons", M.-Y. Song from National Fusion Research Institute, Daejeon, Republic of Korea on "Cross Sections for Electron Collisions with Acetylene", V. Stancalie from National Institute for Laser, Magurele-Ilfov, Romania on "Studies on the Electron-Correlation and Relativistic Effects in Target Representation and Low-Energy Collision Calculation", P. Verma from Indian School of Mines, Dhanbad, JH, India on "Electron Scattering By Silane". Four posters were presented by invited speakers, K. Fujii, D. Fursa, D. Stotler and M. Baustista, to complement their oral presentations.

The second day proceeded with four oral sessions and one technical discussion session. The first session chaired by T. Kirchner was on the topic of **Theoretical Atomic Collision Data** and presentations were given by K. R. Bartschat from Drake University, Des Moines, IA, USA on "Estimating Uncertainties of Theoretical Data for Electron Collisions with Atoms and Ions", O. Zatsarinny from the same institution "Benchmark Calculations for Electron Collisions", C. Ballance from Queen's University Belfast, UK on "The Integrated Propagation of Atomic Structure and Collisional Uncertainties Through to Plasma Diagnostics", J. Colgan from Los Alamos National Laboratory, NM, USA on "Theoretical Approaches to Electron-Impact Ionization" and D. Fursa from Curtin University, Australia on "Electron Scattering from Molecular Hydrogen".

The second session chaired by G. Garcia on the topic of **Experimental Atomic Collision Data** proceeded with presentations by A. Wolf from Max Planck Institute for Nuclear Physics, Heidelberg, Germany on "Storage-Ring Merged Beams Experiments on Electron Ion Recombination: Benchmarking and Accuracy Limits", M. Kitajima from Tokyo Institute of Technology, Japan on "High-resolution Measurements of Total Cross Section for Electron Scattering from Atoms and Molecules at Very-low-energy" A. Müller from Justus-Liebig-Universität Gießen, Germany on "Experimental Studies on Interactions of Atomic Ions with Single Electrons" and H. Tanuma from Tokyo Metropolitan University, Japan on "Atomic and Molecular Data Provided by Multiply Charged Ion Beam Collision Experiments at Low Energies".

The third session chaired by J. Colgan on the topic of **Theoretical Heavy Particle Collision Data** proceeded with presentations by L. Mendez from Autonomous University of Madrid (UAM), Madrid, Spain on "Numerical Calculation of Charge Exchange and Excitation Cross Sections for Plasma Diagnostics", I. Tolstikhina from Lebedev Physical Institute of RAS, Moscow, Russia on "Charge Exchange in Slow Collisions of Ions with Hydrogen Isotopes - Adiabatic Approach" and T. Kirchner from York University, Toronto, ON, Canada on "Basis Generator Method Calculations for Charge-Transfer Collisions Involving Few-Electron Systems".

The last oral session of the 2nd day was chaired by E. Krishnakumar on the topic of **Experimental Heavy Particle Collision Data**. Presentations were given by R. Ali from University of Jordan, Amman, Jordan on "Experimental Studies of the Energy Dependence of State-Selective Non-Dissociative Single Electron Capture in He^{2+} on H_2 Collisions", W. Wolff from Institute of Physics, Federal University of Rio de Janeiro, Brazil on "Multiple Ionization of Atoms and Molecules by Impact of Light -charged Ions at the Intermediate Energy Range" and P. M. Limão-Vieira from New University of Lisbon, Lisbon, Portugal on "Charge Transfer Processes in Atom-molecule Collision Experiments". They were followed by the technical discussion on the topic of **Benchmark of atomic, molecular, heavy particle collision theory and experiment** chaired by K. Bartschat and J. Tennyson

Three oral sessions and one technical discussion session were scheduled on the last day of the meeting. The first session chaired by T. Nakano on the topic of **Data Evaluation and Uncertainty Propagation** had 3 presentations by I. Murakami from National Institute for Fusion Science, Toki-City, Japan on "Evaluation on Atomic Data and Collisional-Radiative Models for Spectroscopic Diagnostics and Collaboration Network in Japan", M. Bautista from Western Michigan University, Kalamazoo, MI 49008, USA on "Uncertainties in Atomic Data and their Propagation" and A. G. Császár from Eötvös Loránd University, Hungary on "Uncertainty Quantification of Ideal-gas Thermochemical Functions".

The second session was chaired by D. Fursa on the topic of **Atomic Data Evaluation** and proceeded with presentations by G. W. F. Drake from University of Windsor, Canada on "Uncertainty Estimates for Atomic Structure Calculations", P. Jönsson from Malmö University, Sweden on "Assessing Uncertainties for Theoretical Atomic Data", N. Nakamura from University of Electro-Communications, Tokyo, Japan on "Observation and Identification of Tungsten Spectra Observed with an Electron Beam Ion Trap", R. Hutton, on "Benchmarking Visible Spectral Line Data", D.-H. Kwon from Korea Atomic Energy Research Institute, Daejeon, Republic of Korea on "Theoretical Electron Impact Ionization, Recombination, and Photon Emissivity Coefficient for Tungsten Ions" and Y. Yang from Fudan University, Shanghai, China on "KLL DR Resonant Strengths".

The last oral session was chaired by V. Kokoouline on the topic of **Molecular and Heavy Particle Data Evaluation** and proceeded with presentations by G. Karwasz from Nicolaus Copernicus University, Toruń, Poland on "Electron Scattering on Molecules: Partial Cross Sections", J.-S. Yoon from National Fusion Research Institute, Daejeon, Republic of Korea on "Data Evaluation of Helium and its Isotopes" and A. M. Imai from Kyoto University, Japan on "First Step Benchmark of Inelastic Collision Cross Sections" and was followed by a special talk of U. von Toussaint from Max Planck Institute for Plasma Physics, Garching, Germany on "Uncertainty Quantification".

The last technical discussion on the topic of **A&M Experimentalist Network** was chaired by A. Wolf, E. Krishnakumar and A. Müller. H. Chung of IAEA opened the technical discussion session with a presentation on "IAEA Evaluation Activities". After the technical session, the meeting concluded.

Abstracts of presentations and posters of participants are found in the Appendix 3. Presentations are available at the Unit's website at https://www-amdis.iaea.org/meetings/DataExchange2016/.

3. Technical Discussions

Discussions of three technical sessions are summarized here by Chairs and meeting participants.

3.1. Priorities of A&M Data for Fusion Applications

D. Reiter and I. Murakami

In this first discussion session, atomic and molecular (A&M) data required for current and future fusion machines were discussed, guided by the plasma conditions and spectroscopic equipment expected in ITER and beyond. A distinction is made between A&M data needs for the boundary plasma (near solid surfaces) and for the core plasma, because of the quite different energy ranges for relevant collision data. In the former domain also plasma chemistry aspects (molecules and their ions) are relevant, while for the latter domain data needs are defined by (hot) plasma spectroscopy, with all chemical bonds broken, and mostly involving nearly fully stripped ions.

Background and general remarks:

Atomic and Molecular data needs for controlled nuclear fusion research have been formulated since the eighties of the last century and have triggered a wide range of significant efforts in the A&M community. These data needs have been and continue to be driven either by (fusion) plasma spectroscopy or by plasma edge physics (boundary plasmas near the walls of the plasma chamber. In the latter significant fractions of neutral atomic and even molecular components coexist and are strongly coupled to the powerful fusion plasma flows (electrons, ions). Atomic and molecular species and collision processes and energy ranges relevant for fusion are quite different in boundary and core plasma regions.

Common to both is that: strong needs exist for large amounts of atomic and molecular data, new and refined spectroscopic instruments challenge the availability and quality of existing data sets, and the number of data users in fusion is increasing, not least due to the ongoing ITER construction and forthcoming exploitation.

In the past decades the data needs (existence of data) have been most pressing and most frequently been discussed and revisited. Due to the (still ongoing) large and successful efforts and the progress made, the enhanced powerful computational, experimental and theoretical capabilities in the A&M community, this is now, at least partially, often replaced by the need to select amongst the data (data evaluation). The present data selection process in fusion is inefficient, because each fusion scientist makes his own choices, driven by criteria such as convenience, availability of a nearby expert, or else. Comparing to (here even copying statements from) the similar situation in the solar spectroscopy community prior to the CHIANTI project (E. Landi, 2013) this inefficiency results from:

A: selection: fusion scientists typically are not atomic physics experts. And there is a disconnection between fusion and atomic physics communities.
B: implementation: this is very time consuming, software duplication
C: results: comparison between results from different authors also depends on the atomic data used.

Also the same general consequences as in solar spectroscopy (and plasma chemistry) can be drawn for A&M data bases in fusion science:

Apart from obvious requirements such as exactness, completeness, evaluation, referencing, etc., in particular the international character of the ITER project and fusion research in general requires the data to be: publicly exposed, as unprocessed as possible, complete transparency to the end user, compactness and free availability. The IAEA A&M data unit is seen to be in a key position to further establish and provide such A&M data frameworks for the worldwide collaborative fusion projects.

1.   Boundary plasma

Plasmas in the boundary region of fusion devices have densities of electrons, protons, hydrogen atoms, and hydrogen molecules up to the 10^{19} to several 10^{20} m^{-3} range and densities of helium and helium ions of (less than) 10 % of that plasma density, with collision energies in the 0.5-200 eV range. The terms hydrogen and proton are used here synonymously to mean all hydrogen isotopes and all hydrogen molecule isotopomeres. In the envisaged 500 MW fusion power burning plasma scenario at ITER the plasma itself will consist mainly of a near 50-50 % mix of D and T. Typical characteristic dimensions and plasma gradient lengths in the boundary are in the 1 to 100 cm range. The relevant collision processes of electrons, protons, and helium ions with hydrogen molecules, hydrocarbons, beryllium hydrides, nitrogen (atomic and molecular), and noble gases (neutrals and all ionization stages) are to be considered. Noble gases, especially xenon and krypton, but also argon and neon are used as cooling gas as well as tracer for diagnostics, both in current fusion experiments and in ITER and maybe in DEMO. Molecules are expected to be formed at surfaces of plasma exposed walls, and probably to a much lesser extend by associative processes also in the plasma volume. As wall materials, W, Fe (stainless steel), Be (ITER, JET) are most relevant, and also C (in the largest current and future experiments W7X (start in 2015) and JT60-SA (start in 2019)) continues to be used. In

addition to those, liquid metals of Li, Ga and Sn are examined currently as relevant candidate materials in fusion reactors. By surface erosion processes these elements and their ions also are present as plasma components. From these walls hydrocarbons and various other molecules may penetrate the boundary plasmas and also the vacuum (pumping) system.

Formation and destruction channels of HeH^+, BeH, BeH_2, BeH^+ still need to be clarified. Experimental measurements in tokamaks for CH, CH_2, BeH, BeH_2, lines etc. have been performed, but interpretation of these results (e.g. leading to quantification of surface erosion rates, aka "source term spectroscopy") requires knowledge of the full (catabolic) collisional reaction chain (and transport) in boundary plasma relevant temperature and density conditions. Data on rotational and vibrational state resolved collision processes of many of the relevant molecules, notably also hydrocarbons, are either not available or not well prepared for fusion applications and are necessary for further enhancing quantitative spectroscopic access to the plasma. Branching ratios for the various excited product states (i.e. final state resolved cross section information) need to be improved, or be made available to fusion scientists.

For hydrogen molecules, many collision data are available now but with large uncertainties still in particular for processes involving the excited states of H_2. It appears that existing H_2 data are not well implemented in fusion modeling, although there are extensive efforts on plasma modeling and collisional-radiative models with H_2 being carried out by various other, often low temperature plasma physics applications outside fusion research. The challenge in fusion is due to the strong coupling with complex plasma transport phenomena, to identify sufficiently reduced but still accurate underlying plasma chemistry sub-models (data condensation) before implementation into physically complex and high dimensional plasma transport models.

Information on plasma and gas surface interaction is also important for peripheral (technical, low temperature) plasmas used in fusion, such as plasma sources to produce hydrogen beams based on negative ion sources. Also here, as in the boundary plasma itself, the relative role of volume or surface processes in formation of particular molecules (or molecular ions) still needs further clarification. For the fusion plasma flame itself, there have been discussions during the meeting whether tungsten molecular compounds such as tungsten hydrides and tungsten oxides are formed or not, and if yes: how they are formed. Chemistry on wall surfaces depends on surface conditions. Fusion plasma experiments typically do not have clean surfaces, and these surfaces are difficult to characterize and to model. In particular estimates on wall erosion rates for all relevant wall materials needed to be refined. A mass spectrometer for molecule gas analysis near the boundary is planned to be installed in JET and installation of an erosion monitor is planned in ITER.

2. Core plasma

For core plasmas, the plasma-thermal (up to 20 keV temperature) range is relevant, but also collision energies up to 1 MeV are to be considered for electron, proton collisions with plasma heating beams and their charge exchange and ionization products. Even higher energies (up to 3.5 MeV) are relevant for collisions involving the fusion product He^{2+}, e.g. with electrons, impurities (W ions up to charge state around 55) and tracers for diagnostics. Within the neutral hydrogen particle beams (energies in 100-1000 keV range) collisions with the thermal plasma constituents from the hot core to colder boundary plasma, are to be considered, for quantification of beam attenuation, beam emission, and charge exchange recombination spectroscopy. Notably also accounting is needed for the motional Stark effects caused by the fast (up to 1 MeV) beam particles crossing the strong plasma confining magnetic field (5-10 Tesla).

Behavior of tungsten impurities, across the boundary plasma and deep into the core plasma (transport, intermixed with local ionization-recombination balances) is a big concern for the overall fusion plasma performance (fusion power), due to related fuel dilution and radiation losses. Ionization / recombination and radiation rates as well as charge exchange recombination (with H atoms from beams) should be obtained and evaluated (uncertainty quantification) for all relevant ionization stages, likely from neutral (Z=0) up to Z=55 - 60.

Background magnetic (mostly external) and electric (mostly micro) fields may affect collision cross sections. It has been reported during the meeting that recombination rate coefficients for low charged ions can be enhanced by electric fields by as much as a factor 50, under certain conditions.

For the purpose of spectroscopic diagnostics, the same criteria apply as those in other fields with plasma chemistry and plasma spectroscopy applications, see above (background). Detailed spectroscopy needs to identify specific important transitions with highest sensitivity to plasma parameters, otherwise huge databases would be needed, which are neither convenient nor easily usable. On the other hand, estimation of radiation power better than at the present approximate level of accuracy needs all transitions and construction of convenient and flexible collisional-radiative model tools.

The tolerable degree of condensation ("charge state bundling, or "QSS approximation for meta-stables) in effective (reduced) rates coefficients from collisional radiative models is highly case dependent (plasma conditions, plasma size, gradient scale length), and also has to be discussed with reference to transport time scales competing with the collisional time scales, on case by case basis.

Accuracy of basic atomic and molecular data should be known. Uncertainties of atomic data propagate in models and spectroscopic applications, so sensitivity analysis and uncertainty propagation from A&M data in models is a quite important challenge and a field at its infancy in fusion science. Currently, in fusion applications of A&M data, uncertainty estimates depend on human judgements, i.e. often experimentalist and individual modelers' intuition. This should, wherever possible, be replaced by more rigorous and quantitative strategies as they are for example well established in the case of nuclear data applications. Again: the IAEA data unit, being part of the IAEA nuclear data section, is probably in a very good situation and may take a key role to initiate and guide this process.

A starting point may already be the uncertainty propagation from raw A&M data into effective (collisional radiative) rate coefficients, for which systematic approaches are well established and in place in other areas of atomic data applications, outside fusion research

3.2. Benchmark of Atomic, Molecular, and Heavy-Particle Collision Theory and Experiment

K. Bartschat and J. Tennyson, I. Schneider, T. Kirchner

The summary below is separated into sections for electron collisions with atomic ions, atomic neutrals, molecular ions, molecular neutrals, and finally heavy-particle impact. As a general observation, it was pointed out that all experiments, in which light is observed, can be affected by cascades that are not easy to disentangle from the direct excitation cross section – should this actually be required. Also, optical emission data are difficult to bring onto an absolute scale for the underlying cross sections.

1. Electron Collisions with Atomic Ions

First, it is important to identify key systems. It was pointed out that advanced theoretical methods such as convergent close-coupling (CCC) and R-matrix with pseudo-states (RMPS) seem to be able to handle the most important processes involving targets with 12 (i.e., Mg-like) or less electrons, possibly with the exception of inner-shell excitation and ionization. In this context, it was noted that Carbon is used in the W7-X stellarator at Greifswald (Germany).

In general, targets with closed (sub) shells are more frequently used for diagnostics. When the ions are highly charged, e.g. Ni-like W or Xe^{24+}, distorted-wave theories should be able to handle the collision part, since the Coulomb interaction with the nucleus will generally dominate the electron-electron correlations and channel-coupling effects that require more sophisticated theoretical

approaches. Nevertheless, challenges remain, since resonances may interfere with the direct processes and the number of transitions, for which data are required, may be very large. The Giessen group has measured electron-impact ionization cross sections for Zn-like Xe^{24+} ions using their electron-ion crossed-beams setup and found strong contributions of resonant processes which are not included in distorted-wave approaches. It was also noted that the ADAS database contains configuration-averaged data.

Regarding Dielectronic Recombination (DR), the Giessen/Heidelberg group has provided a number of experimental datasets. It would be nice to have more, but there are several organizational issues that need to be accounted for. To begin with, the Heidelberg TSR storage ring has been de-commissioned and the the GSI storage ring (ESR) is currently unavailable for measurements due to ongoing reconstruction. At ESR, even when it becomes available, the competition for beamtime will be high. The experiments are expensive, and it would be necessary to make a very strong scientific case for the scientific interest of such measurements. While those data are certainly desirable to benchmark theoretical efforts (the actual target is not particularly important), making this case will be a serious challenge for our community. Regarding ions in very high charge states, there may be some hope (still with a timeframe of 2-3 years) for measurements with the Cryring at GSI that was brought from Stockholm to Germany. DR experiments are also planned in Lanzhou (China), possibly in 2018. Chances are that they will involve relatively light ions with low charge – not yet tungsten. There is also the cryogenic storage ring CSR in Heidelberg. Here, DR measurements for complex atomic ions in low charge states can be envisaged from about 2018 on.

Another possibility for data is experiments using Electron Beam Ion Traps (EBITs). One can observe lines with high precision, which could be used to check atomic structure calculations. Note that care has to be taken in processing the raw data, which are generally convoluted. It is hard to measure absolute rate coefficients, but the ionization balance can be determined.

2. Electron Collisions with Neutral Atoms

Neutral targets are clearly less important for the fusion community than ions, even though they might occur at the edges of the divertor. Nevertheless, they are an excellent testing ground for advanced collision theories. One system of significant interest is electron-impact excitation of xenon in the 10 eV – 100 eV incident-energy range, which is currently under investigation in Fedor's group at Prague. [This is the setup originally developed in Fribourg (Switzerland) by Allan.]

It was noted that neutral tungsten may enter an area of high temperature and develop from there into various charge states (W^+, W^{2+}, ...). Some spectroscopy work is going on in France. Overall, near-neutral tungsten targets seem to be too much of a challenge for current theories, and this rather unsatisfactory situation is not helped by the fact that the available experimental data are very limited as well.

3. Electron Collisions with Molecular Ions

Storage ring experiments have left a rich legacy of data particularly on dissociative recombination (DR). The first generation facilities (3 in Europe, 1 in Japan) have now all closed, but new ones, such as CSR in Heidelberg, have become operational. Storage ring experiments give benchmark quality measurements of DR from the vibrational ground state (v=0) of (mainly asymmetric) molecular ions. Data are available on fusion-relevant species such as HD^+, CH^+ and HeH^+. The situation with N_2^+ is less satisfactory due to problems with cooling symmetric species. NH^+, which is also astrophysically relevant, has not been studied experimentally. There has been significant work on the theory of electron/molecular cation collisions. Theory is necessary to extend studies to excited vibrational states

and triterated species. DR of BeH$^+$ has been extensively studied theoretically, and detailed extensions to its isotopomers are ongoing.

There are less data on electronic and vibrational excitation or impact dissociation. These processes are in principle accessible experimentally, albeit with more difficulty, and from theory. The theory is continuing to be developed in Le Havre and elsewhere. One of the biggest challenges for it is the prediction of the branching ratios, badly missed by the modelers. It appears that CH$^+$ would provide a good system for benchmarking theory and providing uncertainty quantification. It is a few (six) electron system for which good experimental data are available (and new data may be provided by CSR); it is also an astrophysically important species.

4. Electron Collisions with Neutral Molecules

Many processes are important for electron collisions with neutral species not all of which can be treated using a single, unified theoretical model. For example different methods are generally used to treat electron impact vibration excitation depending on whether the process is driven by a resonance or is non-resonant.

Recent theoretical CCC calculations of electron collision with H$_2$ performed at Curtin University show excellent convergence and, unusual in this field so far, include estimated uncertainties. There remain some issues with the effects of narrow Feshbach resonances at 14 eV, and the CCC model would need to include nuclear motion to allow for the treatment of all processes. This treatment will allow for isotope effects due to H, D or T to be included in the calculations. Although these results for H$_2$ (will) provide a benchmark, the methods used to obtain them are not generally applicable to electron-molecule collisions. There is also a need for a benchmark system that has a greater number of electrons.

For other systems the situation is less satisfactory. Electron-impact dissociation cross-sections are poorly determined from both theory and experiment. The processes generally go via electronic excitation. Similarly, while accurate total ionization cross sections are reasonably straightforward to compute using the BEB method or other semi-empirical procedures, dissociative ionization cross sections are more difficult to obtain. All these processes are very important for fusion applications. There are a diminishing number of groups performing electron collision studies for molecules important for fusion. (There is a larger emphasis on collisions with biological molecules.)

There is a need for a benchmark system with uncertainty-quantified theoretical calculations of electrons collisions for all processes occurring up to the ionization threshold. Ideally this study will involve more than one theoretical group using different methodologies. Electron collisions with N$_2$ would appear to be an appropriate candidate system, as a molecule that is important for both fusion and atmospheric studies. N$_2$ is a 14-electron system diatomic system, which means that both electron collision and nuclear motion studies should be treatable.

5. Heavy-Particle Collisions

The most important heavy-particle collision systems for fusion plasma applications involve neutral atomic hydrogen (H, D, T) and multiply-charged (impurity) ions, and the main process of interest is charge exchange (electron transfer).

At low energies (100 eV or less) charge exchange cross sections are deemed to be small, unless there is an accidental resonance. If the initial state is an excited state the cross section will be larger, but the population of excited states decreases with increasing principal quantum number. Nevertheless, there may be some interest in charge exchange cross sections for excited initial states (e.g. for reactions of

helium with metastables), since mostly scaling laws whose accuracy is not clear are used for modelling purposes.

Diagnostic neutral beams on the other hand have energies around 100 keV, and data for charge exchange to basically anything in the plasma (including carbon and tungsten ions) are deemed very important. It was noted that in addition to ground-state hydrogen one should also consider charge exchange from excited states in this context, since one cannot assume the diagnostic beam atoms to always remain in the ground state.

Benchmark measurements would be desirable, but are probably not feasible for excited hydrogen.
For theory, consideration of excited initial states is challenging, since electron transfer occurs into ion shells with high principal quantum numbers and hence large sets of basis states have to be included in close-coupling expansions. Classical trajectory Monte-Carlo calculations are easier to carry out, but may lack predictive power.

The importance of collisions involving (fast) alpha particles was noted. Not much is known about the energy loss of the alpha particles and the transitions they excite in ions, since these processes are difficult to measure. Likewise, charge exchange from neutral lithium was mentioned as another important problem.

Moving from atoms to molecules, collisions of protons (as well as deuterons and tritons) with hydrogen and beryllium-hydride molecules at very low energies (below 5 eV) are of some interest, e.g. in the context of beryllium-hydride formation. If the molecule is vibrationally excited resonance transitions can occur but adequate, first-principle calculations would be very challenging.

3.3 Atomic and Molecular Experimentalist Network

A. Wolf, E. Krishnakumar, A. Müller

1. Data requirement summary and the role of experiments

In fusion devices different atomic and molecular processes are important depending on the plasma region considered. Low-charged ions and some small molecules are most relevant in the edge and divertor plasma regions, while highly charged ions, also of heavier elements occurring as impurities or injected as probe substances, are important in the core plasma.

It is of interest to predict abundances and excitation states for the atomic and molecular, ionized and neutral components of the fusion environment. The important processes are ionization, recombination, excitation, elastic scattering with momentum transfer, dissociation, molecular reactions and also surface reactions; for diagnostics applications, line-emission data are needed.

Reliable predictions require in particular the knowledge of reaction rate constants, including unimolecular processes. They are in general obtained from theoretical calculations or, sometimes, estimations. The role of experiment is twofold: first, to verify or to challenge theoretical predictions by direct measurements of rate constants under well-defined conditions; second, to verify primary assumptions and methods of the many-body quantum calculations underlying these predictions. The sound understanding of quantum processes in the many-body domain is the prerequisite of any reliable data base on atomic and molecular processes.

2. A&M experimental research

The experimental studies most applicable to the fusion environment are those where the quantum systems are interrogated in a state closely representing this environment. Thus, the A&M experimental

research discussed here in the first place concerns what may be termed "real-world quantum systems". A&M research on these systems, also considering the fusion-related data requirements, is significantly distinct from other research lines of present atomic, molecular, and optical (AMO) physics, such as ultra-cold quantum systems, ultra-high-precision and fundamental-symmetry studies, and quantum computation. As for the A&M experimental research on real-world quantum systems, in the focus of this meeting, important activities exist world-wide and involve many excellent research groups. Interaction between them is at a good level and at present mainly assured by well-established international conference series such as ICPEAC (Int. Conf. on Photonic, Electronic and Atomic Collisions) and HCI (Int. Conf. on the Physics of Highly Charged Ions). The research groups have a treasure of powerful laboratory facilities available to them, which are widely distributed geographically.

The present IAEA meeting successfully brought together representatives from a good part of these A&M experimental research groups, as well as representatives of theoretical A&M research and the nuclear-fusion community. It is acknowledged that this wide scope, in particular, enabled fruitful discussions of the research needs and allowed to define priorities for experimental studies. The agreed opinion was that research leading to wider and more reliable knowledge on A&M processes will be of great importance for a better understanding of the fusion plasma environment.

3. Experimental research priorities

The following processes were identified as particularly interesting for benchmark experiments. In general, they concern areas where theoretical predictions are still uncertain considering the complexity of the systems, but experimental benchmarking will allow stepwise improvement of the theoretical approaches.

Electron collisions with neutral systems.
This in particular concerns excitation and ionization of atoms heavier than Mg, as well as the dissociative electron attachment (DEA) to small molecules, being an important molecular destruction process.

Electron collisions with complex ions.
Here, fruitful theory–experiment interaction was demonstrated recently for dielectronic recombination (DR) of W ions in charge states with an approximately half-filled 4f shell. It was pointed out that further studies with less (<4) electrons or vacancies in the 4f shell are desirable. Considered very interesting for experimental benchmarking are also electron-impact ionization for complex ions and electron-impact excitation, in particular to metastable ionic states.

Charge-exchange reactions of multiply charged ions.
Sensitive, recently improved methods are available for experiments on these processes. Regarding the fusion environment, they should focus on the interaction with H atoms for a wide range of complex ions, including multiply charged W, Mo and Xe.

It is emphasized that level lifetime measurements in multiply charged ions (including forbidden transitions) should be further pursued. They allow sensitive tests of the atomic structure calculations underlying spectral line predictions.

Ion and neutral collisions with surfaces and surface-adsorbed species.
This is a rich and diverse field of activity. Of importance in the context of fusion are data on ion – surface collisions and neutral collisions with specific adsorbed species on surfaces.

This list is not considered complete and can grow in future expert-group activities, as further addressed below.

AMO physics has advanced to allow very sensitive benchmark tests of theoretical calculations to be performed for collisional processes and for transient states in complex atoms, molecules and ions. Among these advances and emerging tools are, e.g., (e,2e) experiments detecting the complete kinematics and angular correlations of outgoing particles in individual collision processes, and recent attosecond time-dependent studies on doubly excited states. Both techniques address in particular the electron correlation the treatment of which is notoriously difficult in many-particle atomic calculations. Another research area with potential benefit for fusion-related processes is that of intense laser-matter interactions. As a further example it was pointed out that the understanding of electric and magnetic field effects could profit from spectroscopic work on laser-cooled atoms.

By disentangling basic quantum processes and validating theoretical approaches of many-body atomic calculation, these more fundamental AMO studies can also bring great benefit to understanding the fusion environment. Studies of this type do not necessarily have to be carried out on systems present in the fusion plasma inventory. Methodical aspects of this theoretical model validation by experimental benchmarking need to be further considered and worked out. Some recent activities of IAEA and ITAMP workshops can be considered as first steps towards recognizing these research opportunities and it appears attractive to push this discussion further.

4. Identification of research groups

IAEA can play a strong role in organizing fruitful interactions of theoretical and experimental research groups to realize work along these lines. It was generally acknowledged that among the attendants of the present meeting, a nucleus for an expert group on A&M experimental data could be formed. With a world-wide scope, this A&M experimental network should identify goals of specific experimental work including a wide range of laboratories, and work together with theoretical as well as fusion-plasma related research groups.

The discussions indicated that an international framework (of various possible ones) could be an EU-funded (but world-wide active) expert group on A&M physics research for fusion applications. The present engineering phase of ITER, requiring cost-intensive components to be realized, may also offer a background (financial and/or organizational) for the expert group.

As a desirable next step to strengthen A&M experimental activities related to the fusion environment, a widely visible review publication was mentioned that would explain the research situation and future needs. It should address the AMO community and also identify fundamental questions in many-body physics where emerging AMO research tools (such as multi-coincidence, kinematically complete collision detection, attosecond laser interaction and, possibly, ultracold gases) can be used for model validation in fusion-related atomic theory. Which fundamental questions in many-particle quantum physics can help to make large-scale atomic theory calculations realistic and reliable for unsolved cases entering models of the fusion environment?

A suitable composition of the expert group was identified as experimentalists, atomic theorists, fusion-oriented data users, plasma experimentalists, and data-base and data-assessment managers (data curation and evaluation). A web site organized by the IAEA could point out which groups can provide which expertise and experimental facilities to resolve issues relevant to fusion-oriented research and development.

4. Conclusions

This technical meeting was one of the largest meetings that the Unit has organized in its 30 year history. It brought together experts from atomic and molecular data-producing communities and fusion data user communities. It was highly successful for experts with diverse backgrounds to interact with each other and learn from other communities. Fusion scientists had a chance to examine the sources of data used in their fusion research, learned the complexity of validating data and appreciated the opportunity to interact with data producers. Atomic and molecular physicists learned the priorities of data needs in fusion research and get ideas of data to be explored, and investigate the ways to improve and benchmark data as well as to find benchmark systems critical to fusion research. During and after the meeting, participants recommended that the similar events should be organized regularly.

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Uncertainty Assessment and Benchmark Experiments for Atomic and Molecular Data for Fusion Applications

19-21 December 2016, IAEA Headquarters, Vienna, Austria

Meeting Agenda

Monday, 19 December

09:00   Registration (IAEA Registration Desk, Gate 1)

09:30   Welcome address by Director Meera Venkatesh, Section Head Arjan Koning

Meeting Objectives by B. Braams

Atomic and Molecular Data Needs for Fusion Applications (Chair: B. Braams)

09:50   R. Barnsley, ITER Organization;

10:10   D. Reiter, Atomic, Molecular and PMI Database In Current Edge Plasma Transport Codes, And Forward Sensitivity Analysis

10:30   D. P. Stotler, Sensitivity of Tokamak Transport Modelling to Atomic Physics Data: Some Examples

10:50   T. Nakano, Contribution of quantitative spectroscopy to fusion plasma research

11:10   Coffee Break

11:30   U. von Toussaint, Bayesian Approaches to Uncertainty Quantification in plasma-wall interaction modelling

11:50   K. Fujii, Bayesian Inference for the LHD Experiment Data

12:10   I. Zhang, Application of atomic data to W spectra on EAST tokamak

12:30 Lunch

Theoretical Molecular Collision Data (Chair: C. Ballance)

13:50   J. Tennyson, Uncertainty quantification in calculations of molecular processes

14:10   B. K. Antony, A Stepwise Procedure to Explore Uncertainty and Reliability in Theoretical Cross Section Data for Electron and Positron Scattering

14:30   V. Kokoouline, Uncertainty evaluation in theoretical calculations of cross sections for electron-molecule collisions

14:50   Coffee Break

Experimental Molecular Collision Data (Chair: A. Müller)

15:10   G. García, Evaluated electron and positron-molecule scattering data for modelling particle transport in the energy range 0-10000 eV

15:30   J. Fedor, Dissociative electron attachment cross section in H2 and D2 at the 4 eV resonance

15:50   E. Krishnakumar, Recent developments in absolute cross section measurements for dissociative electron ionization of and attachment to molecules

16:10   **Priorities of A&M Data for Fusion Applications (Chair: D. Reiter, I. Murakami)**

Poster Session

16:50   Poster Session

17:30   Reception / Poster Session

Tuesday, 20 December

Theoretical Atomic Collision Data (Chair: T. Kirchner)

09:00   K. R. Bartschat, Estimating Uncertainties of Theoretical Data for Electron Collisions with Atoms and Ions

09:20   D. Fursa, Electron scattering from molecular hydrogen

09:40   C. Ballance, The integrated propagation of atomic structure and collisional uncertainties through to plasma diagnostics

10:00   J. Colgan, Theoretical Approaches to Electron-Impact Ionization

10:20   O. Zatsarinny, Benchmark calculations for electron collisions

10:40   Coffee Break

Experimental Atomic Collision Data (Chair: G. Garcia)

11:00   A. Wolf, Storage-Ring Merged Beams Experiments on Electron Ion Recombination: Benchmarking and Accuracy Limits

11:20   M. Kitajima, High-resolution Measurements of Total Cross Section for Electron Scattering from Atoms and Molecules at Very-low-energy

11:40   A. Müller, Experimental Studies on Interactions of Atomic Ions with Single Electrons

12:00   H. Tanuma, Atomic and Molecular Data provided by Multiply Charged Ion Beam Collision Experiments at Low Energies

12:20   Lunch

Theoretical Heavy Particle Collision Data (Chair: J. Colgan)

13:40   L. Mendez, Numerical calculation of charge exchange and excitation cross sections for plasma diagnostics

14:00   I. Tolstikhina, Charge exchange in slow collisions of ions with Hydrogen isotopes - Adiabatic approach

14:20   T. Kirchner, Basis Generator Method Calculations for Charge-Transfer Collisions Involving Few-Electron Systems

14:40   Coffee Break

Experimental Heavy Particle Collision Data (Chair: E. Krishnakumar)

15:00   R. Ali, Experimental Studies of the Energy Dependence of State-Selective Non-Dissociative Single Electron Capture in He2+ on H2 Collisions

15:20   W. Wolff, Multiple ionization of atoms and molecules by impact of light -charged ions at the intermediate energy range

15:40   P. M. Limão-Vieira, Charge transfer processes in atom-molecule collision experiments

16:00   Benchmark of atomic, molecular, heavy particle collision theory and experiment (Chair: K. Bartschat, J. Tennyson)

Wednesday, 21 December

Data Evaluation and Uncertainty Propagation (Chair: T. Nakano)

09:00   H. Chung, IAEA Evaluation Activities

09:20   I. Murakami, Evaluation on Atomic Data and Collisional-Radiative Models for Spectroscopic Diagnostics and Collaboration Network in Japan

09:40   M. Bautista, Uncertainties in Atomic Data and their Propagation

10:00   A. G. Császár, Uncertainty quantification of ideal-gas thermochemical functions

10:20   Coffee Break

Atomic Data Evaluation (Chair: D. Fursa)

10:40   G. W. F. Drake, Uncertainty Estimates for Atomic Structure Calculations

11:00   P. Jonssen, Assessing Uncertainties for Theoretical Atomic data

11:20   N. Nakamura, Observation and Identification of Tungsten Spectra Observed with an Electron Beam Ion Trap

11:40   R. Hutton, Benchmarking Visible Spectral Line Data

12:00   D.-H. Kwon, Theoretical Electron Impact Ionization, Recombination, and Photon Emissivity Coefficient for Tungsten Ions

12:20   Lunch

13:40   Y. Yang, KLL DR resonant strengths

Molecular and Heavy Particle Data Evaluation (Chair: V. Kokoouline)

14:00   G. Karwasz, Electron Scattering on Molecules: Partial Cross Sections

14:20   J.-S. Yoon, Data evaluation of helium and its isotopes

14:40   A. M. Imai, First Step Benchmark of Inelastic Collision Cross Sections

15:00   Coffee Break

15:40   A&M Experimentalist Network (Chair: A. Wolf)

16:20   Meeting Conclusion

Poster Presentations

A. A. Buchachenko   Ab Initio Studies of the Collisions Involving Lanthanide Atoms and Ions

K.-B. Chai   Plasma Emission Spectroscopy When There Is Magnetic Reconnection Associated with Rayleigh-Taylor Instability in the Caltech Spheromak Jet Experiment

D. Darby-Lewis R-Matrix Calculations of Electron Impact Electronic Excitation of BeH

J. Kaur   Electron Interactions With Plasma Reactive Carbon Tetrachloride Molecule: An Extensive Cross Section Study

J. Liu   A+M Data Application in EAST Tokamak Edge Simulation of Impurity Seeding Plasma

Priti   Calculation of Detailed Relativistic Electron Excitation Cross Sections and Application to Hydrogen-Caesium Plasma

I. F. Schneider Resonant electron-molecular cation collisions in the edge plasmas of fusion devices: new state-to-state cross sections and rate coefficients

J. M. Seminario Towards the Simulation of Plasma Chemistries from Atomistic and Molecular First Principles Methods

S. Singh   Positron Scattering Cross Sections For Plasma Relevant Hydrocarbons

M.-Y. Song   Cross Sections for Electron Collisions with Acetylene

V. Stancalie   Studies on the Electron-Correlation and Relativistic Effects in Target Representation and Low-Energy Collision Calculation

P. Verma   Electron Scattering By Silane

Supplementary Posters

K. Fujii   Bayesian Inference for the LHD Experiment Data

D. Fursa   Convergent Close-Coupling e- - H2 Excitation Cross Sections

D. Stotler   Sensitivity of Tokamak Transport Modelling to Atomic Physics Data: Some Examples

M. Bautista   Uncertainties in Atomic Data and their Propagation

Abstracts

Atomic, Molecular And PMI Database In Current Edge Plasma Transport Codes, And Forward Sensitivity Analysis

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Magnetic fusion edge plasma transport codes resort to a large number of atomic, molecular and PMI data, in order to quantify these processes within the context of plasma dynamics in the outer and near target area of magnetic fusion devices. Many different edge plasma codes are in use, common to most of them is a 2D or 3D CFD treatment of the main plasma (electrons, ions) components, and a kinetic (often Monte Carlo) treatment of the neutral atomic, molecular components and some low concentration impurity ions. The B2-EIRENE family of codes is such an example. It constitutes amongst others the transport part of the SOLPS code suite, notably the SOLPS_ITER code hosted by ITER-IO.

These primary computational tools, which take A+M+PMI data as input, have to deal with the much more involved 'plasma state of matter' issues first. They are far less mature and limited in their predictive quality as compared to computational tools in other areas of sciences, e.g. to those taking nuclear data as input.

The data challenge (A+M+PMI data) in fusion edge plasma codes, and their uncertainty quantification, often comes in at a peripheral level. These codes isolate this A&M data sub-component of the model, computationally, and make them accessible for experimental quantification. If this separation is made, A+M data fall into the category 'known' parameters, plasma turbulence and flows, also PMI data, and all their consequences fall in the category 'unknown', uncertain, parameters.

In the present contribution we publicly expose the status of atomic, molecular and PMI data in fusion edge plasma codes, and we discuss their journey from the raw, unprocessed data towards condensed, properly averaged data used in integrated code models, as well as first attempts to quantify the uncertainty propagation during this data processing step. This latter is achieved by a (linear) forward sensitivity analysis option build into collision radiative codes for fusion plasma transport applications [1].

Pilot studies for propagation of the collision radiative A&M related uncertainties further, across the plasma flow simulations, governed by a system of partial differential equations (PDEs), onto the final quantities of interest, have meanwhile also been initiated. Efficient, adjoint-based sensitivity calculations establish the fundaments for this uncertainty propagation step. First results are discussed for a plasma flow model with a still simplified (fluid) treatment of the A&M aspects.

[1] See: http://www.hydkin.de/.

Sensitivity of Tokamak Transport Modeling to Atomic Physics Data: Some Examples

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A central concern in the design of burning plasma devices, such as ITER or DEMO, is that they represent extrapolations in dimensionless parameters from existing devices. The only means by which one can confidently predict their operation is via a well validated simulation based upon a first principles, or as close as possible, model. Accurate atomic physics data are essential to this task, not only for these predictive applications, but also for the validation of the model against the available data. In this talk, we present examples illustrating the sensitivity of such simulations to uncertainties in atomic physics data.

The Gas Puff Imaging (GPI) diagnostic [1] provides spatially and temporally resolved data ideal for validating plasma turbulence simulations. To date, those validation tests have been based on statistical characterizations of the turbulence, such as correlation lengths and times. In using those data, one must account for the spatial extent of the neutral gas cloud that is being "lit" by the plasma turbulence. Neutral transport simulations of that gas cloud have essentially no free parameters and are themselves amenable to quantitative validation tests [2]. We will describe a couple of these, utilizing deuterium or helium gas puffs, and examine the sensitivity of the results to the atomic physics data for those systems.

The use of tungsten in ITER as a principal plasma facing material has led to its introduction in a growing number of existing devices. Experiments conducted on those surfaces are frequently targeted at assessing tungsten erosion and its transport into the tokamak core. We will highlight two such recent investigations. In both cases, factor-of-a-few variations in the tungsten atomic physics data result in order of magnitude, or more, changes in the analysis results [3].

Finally, the drive towards truly first principles simulations entails, at least in some regimes, a shift from fluid descriptions of the plasma to ones that are fully kinetic [4]. The development of ever more capable computers and simulation algorithms has been steadily relaxing restrictions on the dimensionality and spatial coverage of such simulations. As they become more detailed and practical, additional atomic physics data will be required, e.g., doubly differential ionization cross sections.

[1] S. J. Zweben et al., Plasma Phys. Control. Fusion **56**, 095010 (2014).

[2] B. Cao et al., Fusion Sci. Tech. **64**, 29 (2013).

[3] J. D. Elder et al., "OEDGE Modeling for the Planned Tungsten Ring Experiments on DIII-D", presented at the 22nd PSI Conference (Rome, 2016).

[4] D. Tskhakaya, Contrib. Plasma Phys. **56**, 698 (2016).

Contribution of Quantitative Spectroscopy to Fusion Plasma Research

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National Institutes for Quantum and Radiological Science and Technology

In fusion plasmas, different roles are required for impurities in terms of atomic number, Z; in low temperature peripheral (divertor) plasmas, enhancement of low Z impurity radiation is of importance for mitigating plasma heat load onto plasma-facing walls, while in high temperature core plasmas, suppression of impurity radiation, particularly by high Z impurity ions, is essential for maintaining high temperature. This talk discusses a mechanism, which enhances low Z impurity radiation in divertor plasmas and a method available for validating ionization and recombination rates of high Z impurity, tungsten (W) based on quantitative spectroscopy.

In the divertor plasma of JT-60U tokamak, we successfully provided a comprehensive picture of the carbon radiative cooling process [1]. In high-density divertor plasmas, typically an electron density above 1×10^{20} m^{-3}, strong radiation zone appeared, and intense line emissions from carbon ions, originating from the carbon divertor targets, were observed. It was found, in this radiation zone, that the C III line emission contributed 30% of the total radiation power, and C IV 60%, and that the C IV ions were produced by ionization of C III ions and at a higher rate by recombination of C V ions (He-like). These indicate that C III and C V ion flowed into the radiation zone, and were converted into the biggest radiator, C IV. In particular, a newly discovered channel [2]*,* conversion of an inefficient radiator C V into an efficient C IV contributed to enhance the radiative cooling more than that of C III to C IV. Interestingly, in Ne-seeded plasmas, recombination of Ne IX (also, He-like ion) was observed in the Ne radiation zone [3], suggesting recombination of impurity He-like ion is one of common key processes to enhance the impurity radiation.

In the core plasma of JT-60U tokamak, W density was determined from the intensity of W^{45+} spectral line (4s-4p: 6.2 nm). The determined W density over electron density ranged from 1×10^{-5} up to 1×10^{-3} [4]. In addition, to investigate the validity of W^{44+} ionization rate and W^{45+} recombination rate, a density ratio of W^{45+} to W^{44+} calculated with an ionization equilibrium model was compared to that determined from an intensity ratio of W^{45+} to W^{44+} 4s-4p lines. One of the advantages of this method is cancellation-out of electron temperature dependence of excitation rates of 4s to 4p by taking the intensity ratio. This is due to similar transitions in simple systems; closed 3d shell + 4s electron, exciting to 4p level for W^{45+} and one additional 4s for W^{44+}. This analysis resulted in agreement between measurement and calculation within experimental uncertainty (~30%), showing the validity of the ratio of W^{44+} ionization rate to W^{45+} recombination rate. Similar analysis performed in the JET tokamak [5], but for the density ratio of W^{46+} to W^{45+} determined from the intensity ratio of W^{46+} to W^{45+} 3p-4d lines (0.52 nm), showed the measured W^{46+}/W^{45+} ratio was systematically higher by 16% than that calculated. This indicates a possibility that the calculated W^{46+} recombination rate is overestimated or the calculated W^{45+} ionization rate is underestimated. The reason for this deviation is not yet clear.

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Bayesian Approaches to Uncertainty Quantification in plasma-wall interaction modelling

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Computer models play a crucial role in providing insight in complex systems. Increasingly the need for verification, validation and uncertainty quantification of computer simulations has become evident. We discuss uncertainty estimates and approaches to uncertainty estimation in plasma-wall interaction with particular attention to hydrogen transport in tungsten and erosion in mixed-material systems.

On the theoretical side closed-loop optimal experimental design algorithms provide a key component for the extension of Uncertainty Quantification (UQ) to higher dimensional settings. Here, we will present an approach for a closed-loop experimental design .

However, in practice the main shortcomings are rarely dictated by limited computational power but more often by the inadvertently use of inadequate models. Examples for that will be given as well as possible approaches to alleviate the problem.

Bayesian Inference for the LHD Experiment Data

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Bayesian statistics is becoming more popular in wide range of science. However, its application to the fusion study is still limited except for a few basic studies [1-3]. In this talk, I will present some basics of Baysian methods, a few of recent machine learning methods, as well as our recent applications to the fusion study in Large Helical Devices (LHD).

One of our applications is the estimation and calibration of the systematic noise in Thomson scattering diagnostics for LHD [4]. Classical statistical analysis, which has been adopted for a long time, is effective to consider the *random* noise, however one of its limitations is the difficulty to take *systematic* noise into account. In case of Thomson scattering diagnostics, the uncertainty of the sensitivity calibration makes additional scatter in the observation. We have modelled such a systematic noise within one of Bayesian statistical frameworks, Gaussian process regression. From a large set of observation data by Thomson scattering diagnostics and the statistical modeling, we have separate the observed signal into the latent plasma parameters, random noise, and the systematic noise. This inference techniques decreases the scatter in the electron density inference by factor of 5 and revealed small spatial structures of electron density distribution in LHD.

Another our application is the atomic data evaluation related to highly charged tungsten ions [5]. Based on large experimental data for the near-ultraviolet emission line intensity of highly charged tungsten observed from LHD plasmas, we derived the electron temperature dependence of the fractional abundance for charge states of 23-28 and the spatial profile of the tungsten density. Since this result purely comes from experiment, it could be a benchmark for the future theoretical calculation.

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Application of atomic data to quantitative analysis of tungsten spectra on EAST tokamak

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ITER has adopted tungsten as the divertor material for the D-T operation. In order to improve the divertor heat load capability, the tungsten mono-block has been equipped on upper divertor of EAST tokamak at 2014 [1]. The tungsten accumulation has been often observed in NBI-heated H-mode discharges suggesting a sufficient improvement of tungsten confinement [2], which is one of the critical issues to achieve long pulse H-mode discharges. Then, a quantitative analysis on tungsten behaviors is urgently desired for maintaining the high-performance plasma of EAST.

In order to study the tungsten behavior in long pulse discharges, tungsten spectra have been measured at 20-140Å with a newly installed extreme ultraviolet (EUV) spectrometer fulfilled a fast time response charge-coupled detector (CCD) of 5ms/frame [3]. It is found that emission lines from highly ionized W ions of W^{40+} to W^{45+} can be easily observed with strong intensities in longer wavelength range of 120-140 Å when the central electron temperature exceeds 2.5keV.   Unresolved transition array (UTA) is always observed at 45-70 Å.

In this work, several isolated lines from W^{40+} – W^{45+} in the longer wavelength range are used for the quantitative evaluation based on the absolute intensity measurement, i.e., W^{40+} ($3d^{10}4s^24p^4$ $^3P_2$ – $3d^{10}4s^24p^4$ $^3P_1$) at 134.87Å, W^{42+} ($3d^{10}4s^24p^2$ $^3P_0$ – $3d^{10}4s^24p^2$ $^1D_2$) at 129.41Å), W^{43+} ($3d^{10}4s^24p$ $^2P_{1/2}$ – $3d^{10}4s^24p$ $^2P_{3/2}$) at 126.29 Å and W^{45+} ($3d^{10}4s$ $^2S_{1/2}$ – 3 $d^{10}4p$ $^2P_{1/2}$) at 126.998Å. In the analysis the photon emissivity coefficient (PEC) of tungsten lines and fractional abundance (FA) of tungsten ions under ionization equilibrium are utilized as the atomic data. In practice, the effective ionization and recombination coefficients from Atomic Data and Analysis Structure (ADAS) database are used in a set of rate equations to calculate the FA in EAST plasmas with measured electron temperature and electron density profiles. An effect of the impurity transport is also considered. Meanwhile, the PEC is directly obtained from ADAS database (arf40_ic series). The tungsten concentration is evaluated from tungsten radiation power coefficient calculated with ADAS database based on the total radiation loss measurement. The results obtained with these approaches are compared with each other.

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Uncertainty quantification in calculations of molecular processes.

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Models of fusion plasma and other important natural and technological processes are becoming increasingly relient on calculated data. Uncertainty quantification (UQ) for processes containing molecules remain unusual; however there are recent recommendations on how to approach this problem [1]. First principles quantum mechanical calculations on molecular structure and collision processes have a number of important characteristics. Firstly the equations of these problems are well known and effectively exact, so the problem is fully and precisely specified. Secondly most solution techniques are relatively free from issues with numerical uncertainties. This means that the uncertainties are dominated by systematic errors associated with the model chosen to represent the problem. Understanding and quantifying these systematic errors can provide important insights and improved UQ for key problems.

The process of UQ in molecular systems will be illustrated by considering the question of how much radiation does one molecule of CO_2 absorb. Recent high-accuracy ab initio calculations of transitions intensities for CO_2 give excellent ($< 0.5\%$) agreement with a few lines measured to high accuracy [2]. However comprehensive lists of transitions generated for atmospheric monitoring [3] give significant (1%) differences with laboratory measurements of spectra performed for the same purpose and other systematic differences as a function of CO_2 rotational state. The talk will describe how detailed interaction between theory and experiment has allowed these studies to be reconciled yielding a consistent, high quality list of transitions which are currently being considered for use by the OCO-2 mission for use their spectral retrievals. The prospects for systematic UQ for molecular processes will be discussed.

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A Stepwise Procedure to Explore Uncertainty and Reliability in Theoretical Cross Section Data for Electron and Positron Scattering

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Many areas of science require accurate values of electron/positron induced scattering cross section data to probe various physio-chemical reactions occurring in those environments. For instance, electron collision data have applications in areas like modeling of electrical discharges, semiconductor processing, gas lasers, low and high-temperature laboratory plasmas, fluorescent lighting, the upper atmosphere, interstellar medium and quantitative mass spectrometry [1]. Similarly, interactions of positrons have potential technical applications in atomic physics, surface sciences, mass spectrometry, atmospheric modeling and medical imaging technique like positron emission tomography (PET) [2].

There is large amount of data set on electron scattering cross sections reported and compiled by various experimental and theoretical groups around the globe. However, we lack a mechanism to check the reliability of such data. Hence, it is critical to qualify and quantify legitimate data in the present scenario to benchmark the prevalent experimental and theoretical datasets. Experimentalists usually provide uncertainties to their measured data. However, theoretically it is quite demanding to envisage an effective methodology to estimate uncertainty for the calculated cross section data, but has been the urge of atomic and molecular physics community today. Hence, the present report is intended to address this issue and contribute a productive effort in this direction.

The first step in our approach is to benchmark the theoretical methodology employed against existing measurements/calculations. Next, a set of correlation relations are studied and verified for the calculated data to ensure consistency. This step is to make sure the reliability of the computed results. Then the variation in cross section due to a change in each input parameter used is quantified. This step is very crucial in speculating the sensitivity of cross sections for various input properties intrinsic to a target. Finally the spread in cross section due to various approximation methods used will be probed. It is to be noted that the aforementioned steps for uncertainty estimation are exclusive to the present method.

The atomic and molecular physics group at Indian Institute of Technology (ISM) Dhanbad, India has been in the forefront of calculating various cross section data for about a decade now. Electron and positron scattering cross sections are computed through SCOP formalism [3,4] (and R-matrix method) for a number of targets having applications in thrust areas of science. The cross section data includes electron induced DCS, total elastic, inelastic, ionization and momentum transfer cross sections [3] and positron impact cross sections like total, positronium formation and ionization (both direct and total) cross sections [4]. Employing above steps, we intend to provide recommended cross section dataset for many unknown targets to form a unified and complete database [5] with appropriate uncertainties.

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Uncertainty evaluation in theoretical calculations of cross sections for electron-molecule collisions

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In this talk, two approaches for uncertainty assessment in theoretical calculations of cross sections for electron-molecule and atomic collisions will be discussed. In particular, a systematic Monte-Carlo approach, used in nuclear physics, for the uncertainty quantification will be reviewed and presented in the framework of electron-molecule collisions. The approach allows one to evaluate the uncertainty of final theoretical cross sections if uncertainties of all parameters used in the model are available. It can also deal with parameters of the theoretical model that are correlated. Correlations between parameters often reduce uncertainties of final results and, therefore, should be accounted for if data of a high value is under consideration. The approach allows also a systematic comparison with experimental data (if they are available). The procedure gives a standardized way to produce evaluated (recommended) cross sections and uncertainties combining information from different theoretical and experimental sources.

Evaluated electron and positron-molecule scattering data for modelling particle transport in the energy range 0-10000 eV

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Particle transport in molecular media, both liquids and gases, and radiation damage are customary modelled using atomic scattering data based on the Born-Bethe theory [1]. However, this approach tends to overestimate electron and positron scattering cross sections for incident energies below 10000 eV, especially for elastic processes. Here we present a method to obtain evaluated electron and positron scattering data for some molecular prototypes (N2, CH4, H2O) by combining experimental and theoretical methods, validated within their corresponding energy range of applicability, in order to achieve a consistent data set over a broad energy range (0-10000 eV).

These data are used as input parameters for an event by event Monte Carlo simulation procedure [2] which will be applied to some validating experiments. The assigned uncertainty limits for the input data will be checked by comparing the observed results with the predictions of the simulation. Possible applications to model transport processes in fusion plasmas will be also discussed.

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Dissociative Electron Attachment Cross Section in H_2 and D_2 at the 4 eV resonance

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The 4 eV resonance in electron-H_2 collision is in principle the simplest resonance in electron-molecule scattering. Due to its large width, the isotope effect in the dissociative electron attachment cross section is very large. So far there have been two quantitative measurements of the $\sigma(H^-/H_2) / \sigma(D^-/D_2)$ ratio: Schulz and Asundi[1] measured the often quoted value of 200, more recently Čadež and co-workers [2] determined this ratio to be 325.

We have determined cross sections for dissociative electron attachment in H_2 and D_2 using a trochoidal electron monochromator in combination with an anion time-of-flight mass analyzer. The use of time-and-position sensitive delay-line detector for anion detection has enabled an efficient signal-background separation, which is crucial for measuring cross sections that are as low as in the present systems. We have examined only the cross sections at the 4 eV and 14 eV resonances, since in both energy ranges the DEA is a threshold process yielding slow fragments. The cross sections were calibrated against those of O^- from CO_2 and $HCOO^-$ from HCOOH.

For the 14 eV resonance the present energy-integrated cross sections (independent on electron energy resolution) are in very good agreement with recent measurements using the velocity-map imaging technique [3]. However, the isotope ratio of integrated cross sections in H_2 and D_2 at the 4 eV resonance is 800. The critical re-examination of previous experiments shows, that the difference with present results is to a large degree caused by an insufficient separation of background signals in those experiments.

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Recent developments in absolute cross section measurements for dissociative electron ionization of and attachment to molecules

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Measurement of absolute cross sections for the production of various positive and negative ions from molecules by electron impact has been a difficult problem till very recently. While the total ion cross sections could be obtained fairly easily using a total ion tube [1], the partial cross section measurements posed problems due to the initial kinetic energy and angular distributions of the fragments ions. In order to obtain the absolute cross sections, it was necessary to collect and detect all the ions from an interaction volume of known target density and electron current density. While the relative flow technique [2] considerably reduced complexity of determining the target density and the electron current density and their overlap volume, the problems persisted in collecting, mass analyzing and detecting the fragment ions without discrimination against their initial kinetic energies, angular distributions and mass to charge ratios. A segmented time of flight mass spectrometer along with pulsed electron beam and pulsed ion extraction arrangement provided a very simple and clean solution for these problems [3]. A more recent advancement of this for the case of positive ions from simple molecules has been a combination of total ion tube technique with position sensitive detector, where mass to charge ratio separation was carried out using time of flight [4]. The latest advancement in these measurements applicable to both positive and negative ions has been the use of a momentum imaging time of flight mass spectrometer in combination with the relative flow technique to solve the 50 year old puzzle in the dissociative electron attachment cross sections for H_2 and D_2 [5]. While all these techniques could be used for molecules which have large enough vapour pressure at room temperature, a wide variety of important molecules remain as solids at room temperature with very small vapour pressure. Here again, a variation of the relative flow technique coupled to time of flight mass spectrometry has provided a relatively simple solution to the problem [6]. While presenting these techniques, the talk would cover various sources of systematic uncertainties and common pitfalls in these measurements

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Estimating Uncertainties of Theoretical Data for Electron Collisions with Atoms and Ions*

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The recommendations of how to go about estimating the uncertainties in theoretical predictions of electron collision data for atomic and ionic targets, as outlined in a recent Topical Review [1], will be discussed. In order to do so, the basic ideas behind various methods used in such calculations will be summarized, as well as their (perceived) strengths and weaknesses. Examples, however, show that some of the statements made in standard textbooks on atomic collisions are not necessarily valid when it comes to electron collisions with complex, open-shell targets.

[1] *TOPICAL REVIEW: Uncertainty Estimates for Theoretical Atomic and Molecular Data*
   H. K. Chung, B. J. Braams, K. Bartschat, A. G. Császár, G. W. F. Drake, T. Kirchner,
   V. Kokoouline, and J. Tennyson, J. Phys. D **49** (2016) 363002.

Electron scattering from molecular hydrogen

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We have recently extended the convergent close-coupling (CCC) method to model electron and positron collisions with molecules [1,2,3]. For these types of collisions it is our aim to provide a comprehensive set of cross sections that are demonstratively convergent and valid over a wide range of incident energies.

Molecular hydrogen is the simplest neutral molecule. For theorists the H_2 molecule is a natural starting point for developing and testing computational techniques. A large number of theoretical methods have been applied to study e-H_2 collisions in the past, however modern large-scale close-coupling techniques have not yet been applied to the problem (with the exception of R-matrix with pseudo-state and time-dependent close-coupling methods applied to calculation of ionisation). The largest and most detailed calculations are more than ten years old. They included no more than the first nine states of H_2 therefore neglecting coupling to the high lying excited states and ionisation channels. No convergence studies have been performed for e-H_2 scattering to date and the accuracy of the calculated cross sections is largely uncertain.

This unsatisfactory situation is surprising given the importance of the H_2 molecule in fundamental science and applications. Molecular hydrogen is the most abundant molecule in the Universe, particularly in interstellar space and in the atmospheres of gas giants and the outermost planets in our Solar System. It is present at the edge region of fusion devices and widely used in plasma processing. A comprehensive dataset of e-H_2 collision data is in great demand for modelling various astrophysical and technological plasmas. It is our aim to provide such data.

In this report we will present results of large-scale fixed-nuclei close-coupling calculations of electron scattering from the ground state of H_2 [3] for incident electron energies from 10 to 300 eV. The calculations have been performed using a single-centre implementation of the CCC method. We have established convergence of the close-coupling expansion by increasing the size of the calculations from nine to 491 states. A partial wave expansion of the projectile electron wave function has been performed to the maximum angular momentum value $L_p=8$ and total angular momentum projection $M_{tot}=8$. Higher partial waves have been accounted for using a Born top-up procedure. Differential and angle integrated cross sections will be presented for a number of excited states ($b^3\Sigma_u^+$, $a^3\Sigma_g^+$, $c^3\Pi_u$, $B^1\Sigma_u^+$, $EF^1\Sigma_g^+$, $C^1\Pi_u$, $e^3\Sigma_u^+$, $h^3\Sigma_g^+$ $B'^1\Sigma_u^+$, $D^1\Pi_u$, $B''^1\Sigma_u^+$, $D'^1\Pi_u$) together with total and total ionization cross sections.

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The integrated propagation of atomic structure and collisional uncertainties through to plasma diagnostics

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Although the atomic and molecular collisional communities have invested considerable effort in developing various highly accurate approaches to electron-impact excitation, ionization and dielectronic-recombination, systematic studies of the uncertainty for each process has not been given the same amount of attention.

Furthermore we are finding that uncertainty in plasma diagnostics is not simply the sum of these isolated collisional rates, but are often the product of multiple interacting processes that are a function of electron density and temperature. For example, an effective ionization rate [1] for a particular ion stage is a weighted summation over the groundstate and meta-stable ionization cross-sections. The contribution from the excited state ionization to the effective ionization rate depends directly on the population of the excited states relative to the groundstate, therefore sampling the variation in a wide variety of radiative and electron-impact excitation transitions.

Therefore, although associating a meaningful uncertainty in each fundamental collisional process is the first step, the propagation of these variations into plasma diagnostics requires an uncertainty grid which is a function of electron density and temperature and is the longer term goal. We outline in [2] a method by which these uncertainty contributions can be propagated through to plasma diagnostics.

In order to provide one aspect of these uncertainties, a perl-script front-end to an R-Matrix with Pseudo-States (RMPS) package has been written, through which a Monte-Carlo approach varies the underlying atomic structure behind these collisional calculations many, many times. The subsequent excitation, ionization and di-electronic recombination results from these calculations will provide more realistic variation in the uncertainty from an atomic structure foundation upwards. We intend not only to provide an uncertainty file for each of the fundamental collisional processes, but also on the secondary derived parameters such as effective recombination/ionization rates.

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Theoretical Approaches to Electron-Impact Ionization

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Electron-impact ionization cross sections are one of the fundamental constituents of the myriad sets of atomic data required for plasma modeling. A short review will be given of the various theoretical approaches to computing such ionization cross sections. Examples include perturbative approaches based on distorted-wave theory, and non-perturbative approaches based on close-coupling expansions. Non-relativistic, semi-relativistic, and fully-relativistic versions of these methods are generally available. The availability of computing packages to generate such cross sections is also discussed. For example, ionization cross sections may be obtained using distorted-wave (and/or scaled hydrogenic) methods using the Los Alamos suite of atomic structure and collision codes [1], available online [2]. Such methods are relatively computationally inexpensive, and increase in accuracy as the charge of the target ion increases.

Close-coupling approaches to electron-impact ionization include the convergent close-coupling method [3], R-matrix approaches [4], and time-dependent close-coupling methods [5]. These approaches have, for the most part, been applied to neutral and near-neutral systems, where differences with perturbative methods can become significant. However, all of these calculations are normally quite computationally expensive.

This talk will provide some examples of the ionization cross sections for a selection of atoms and ions, and present comparison with measurements, where available. We will also start a discussion of how the uncertainty of these cross sections can be determined, and what calculations are most needed for future fusion modeling efforts.

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Benchmark calculations for electron collisions with complex atoms

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Over the past decade, we have developed a highly flexible *B*-spline *R*-matrix (BSR) method [1] that has some advantages compared to the standard *R*-matrix (close-coupling) approach. The two essential refinements are i) the capability for using the flexible term-dependent one-electron orbitals, and ii) the use of *B*-splines as a universal and effectively complete basis to generate the *R*-matrix basis. These features allow us to achieve a high accuracy in the target description, as well as a truly consistent treatment of the scattering system. The BSR code was successfully applied to many problems of electron collisions from atoms and ions, with special emphasis was placed on complex, open-shell targets. Often considerable *improvement* was obtained in comparison with previous calculations. Many examples can be found in a recent Topical Review [2].

More recently, the BSR complex has been extended to i) the fully relativistic Dirac scheme and ii) intermediate energies using the continuum pseudo-state approach. These extensions allow for an accurate treatment of *heavy targets* as well as a fully non-perturbative way to handle electron-impact *ionization*, including such highly correlated processes as ionization plus simultaneous excitation..

During the last years we developed parallel versions of our BSR and DBSR codes. They made it possible to carry out large-scale *R*-matrix with pseudo-states (RMPS) calculations and thereby provide *converged* (with respect to the number of coupled states) results for electron impact excitation of individual target states. For many systems our calculations revealed dramatic reductions of the predicted excitation cross-sections at intermediate energies, due to the strong influence of coupling to the target continuum. These results raise questions about the absolute normalization in several published measurements. Our RMPS calculations represent the extensive and *complete* sets of electron scattering data ready for applications.

Finally, we can *systematically analyse the convergence pattern of our results* by performing a series of calculations, in which we couple a varying number of bound and pseudo-states. Furthermore, the influence of the target description on the quality of the final results can be analysed. Such studies allow for *common-sense estimates regarding the uncertainty of our theoretical predictions*.

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Storage-Ring Merged Beams Experiments on Electron–Ion Recombination: Benchmarking and Accuracy Limits

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Ion storage rings are a powerful tool for measuring inelastic electron–ion collision rates, using merged ion and electron beams. Such measurements yield benchmark data for important atomic and molecular ions, offering high resolution in the collision energy and good accuracy for absolute cross-section values. This way, the results contribute to the understanding of the underlying physics mechanisms and can verify theoretical calculations, including their scaling to other systems (such as, e.g., along isoelectronic sequences for atomic ions).

The main experimental focus is electron recombination with positive atomic and molecular ions [1, 2]. Also ionization cross sections are measured [3] and deexcitation of internal levels by electron collisions was observed for molecules [4]. After an overview of the technique, we discuss some results that demonstrate the degree of quantitative control reached in the measurements, and identify aspects critical for best accuracy.

In merged-beams experiments, collision energies can be tuned from the milli-eV range up to a keV or more, changing the beam energies. The geometrical overlap and the beam currents can be defined with good accuracy, and the reactions are detected with high efficiency using event-by-event counting. For comparisons with theoretical cross sections at high energy resolution, collision velocity distributions specific to the merged-beams situation are used [5]. Control of metastable internal states of the interacting ions is gained by the extended storage time of the ions and by investigating time-dependent variations of the reaction rates.

In finding the rate coefficients from measured product-counting rates, monitoring the stored ion beam intensity plays an important role. Absolute reaction rates can in some cases be determined also from electron-induced ion loss rates [6]. Careful modeling of the electron–ion collision zone improves the accuracy in extracting absolute cross sections and energy dependences [5]. The detection efficiency of reaction products can reduced when they are highly excited or when the electron-induced reactions lead to large momentum transfer to the products. Finally, the populations of internal quantum states in the stored ions need to be considered carefully. Often, rate equation models using lifetime data of metastable levels are used to simulate the state populations. In some studies, also the modification of the internal state populations by inelastic electron collisions may become relevant. The discussion will consider results from magnetic ion storage rings. A short outlook will be given to planned merged beams experiments at a cryogenic electrostatic storage ring [7].

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High-resolution Measurements of Total Cross Section for Electron Scattering from Atoms and Molecules at Very-low-energy

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Accurate absolute cross section data for electron scattering from atoms and molecules provide important information not only for the fundamental physics of electron collisions but also for many fields such as electron-driven processes in the Earth and planetary phenomena, gaseous discharges, radiation chemistry and plasmas physics. Consequences of several interesting scattering phenomena such as Ramsauer - Townsend minimums, shape resonances, vibrational Feshbach resonances, and threshold structure due to a virtual state, appear in the scattering cross section curves especially at very-low collision energies, The low energy behaviors of the electron scattering cross sections are also related to the scattering length which gives zero-energy scattering cross section.

In the present report, absolute total cross sections for electron scattering from noble-gas atoms and some small molecules obtained with a technique employing the threshold-photoelectron-source combined with Synchrotron Radiation (SR) are presented. The technique makes use of photoelectrons produced by the photoioniztion of atoms using SR instead of using the conventional hot-filament electron sources [1-4]. In the present work, cross section measurements at very-low energies down to 5 meV with a high energy resolution were realized the in the single collision condition.

The measured cross sections for lighter noble-gas atoms, especially for He, agree very well with the theoretically obtained cross sections known as 'standard' [5-7] in the electron energy range down to 6 meV. On the other hand, heavier noble-gas atoms such as Kr and Xe were significantly smaller compared to the values reported by the previous swarm studies at energies below 100 meV. Comparison of scattering length for noble gas atoms obtained in the present work with those obtained in the swarm experiments also show systematic disagreement for heavier noble-gas atoms. Present high-resolution measurement also enabled to observe the structures on the total cross section curves of Feshbach resonances. Natural width of these resonances are also analyzed based on the spin-dependent resonant scattering theory. Total cross sections for electron scattering from some small molecules such as H_2, N_2 O_2, CO_2, and N_2O will also be presented.

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Experimental Studies on Interactions of Atomic Ions with Single Electrons

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Collisions of single electrons with atomic ions can lead to recombination, elastic scattering, excitation or ionization [1]. The most important quantities characterizing such processes in ionized gases are the temperature-dependent plasma rate coefficients α_{if} for transitions from an initial state i to a final state f. The temperature range of interest in the context of fusion plasmas is from essentially zero to hundreds of millions of Kelvins. Charge states of atoms with atomic numbers Z possibly playing a role in a fusion plasma range from 0 to Z where only the heaviest contaminants in the plasma cannot be fully stripped of electrons. Hence, experiments have to cover an extremely wide range of parameters.

Recombination of a single electron with an ion can happen as a direct radiative recombination or in a multi-step resonance process including single or multiple excitation of the ion plus capture of the electron and subsequent relaxation by photoemission. Elastic scattering and excitation can also be the result of a direct or a resonant multi-step process but with an electron ejected instead of photons. Electron-impact single or multiple ionization can proceed via direct knock-off of electrons or via (direct or resonant) excitation to an intermediate autoionizing state with subsequent emission of electrons. The indirect contributions produce rich structures in the energy dependence of the associated cross sections.

Crossed- and merged-beams experiments have provided a wealth of data on recombination and ionization of ions in a wide range of charge states while measurements on elastic scattering and electron-impact excitation of ions remain to be scarce. Much of the progress accomplished over the last decades has been made possible by the use of heavy-ion storage rings. This is particularly true for recombination of highly charged ions for which the interaction of cold beams of electrons with stored and cooled ions in a merged-beams configuration provides the method of choice to study cross sections and resonance energies. The most precise measurements on electron-impact ionization of ions were performed using crossed-beams arrangements which have the advantage of relatively low cost and high availability. Total relative uncertainties of colliding-beams cross-section data are typically 10 ± 5 %. Statistical uncertainties have been reduced even to the 0.01 % level in some cases.

Problems in most beams experiments arise from the possible presence of mixtures of electronic levels in the parent ion beam used for cross-section measurements. Storage rings allow for relatively long delay times between the production of a desired ion charge state and the start of a measurement so that excited states can decay. However, these delay times are limited by the lifetimes of the stored ion beams and, therefore, long-lived excited states can also be present in an ion beam prepared for storage-ring measurements. As a result, cross-section data from colliding beams experiments may have additional uncertainty.

Recent experimental results on recombination and ionization will be presented to illustrate the present status of the field. By employing the principle of detailed balance independent cross-checks can be made between results of electron-ion recombination and photoionization experiments. The remarkable agreement of absolute cross-section results obtained with very different experimental arrangements provides proof for the validity of both measurements.

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Atomic and Molecular Data provided by Multiply Charged Ion Beam Collision Experiments at Low Energies

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Fundamental atomic and molecular data consist of spectroscopic data and dynamical data. Ion beam experiments have been used for the measurements of both kinds of data. Historically, beam-foil spectroscopy has provided atomic spectroscopic data including the radiative transition rates of for highly charged ions. In the experiments with gaseous targets, various kinds of elastic, inelastic, and reactive processes have been measured in collisions of ions.

In Tokyo Metropolitan University, a 14.25 GHz electron cyclotron resonance ion source (ECRIS) have been used to produce various multiply charged ions, namely, C^{q+} (q = 4-6), O^{q+} (q = 6-8), Fe^{q+} (q = 7-16), Sn^{q+} (q = 3-21), and Xe^{q+} (q = 7-23), and photo-emission spectra following charge transfer collisions with neutral gases have been observed in visible-ultraviolet [1], extremely ultra-violet (EUV) [2], and soft X-ray regions [3]. Charge exchange spectroscopy is very useful technique to obtain transition wavelengths of multiply charged ions and measure the emission cross sections.

As tungsten will be used as a component of plasma-facing devices in the ITER, a number of spectroscopic studies have been reported in this decade. Recently, we observed emission spectra from tantalum ions. Because tungsten has five isotopes of the mass numbers from 180 to 186, it is not suitable for the ion beam experiment with the charge state separation. On the other hand, tantalum has 181-Ta with the natural abundance of 99.988%, and it is suitable for the charge-selected ion beam experiments. Because the atomic number of tungsten is 74 and that of tantalum is 73, the electronic structure and spectroscopic properties might be similar for isoelectronic ions. Therefore, we have decided to use tantalum ions instead of tungsten ions, and the measurements of EUV spectra of multiply tantalum ions after charge transfer collisions are now in progress.

It is well known that remarkable amounts of metastable helium-like ions, 1s2s $^3S_1$, are produced in the ECRIS. Therefore, in the cross section measurements of helium-like ions, we should consider the contribution of metastable state. According to the classical over the barrier model, we suppose that the ground and metastable states of ions have similar capture cross sections in collisions with the same target. However, in the collisions of helium-like C, N, and O ions with neutral gases, we have observed soft-X ray emissions corresponding to $1s^2 2s$ - 1s2snl transitions. As the 1s2snl state should be autoionized, the capture cross section will be reduced by this effect. Therefore, for the accurate cross section measurements, we should consider the fraction of metastable states and the detail mechanism in the collisions of metastable ions with neutrals.

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Numerical calculation of charge exchange and excitation cross sections for plasma diagnostics[*]

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Cross sections for charge exchange in ion-H collisions are the basic data required in charge exchange diagnostics of tokamak plasmas [1]. However, these data are in general not accessible experimentally and they are commonly obtained theoretically. The precision of the calculations depends on the collision energy and is in general unknown. In the present work we present a method to solve numerically the time dependent Schrödinger equation [2], which is based on the package GridTDSE [3]. In the calculation of charge exchange cross sections the wave function, which is initially an atomic travelling orbital, is evaluated in the points of a 3D Cartesian grid centered on the projectile nucleus and propagated by solving numerically the corresponding first order differential equation. The projections of the final wave function on the different bound states yield the charge exchange probabilities and cross sections. This technique can be employed in a wide energy range, and, given that the computational procedures are completely different, the comparison with the results of other methods (close coupling, classical trajectory Monte Carlo) provides an estimate of the uncertainties of the data. We have employed the grid numerical method to evaluate charge exchange n-resolved cross sections for collisions of Be^{4+} and B^{5+} with $H(1s)$ at collision energies between 1 and 500 keV/u.

In this work we also show that the method can be applied to describe excitation and electron loss of atoms in ion-atom collisions, which are relevant in determining the density of diagnostics beams [4] and in the stopping of heating neutral beams. In this work we present calculations for excitation and electron loss in $Be^{4+} + H(1s)$ collisions and we estimate the uncertainties of these data by comparison with once center atomic orbital expansions [5].

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Charge exchange in slow collisions of ions with Hydrogen isotopes. Adiabatic approach.

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In low-temperature plasmas (near-wall plasma and plasma in a divertor of tokamaks and stellarators), charge exchange is the dominant process in the population of excited states of plasma ions and, therefore, plays an important role in ion charge distribution, radiative cooling, and the transport of particles.

Recently, the strong isotope effect was predicted for He^{2+} + H, D, T charge exchange processes [1], which are of considerable interest for plasma modeling in a fusion reactor. This effect is due to the rotational mixing of electronic states at small internuclear separations R and results in a significant difference in the charge exchange cross sections in collisions of He^{2+} ions with H, D, and T atoms – the heavier the isotope the larger the cross section – at low collision energies (1–500 eV/amu). These findings motivated a series of studies where the results of [1] were confirmed and extended to other collision systems. In particular, in [2,3,4], using the adiabatic approach developed by Solov'ev [5], the strong isotope effect was shown to exist also for heavier projectiles. These results, apart from their general interest for collision physics, have important implications for diagnostics and simulation of elementary processes in fusion edge plasmas.

In the theory of atomic collisions, the adiabatic approximation is used to describe electronic transitions when the collision velocity is small and the nuclear motion can be treated classically. In this theory, there are no assumptions on the specific form of the electronic Hamiltonian, and only the smallness of the relative nuclear velocity is used. It results in a deeper understanding of the nature of nonadiabatic transitions. Since the isotope effect occurs at collision energies where the adiabatic theory applies, the adiabatic approximation is a natural theoretical framework for studying the effect.

The electron-nuclei interaction affects the internuclear motion in slow ion-atom collisions, which in turn affects theoretical results for the cross sections of various collision processes. The results are especially sensitive to the details of the internuclear dynamics in the presence of a strong isotope effect on the cross sections, as is the case, e.g., for the charge transfer in low-energy collisions of He^{2+} with H, D, and T. It was shown in [6] that internuclear trajectories defined by the Born-Oppenheimer (BO) potential in the entrance collision channel, which effectively accounts for the electron-nuclei interaction, are in much better agreement with trajectories obtained in the *ab initio* electron-nuclear dynamics approach [7] than the corresponding Coulomb trajectories. It was also shown that the use of the BO trajectory instead of the Coulomb trajectory in the calculations of the charge-transfer cross sections within the adiabatic approach improves the agreement of the results with *ab initio* calculations.

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Basis Generator Method Calculations for Charge-Transfer Collisions

Involving Few-Electron Systems

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The basis generator method (BGM) has been developed over many years with the objective to devise a general method for the solution of the time-dependent Schrödinger equation (TDSE) [1, 2]. It is based on the idea that completeness of a basis is not a necessary criterion for converged results. Rather, if the basis used to expand the state vector has the ability to adapt dynamically to the problem at hand, a relatively small basis size may be sufficient to obtain accurate (in principle, exact within numerical accuracy) results. The BGM has been applied most extensively and successfully to ion-atom and, more recently, ion-molecule collisions over broad ranges of impact energies [3, 4]. In its two-center (TC) implementation [5] it is similar to the more traditional atomic orbital close coupling method in that atomic bound states (with electron translation factors) and a set of pseudostates are used to represent the solution of the TDSE. It is in the way the pseudostates are constructed in which it differs.

In this talk, I will give a (necessarily brief) overview of recent TC-BGM collision calculations. The focus will be on charge-transfer reactions involving few-electron systems such as the noble gas atoms and water and methane molecules. The multi-electron problem is dealt within an independent particle model which is inspired by density functional theory. This implies that in addition to uncertainties associated with numerical and/or convergence issues model uncertainties have to be assessed. The only currently known way of doing this is via extensive comparisons of different model variants with experimental data and other theoretical results. It will be demonstrated that this is a useful procedure that provides qualitative, albeit not quantitative, information on the achieved accuracy.

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Experimental Studies of the Energy Dependence of State-Selective Non-Dissociative Single Electron Capture in He^{2+} on H_2 Collisions

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The Cold Target Recoil Ion Momentum Spectroscopy (COLTRIMS) technique has been used to investigate non-dissociative state-selective one electron capture processes in $He^{2+} + H_2$ collisions in the intermediate impact energy range 120 keV − 700 keV. The experimental measurements were performed at the Van de Graaff accelerator facility of the University of Jordan.

By contrast with photon spectroscopic studies of the same collision system, the COLTRIMS measurements have the advantage of being able to directly measure capture to the ground state (n=1) of the projectile ion. The measurements showed that capture to the ground state essentially dominates the collective capture to the excited states (n ≥ 2) over the entire impact energy range.

The measurements are found to be in gross disagreement with classical trajectory Monte-Carlo (CTMC) model calculations [1] over the entire impact energy range. The measurements demonstrate that comparisons with cross sections extracted from photon emission may lead to erroneous conclusions. The experimental results call for the development of more accurate theoretical models for the description of the important $He^{2+} + H_2$ collision system.

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Multiple ionization of atoms and molecules by impact of light charged ions at the intermediate energy range

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The ionization of multi-electron atoms and molecules by dressed and bare charged projectiles in the intermediate energy range regime which corresponds to the Bragg peak, where the stopping power of projectiles in matter reaches its maximum, is an important regions of the projectile trajectory for many applications. The understanding of the collision dynamics is essential to obtain the local damage in matter. Bare projectiles give a key benchmark to study the role of projectile screening in collision involving dressed projectile ions.

We report experimental and theoretical ionization and electron-capture cross sections for single, and multiple-electron removal from Ne atoms and H_2O molecules by He^{2+}, B^{2+}, C^{3+} and Li^{3+} ranging from 100 to 1000 keV/u. The experiment was carried out at the Tandem Pelletron accelerator facility of the Physics Institute at the Rio de Janeiro Federal University. Both the final state of the projectile and of the ejected recoils ions or fragment-ions were measured in coincidence to obtain cross sections associated with the pure ionization and electrons-capture channels. By using standard growth-rate method and time of flight mass spectrometry, absolute total and partial cross sections were obtained. These absolute cross sections are needed for comparison and aid to the development of theoretical methods for the collision dynamics over a wide range of projectile velocities as well as for providing reliable input data in simulation of penetration and damage of heavy ions in matter.

The average effective charge of the dressed charged ions along the ionization path and the effectiveness of its electrons in shielding its nucleus was investigated by comparing the cross sections of the multiple ionization of Ne and H_2O targets by B^{2+} and C^{3+} with the bare He^{2+} and Li^{3+} projectiles, respectively. The measurements have shown a strong screening effect for all n-fold recoil ion charge states in the ionization channels at the same velocities. The total ionization cross sections divided by the squared projectile charge as function of the impact energy show a universal, charge-independent scaling law at high energies (above 1000keV/u). On the other hand, at lower energies, the scaling is no longer fulfilled and more sophisticated theoretical approaches must be applied.

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Charge transfer processes in atom-molecule collision experiments

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Several elementary collisional processes are not due to direct electron impact but rather depend upon electron transfer. Electron induced chemistry is prevalent in many natural and industrial processes in a wide variety of media, including the formation of organic molecules within ice mantles on dusty grains in the interstellar medium [1]; the control of fluorocarbon plasmas used to produce silicon chips [2,3]; the chemical modification of absorbates using electron patterning [4] and scanning tunnel microscopy [5], and in edge and divertor plasmas of toroidal fusion devices [6], just to mention a few. Also, studying chemical reactions for molecular systems is relevant to understand radiation induced damage at the molecular level with the uttermost need to develop more efficient radiation therapies.

In the Lisbon laboratory we study gas phase electron transfer processes to molecules yielding ion-pair formation. The setup is of a crossed neutral atom-neutral molecule beam arrangement consisting of a potassium source, an oven, and a reflectron time-of-flight (TOF) mass analyser [7].

In this presentation we will address some of our most recent experimental achievements in anion formation by electron transfer experiments from collisions of neutral potassium atoms with key relevant molecules and their potential relevance to fusion plasmas. Relative cross-sections as a function of the centre-of-mass system will be presented and the dynamics of negative ions discussed. The experimental uncertainty of systematic relative cross sectional values are typically 10-20%.

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Evaluation on Atomic Data and Collisional-Radiative Models for Spectroscopic Diagnostics and Collaboration Network in Japan

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Spectroscopic diagnostics requires an atomic model such as a collisional-radiative (CR) model with atomic data such as electron-impact excitation rate coefficients to get information on plasmas from spectra. These atomic data and models should be reliable. We have evaluated the atomic data and the CR model for some iron ions by comparing available atomic data [1] and comparing calculated spectral line intensities with laboratory measurements [2-7]. The compact electron beam ion traps (CoBITs) and the Large Helical Device (LHD) produce plasmas with different electron densities, i.e., $\sim 10^{10} cm^{-3}$, and $\sim 10^{13}$-$10^{14} cm^{-3}$, respectively, and are useful for evaluations. We applied the same CR model to calculate spectral intensity ratios to compare the measured ratios in the CoBITs and the LHD. This method gave us the validity of the CR model and the atomic data included in the model, and we examined Fe XIII [2, 4], Fe XIV [2], Fe XV [2], Fe XVII [6, 7], Fe XXI [3] and Fe XXII [5].

We have organized collaboration network with atomic physicists in Japan. National Institute for Fusion Science has the collaboration programs with some small budget. Using the program, we organize several collaboration projects to study, for example, some atomic data related to fusion science and applied plasmas, spectroscopy on various elements in LHD and CoBIT, spectra after ion bombardment on metals and ceramics, and so on. This program helps to organize collaboration groups and support activities in atomic physics. We also conduct international collaborations via China-Korea-Japan A3 Foresight Program, National Institutes of Natural Science (NINS) Program on International Hubs for Natural Science Research, NINS Program for Cross-Disciplinary Study, and so on, to construct researcher networks with atomic physicist and plasma physicists.

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Uncertainties in Atomic Data and their Propagation through Spectral Models

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We present a method for computing uncertainties in spectral models, i.e., level populations, line emissivities, and emission line ratios, based upon the propagation of uncertainties originating from atomic data. We provide analytic expressions, in the form of linear sets of algebraic equations, for the coupled uncertainties among all levels. These equations can be solved efficiently for any set of physical conditions and uncertainties in the atomic data.

Regarding the intrinsic uncertainties in theoretical atomic data, we propose that these uncertainties can be estimated from the dispersion in the results from various independent calculations. We apply our approach to the computation of atomic data for O III and Fe II. For these ions we derive data uncertainties by comparing all previous published data with several new calculations employing a variety of different methods, such as Hartree-Fock, Thomas-Fermi-Dirac potential, and Dirac-Fock, and R-matrix methods. Then, we construct excitation balance spectral models, and compare the predictions from each data set with observed spectra from various astronomical objects. We are thus able to establish benchmarks based on observed astronomical spectra.

Uncertainty quantification of ideal-gas thermochemical functions

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Ideal-gas thermochemical functions, in the temperature range of $T = 0 - 6000$ K, play an important role in many scientific and engineering applications. Modelers often request the availability of these functions with an accuracy not less than 0.01 % over a large temperature range. This is the case, for example, with the new international standard equation of state (EOS) for the thermodynamic properties of "light" and "heavy" water under development at the International Association for the Properties of Water and Steam (IAPWS) [1].

The determination of the ideal-gas heat capacity, enthalpy, and entropy functions (sometimes called "caloric properties") of molecules is based on the partition function $Q(T)$ and its first two moments, $Q'(T)$ and $Q''(T)$. The only technique to achieve the accuracy goal stated above is based on the direct summation technique involving rovibronic energy levels of the molecule. Using this technique the accurate determination of thermochemical functions becomes especially challenging at low and at high temperatures.

Highly accurate partition functions have been determined for the parent water isotopologue $H_2^{16}O$ [2] and also for heavy water [3]. In these studies the following sources of uncertainty have been identified and investigated in considerable detail for four water isotopologues: (a) the inherent uncertainty of the (small number of) experimental and (large number of) computed rovibronic energy levels utilized during the direct sum; (b) the uncertainty in the number of (computed) bound rovibronic energy levels close to the first dissociation limit of the molecule; (c) the effect of unbound (scattering and resonance) states; and (d) the uncertainty of the physical constants employed when the thermochemical functions are generated. At low and high temperatures these factors have distinctly different contributions to the overall uncertainty of the caloric properties of "light" and "heavy" water. At high temperatures, the uncertainty in the density of the unbound molecular states determines the uncertainty of the thermochemical properties.

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Uncertainty Estimates for Atomic Structure Calculations

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Atomic structure calculations play a key role not only in plasma diagnostics and astrophysical calculations, but also in fundamental tests of quantum electrodynamics (QED) and elementary particle interactions. The accuracies that can be achieved for one-, two-, and three-electron systems place fundamental limits on what can be achieved for many-electron atoms. The talk will present a brief survey of uncertainty estimates for effects arising from both higher-order physical effects not included in the calculations (such as relativistic and/or QED corrections), and approximate solutions to the few-body Schroedinger (or Dirac) equation. For two- and three-electron atoms or ions, extremely accurate solutions can be obtained by use of explicitly correlated wave functions in Hylleraas coordinates. The results are essentially exact for all practical purposes in the nonrelativistic limit. However, this is not the case for many-electron atoms. Here, the generally applicable, but less accurate methods of atomic physics must be used, such as the Hartree-Fock approximation and its extensions to include electron correlation effects (configuration interaction and many-body perturbation theory). The low-Z and high-Z regions of nuclear charge must be considered separately. Here, uncertainty estimates are much more difficult, but important progress has been made in recent years in quantifying the computational uncertainties [1].

The requirement of uncertainty estimates for theoretical calculations, as appropriate, is now part of the acceptance criteria for papers published in *Physical Review A* [2]. The journal policies and their impacts on the field will be briefly discussed.

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Aassessing uncertainties for theoretical atomic data: bound state energies and transition probabilities

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I review the available experimental techniques for providing transition data for atomic systems. Techniques include picosecond spectroscopy and fast-beam-laser interaction for accurate measurements of neutral or near neutral systems, combined laser induced fluorescence (LIF) and branching ratio measurements (method referred to as gold standard for line list data) and finally storage ring and EBIT measurements of long lifetimes in highly charged systems. Then I continue to discuss what impact these experimental data has had on theoretical calculations and their error estimates. To follow up, I discuss what experimental atomic transition data are needed, and to what precision, to further advance our capacity to provide accurate atomic data along with error estimates. Finally I give a report of the activities, experimental and theoretical, in the Computational Atomic Structure (COMPAS[*]) group that are planned in response to the data needs of the fusion community and also to the data needs of the astrophysical community within the GAIA ESO survey.

[*]Homepage: http://ddwap.mah.se/tsjoek/compas/

Observation and Identification of Tungsten Spectra Observed with an Electron Beam Ion Trap

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Tungsten will be used as a plasma-facing material in ITER, and thus is considered to be the main impurity ions in the ITER plasma [1]. In order to suppress the radiation loss due to the emission from the impurity tungsten ions, it is important to understand the influx and the charge evolution of tungsten ions in the plasma through spectroscopic diagnostics. Thus, atomic data needs for tungsten ions have been noted in recent years, and a lot of experimental and theoretical effort has been made so far. However, further efforts are still strongly needed as the required data spread over wide ranges of charge state and wavelength.

An electron beam ion trap (EBIT) [2] is one of the powerful experimental devices for the spectroscopic studies of highly charged ions. An EBIT produces highly charged ions through successive ionization of trapped ions by a quasi-monoenergetic electron beam. The produced ions, which are mostly in the ground state, can be trapped with a narrow charge state distribution for many hours. It thus provides simple spectra that are useful to identify previously unreported lines [3].

The identification procedure often involves two steps. The first step is to identify the charge state of the ion that should be assigned to each line, and the second is to identify the upper and lower levels of the transitions. The first step can be done without the help of theory. For example, the electron beam energy dependence of the spectra is often used for identifying the charge state based on the fact that the maximum charge state in the trap is determined by the electron energy [3]. On the other hand, the second step needs theoretical support. In order to analyze EBIT spectra, collisional radiative model calculations are needed [4]. In both steps, careful analysis is needed especially for relatively low charge states, e.g. many electron systems, for which the energy level structure becomes complicated. In this paper, we present our recent efforts to observe and identify the relatively low charge state of tungsten ions with a compact EBIT [5].

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Benchmarking Visible Spectral Line Data for Highly Charged Tungsten Using an EBIT and GRASP Calculations.

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In this contribution we will discuss a single spectral line in W_{27+} - an M1 line between the two ground state fine structure levels $4d^{10}4f$ $^2F_{7/2}$ and $^2F_{5/2}$. This is the only transition within the ground configuration of this ion and therefore a challenge to identify spectroscopically. We have studied this line both experimentally using an EBIT and theoretically using the GRASP2K code [1]. These investigations were done independently and the results only compared when both methods had reached a conclusive wavelength, from careful and systematic considerations. One of the motivation for this work was the fact that earlier predictions for this transition showed a spread of over 400 Å for the wavelength [2, 3]. Our experiments were performed using the Shanghai permanent magnet EBIT and an Andor 303 Shamrock spectrometer equipped with an Andor Newton CCD camera. Tungsten was injected into the EBIT using the vaporous compound $W(CO)_6$. Spectra were recorded at several electron beam energies to isolate the W_{27+} line. The spectra were wavelength calibrated using a number of calibration lamps and the final experimental wavelength was determined to be 3377.43 ± 0.26 Å. To confirm the line was really from W_{27+} we determined the lifetime of the upper level of the ^2F term and compared our value with one from a calculation. As the line is from an M1 transition the lifetime of the upper level it is trivial to calculate the rate and thereby the lifetime. Our theoretical studies are systematic in two senses – first we investigate the contributions to the wavelength from different core subshells. These studies implies it is important to include core valence correlation even between the valence 4f and deep subshells – as a matter of fact, the correlation contribution from 3d is more pronounced than from 4d. The second dimension of the systematic approach is an increase of the *active set* of orbitals, and thereby the *space of configuration state functions (CSFs)* to show convergence of the final results.

Finally, after these independent investigation we are able to do *single-line spectroscopy* to identify this transition, since the agreement between our experimental and theoretical wavelength is within the order 0.1%, since the experimental vacuum wavelength is 3378.43 Å whereas the calculated wavelength is 3374.73 Å. This is probably the best agreement for such a transition in the visible region for a highly charged high Z ion.

We will also discuss cases in which this agreement could be even better, allowing for rigorous tests of minute effects – in the realm of Breit and QED interactions.

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Theoretical Electron Impact Ionization, Recombination, and Photon Emissivity Coefficient for Tungsten Ions

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Electron impact ionization (EII), dielectronic recombination (DR) and photon emissivity coefficient (PEC) for tungsten (W) ions have been calculated using flexible atomic code based on fully relativistic *jj*-coupling scheme. Those atomic data for W is necessary for spectroscopic and transport modeling of impurity in a magnetically-confined fusion tokamak since W has been a preferred first wall material in tokamaks.

The calculated EII cross sections for W^+ [1] and W^{17+} [2] were compared with other experiments and theoretical calculations. The calculated DR rate coefficients for W^{q+} (q = 44 - 46) [3] were compared with other ab-initio calculations and semi-empirical predictions. Uncertainties for calculated energies of levels, cross sections of EII, and rate coefficients of DR coming from orbital sensitivities due to local central potential choices and from configuration mixings are discussed. The calculated PEC for W^{q+} (q=5-48) and some results for its use in a prediction for VUV (λ = 14-22 nm) spectra from a tokamak are presented. The sensitivities of the spectra and fractional abundances for W ions to the underlying DR data set are shown and discussed.

DR rate coefficients for W^{5+} and W^{20+} are in the process of calculation with the same methodology for W^{q+} (q = 44 - 46) and of mutual verification with other previous predictions. The results will be also presented and discussed.

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KLL dielectronic recombination resonant strengths of He-like up to O-like tungsten ions

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Dielectronic recombination (DR) is an important process in hot plasma physics as well as in atomic structure and collision theory. Here we report the studies of the KLL DR resonance strengths of He-, Li-, Be-, B-, C-, N-, and O-like tungsten ions, through both experiment and calculation. The experimental resonance strengths were determined within uncertainty below 11% at the Shanghai electron beam ion trap by employing a fast electron beam-energy scanning technique. A fully relativistic configuration interaction method implemented in the flexible atomic code was employed to calculate DR process and also radiative recombination (RR). Also the consideration of the interference effect between DR and RR was revealed to be necessary to determine the resonance strength.

The experimental results of the total resonance strengths of He- to O-like tungsten ions agree very well with our calculations obtained by FAC, as in Fig.1. Furthermore, the total resonance strengths of B- and C-like ions agree well with a scaling law in the heavy ion region [1].
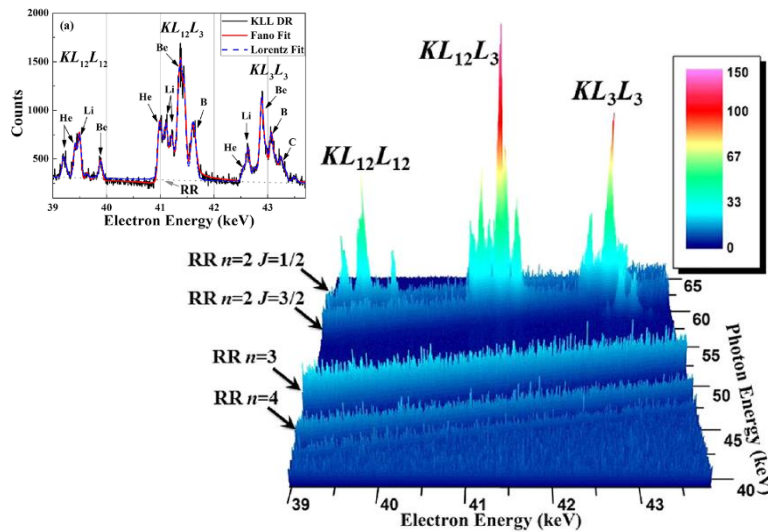

Fig. 1 Three-dimensional spectrum of x-ray intensity, as a function of electron energy for the x-axis and photon energy for the y-axis. The resonance peaks are from KLL DR events of He- up to O-like. More details can be found in [1].

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Electron Scattering on Molecules: Partial Cross Sections

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Total cross sections for electron scattering on atoms and molecules in gas phase, if free from systematic errors, can be determined within 5% accuracy. This is thanks to a simple, beam attenuation method and an absolute determination of target density.

Partial cross sections, like vibrational and electronic excitation must be determined by cross-beam methods, in which geometry of the scattering region and target density are not known directly. Experimental data need normalization (and integration over 0-180º scattering angle). Therefore, declared accuracies of cross sections are not better than 20-25%.

Ionization cross sections are somewhat easier to be measured, but also in this case systematic errors due to non-complete collections of ions produced can alter cross sections. Finally, cross sections for dissociation into neutrals need special techniques and have been determined only for some specific targets, like O_2, N_2O [1] or $CFH_3 - CF_4$ series [2].

Semiempirical methods like Born approximation for vibrational cross sections, Bethe-Born binary encounter model for ionization [3] and electronic excitation [4] give some guidelines for evaluation of experimental inconsistencies. Additionally, electron diffusion coefficients determined in swam experiments are extremely sensitive to partial (inelastic) cross sections. These mutual checks can produce self-consistent set of total and partial cross sections; unfortunately it was demonstrated only for relatively simple targets, like CH_4 [5].

In this paper, evaluation of experimental uncertainties on partial cross sections for selected molecules, like H_2, O_2, C_2H_2, NF_3 will be given. In this validation partial cross sections are compared to semi-empirical models and total cross sections constitute a reference limit for the sum check.

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Data evaluation of helium and its isotopes for fusion plasma

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Hydrogen and helium and their recombination molecules (H_2, HeH^+, etc) are important molecules in fusion plasmas and these molecule properties are studied by theoretically and experimentally. Thus, cross-section data for electron impact with hydrogen and helium and their combination molecules are surveyed and compiled. Cross sections are collected and reviewed for total scattering, elastic scattering, momentum transfer, excitations, electronic states, recombination, ionization, emission of radiation attachment. For each process, the recommended values of the cross section are presented for use. The literature has been surveyed through the end of 2015. A strong emphasis is placed on the consistency of the results determined by different techniques. In cases where only a single set of data is available for a given cross section those data are normally presented, but not designated as recommended, unless there is a strong reason to reject them.

First Step Benchmark of Inelastic Collision Cross Sections for Heavy Ions using Charge State Evolutions after Target Penetration

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In present plasma modelings, a set of accurate cross-sections is essential to checking the validity of introduced models for complicated phenomena taking place in fusion plasmas. Although the number of studies devoted to cross-section measurements has been notably decreased recently, immense improvements of computer power have brought new developments in theoretical procedures, which have synergistically realized more complicated calculations in more details, and the lack of directly-comparable experimental data for that detailed partial cross-sections, or even for total cross-sections, came to be a serious problem.

We propose here to make use of simpler phenomena consisted of various inelastic collision processes, whose model is well-established, as a first order benchmark of the validity of a set of cross-sections. In penetrating through targets, ions change their charge-states until they establish the equilibrium charge-state distribution, in which increases and decreases in population of each charge-state balance each other and the population seems to remain unchanged. Ratios of neighboring equilibrium charge-state fractions are equivalent to ratios of total single-electron capture and loss cross-sections between those charge-states, which has been used in checking consistency of these cross-sections. Before establishing the equilibrium, fractions for each nl-substate dynamically change accordingly to a set of rate-equations

$$\frac{dF_i(x)}{dx} = \sum_j F_j(x)\sigma_{ji} - \sum_j F_i(x)\sigma_{ij}, \quad \sum_i F_i(x) = 1,$$

where $F_i(x)$ denotes the fraction of specific i-substate at the penetration depth x, and σ_{ij} denotes collision cross-section or transition rate from substate i to j, i.e., those for excitation, collisional and radiative de-excitations, ionization, and charge transfer processes.

There exist several codes solving these nl-substate oriented rate-equations, whose results can be compared with experimental charge-state fractions after summed up to. The BREIT code [1] is a complete solver of these rate-equations, requiring separate input of the cross-sections, while the ETACHA code [2] treats 60 orbital-states up to $n = 4$ shell (with some approximation for higher n shells), through calculating the single-transfer cross-sections in the code. Comparison with experimental charge-state evolutions for 2.0 MeV/u C^{q+} ($q = 2$–6) and S^{q+} ($q = 6$–16) ions through C-foil targets [3] proved that the set of cross-sections ETACHA uses were rather good, although an empirical formula [4] better predicted the equilibrium charge-state distributions. The pre-equilibrium charge-state evolutions were quantitatively-well reproduced, but it was also suggested that inclusion of multiple-transfer cross-sections is needed when charge-state of penetrating ion is far separated from the equilibrium charge-state.

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