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IFRC Subcommittee on Atomic and Molecular Data for Fusion: Report on the Activities of the Atomic and Molecular Data Unit, June 2022 – May 2024

Prepared by

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Vienna, Austria

November 2024

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ABSTRACT

The 24th meeting of the Subcommittee on Atomic and Molecular Data of the International Fusion Research Council (IFRC) was held from 6 – 7 June 2024 as a hybrid event, with nine members attending in-person and one online. Activities of the Atomic and Molecular Data Unit for the period June 2022 – May 2024 were reviewed, and recommendations were made for continuing activities in 2024 – 2025 and for new projects in the 2026 – 2027 budget cycle. The proceedings, conclusions and recommendations of the Subcommittee meeting are described in this report.

November 2024

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Executive Summary and Recommendations

The International Fusion Research Council (IFRC) Subcommittee on Atomic and Molecular Data met at IAEA Headquarters in Vienna on 6 – 7 June 2024 to review the work of the Atomic and Molecular Data (AMD) Unit within the Nuclear Data Section. The Subcommittee heard presentations on the Unit's activities since the last meeting in May 2022 and discussed priorities for database development and evaluation, Coordinated Research Projects and Workshops, as well as the Unit's web presence and other planned activities.

The IFRC Subcommittee offers the following specific recommendations.

1. The AMD Unit should consider initiating **a database of experimental Visible / UV / VUV spectra** obtained from EBIT and magnetic confinement fusion plasma experiments to validate and benchmark theoretical models and simulations of atomic processes in plasmas (Section 15.3).

2. The **updated Methods of Work** for the IFRC Subcommittee (Appendix A) are now adopted following their approval by the IFRC Committee in July 2022.

3. The **Duty Travel** undertaken by Unit Staff members since the last Subcommittee meeting (Section 9) has been appropriate and relevant to the goals of the Unit; external publications (Section 10) by staff members were published in suitable journals and aligned with the Unit's activities on Atomic, Molecular and Plasma-Material Interaction data.

4. The AMD Unit should continue to organise **Workshops and Schools** on topics related to its remit (Section 12), and should continue to propose one such event at the International Centre for Theoretical Physics in each calendar year.

5. **The IFRC Subcommittee should seek to enlarge its membership** with suitably-qualified individuals from fusion research institutes in the Member States of India, Spain, Italy and the US (Section 14.2).

6. The AMD Unit's ongoing CRPs concerning Injected Impurities and Molecules in Edge Plasmas (Section 13) should conclude during the coming biennium (2026–27). The CRP on Tungsten Ions, will hold its first Research Coordination Meeting (RCM) in 2025 and will also continue into the next biennium. The Unit staff should seek to **extend the ongoing CRP on Hydrogen Permeation** (Section 15.1) to hold a fourth RCM during the 2026-27 biennium.

7. Given the work demanded by the programmatic activities of the Unit, the activities initiated during Christian Hill's and Kalle Heinola's tenure and those deemed necessary by the Subcommittee, it **recommends that the Unit staff be increased to the appropriate level**.

8. The **next IFRC Subcommittee meeting** should be held in **May or June 2026**.

As a final note, the Sub-committee would like to offer our commendation to the Unit Head (Christian Hill) and Atomic Physicist (Kalle Heinola) for their contributions to the Atomic and Molecular Data Unit over the past six years. They have done outstanding work in maintaining

and expanding the work of the Unit, even in the face of the COVID-19 shutdowns. Their efforts are truly appreciated.

James W. Davis, Chair
University of Toronto
Canada

Rémy Guirlet, Vice-Chair
CEA Cadarache
France

1. Introduction

The Subcommittee on Atomic and Molecular Data of the International Fusion Research Council (IFRC) meets biennially to advise on the work of the Atomic and Molecular Data Unit within the Nuclear Data Section. The meeting time, in the spring of even years is selected to coordinate with the budget and policy preparations of the Agency; meeting and budget plans for the next year are developed over the summer and preliminary CRP proposals for the next biennium (which starts in an even year) are reviewed in August or September.

The most recent previous meeting, the 23rd Subcommittee Meeting, was held from 16 – 17 May 2022 in-person at IAEA Headquarters in Vienna, Austria, and online for participants unable to travel. The report for this meeting is available online at https://amdis.iaea.org/meetings/ifrc-2022/. It provides a record of the projects and activities of the Atomic and Molecular Data (AMD) Unit for the period June 2021 – May 2022 and documents the recommendations made by the Subcommittee concerning planned activities for the current biennium (2024 – 2025).

This report summarizes the findings, recommendations and discussions of the 24th Subcommittee Meeting, held mostly in-person at IAEA Headquarters from 6 – 7 June 2024.

This report is divided into sections describing:

- Staffing and other administrative matters concerning the AMD Unit;
- The status of completed and ongoing Coordinated Research Projects (CRPs);
- Activities relating to data evaluation, data provision and standards recommendations in the Unit;
- Reports of discussions concerning the Data Centres Network (DCN), Code Centres Network (CCN), Global Network for the Atomic and Molecular Physics of Plasmas (GNAMPP) and other Technical Meetings;
- Training workshops conducted at the Abdus Salam International Centre for Theoretical Physics (ICTP);
- Duty travel undertaken by Unit staff;
- A list of publications produced by the Unit staff members;
- Cooperations, Practical Arrangements and other activities;
- A summary of planned activities for the next biennium, 2026 – 2027.

2. Staffing and Administrative Issues

Since the previous meeting, the AMD Unit has continued to operate with its full complement of staff. The roles of the Unit members are as follows:

Christian Hill	*Unit Head*
Kalle Heinola	*Atomic Physicist*
Ludmila Marian	*Scientific Data Manager**
Marco Verpelli	*Nuclear Data Analyst/Programmer**
Dipti	*SSA Consultant, Atomic and Molecular Data** *(Aug 2021 – Feb 2024)*
Khadidja Benyahia	*SSA Consultant, Atomic and Molecular Data* *(Apr 2024 – Jul 2024)*

* The duties and responsibilities of these roles are shared with other Units in the Nuclear Data Section.

Dipti's SSA contract was exceptionally renewed beyond the usual two years, and concluded at the start of 2024. A non-competitively recruited SSA consultant, Ms Khadidja Benyahia started a three-month position in April 2024.

The Unit Head, Mr Christian Hill, will rotate out of his position at the end of September 2024 and the role will be advertised by the Section in due course.

A full-time Junior Professional Officer (JPO), funded by Saudi Arabia at the P2 level will join the Unit as an Associate Data Scientist (Fusion Energy). Liaison with the funding authorities and recruitment is being handled at the Departmental level. This extra-budgetary position is offered in response to the proposal submitted by the Unit to the most recent call for JPO professionals with the following role:

> *The Associate Data Scientist is: 1) an analyst, reviewing and classifying journal literature in the area of atomic, molecular and plasma-material interaction data for fusion and interacting with producers, evaluators and users of such data; 2) a database developer, maintaining data libraries and their implementation as online services; and 3) a team member, carrying out scientific or technical research to support the exploitation of these data through validation and visualization software and the development of novel Machine Learning algorithms to create, manipulate and explore them.*

It is anticipated that the hired individual would spend a year in the Unit.

3. Coordinated Research Projects

F43023: Data for Atomic Processes of Neutral Beams in Fusion Plasma

Neutral beam injection is a standard method to heat the plasma in fusion experiments also has important diagnostic uses. Modelling of beam penetration into the plasma and of photoemission signals relies on detailed data for atomic processes. There are quite significant gaps in these data and the data that are available are often of uncertain quality. This CRP provides evaluated and recommended data for the principal atomic processes relevant to heating and diagnostic neutral beams in fusion plasmas. The primary emphasis is on processes of hydrogen (H and D) neutral beams in the high temperature core plasma.

Three Research Coordination Meetings (RCMs) were held in Vienna in 2017, 2019, and 2021. There are 11 participants from 10 Member States engaged in both the calculation of fundamental atomic collisional data and its application in neutral beam modelling codes.

Two code comparison exercises are associated with the Neutral Beams CRP and are described in detail in the CRP meetings' reports [1] and the report of the 23rd IFRC Subcommittee meeting [2]. A final meeting, to make recommendations of data and to plan the CRP final report, was held from 18 – 20 May 2022 [3]. The final report took the form of a Special Topic article in the journal Nuclear Fusion [4], co-authored by all CRP participants and published in October 2023 [4].

Data resulting from the Neutral Beams CRP has been deposited in the AMD Unit's CollisionDB database [5]. The CRP was officially finalized at a meeting of the Committee for Coordinated Research Activities (Nuclear Applications) (CCRA-NA) on 21 June 2023.

[1] https://amdis.iaea.org/CRP/neutral-beams
[2] https://amdis.iaea.org/meetings/ifrc-2022/
[3] https://amdis.iaea.org/meetings/neutral-beams-cm/
[4] C. Hill, Dipti, K. Heinola, A. Dubois, N. Sisourat, A. Taoutioui, H. Agueny, K. Tőkési, I. Ziaeian, C. Illescas, A. Jorge, L. Méndez, A. Kadyrov, N. Antonio, A. Kotian, T. Kirchner, A. Leung, J. Ko, J. Lee, O. Marchuk, M. O'Mullane, E. Litherland-Smith, G. Pokol, O. Asztalos, P. Balazs, Y. Wu, C. Jia, L. Liu, J. Wang, Atomic collisional data for neutral beam modeling in fusion plasmas, *Nuclear Fusion* **63**, 125001 (2023) [https://doi.org/10.1088/1741-4326/acf5da]
[5] https://amdis.iaea.org/db/collisiondb/

F43024: Atomic Data for Vapour Shielding in Fusion Devices

When wall material is rapidly evaporated or ablated by an energetic plume of hot plasma, a dense expanding plasma cloud is formed in front of the surface. In this dense plasma the incoming energy may largely be converted from fast particle kinetic energy into electromagnetic radiation directed away from the surface, thereby shielding the wall from further damage. This CRP focused on the provision of fundamental atomic and molecular data to accurately model

the vapour shielding phenomenon, with particular focus on novel liquid metal walls that have been proposed for use in magnetic confinement fusion devices.

Three RCMs were held over the lifetime of the CRP (2019 – 2023): 13 – 15 March 2019 (at IAEA HQ), 7 – 9 October 2020 (online event) and 19 – 21 October 2022 (IAEA HQ). There were nine participating groups from nine different Member States:

Participant	**Institution and Member state**	**Topics**
Mohamad AKEL	Atomic Energy Commission of Syria (AECS), Syria	Plasma-focus device exposure of Sn targets; A+M data
Igor BRAY	Curtin University, Australia	CCC applied to p + H, e + Li and p + Li
Roberto CELIBERTO	Polytechnic University of Bari, Italy	QM ro-vibrational properties e + Li_2 and e + LiH
Ronnie HOEKSTRA	University of Groningen, Netherland	Structure and interactions of Sn^{q+}; q<20
Ratko JANEV	Macedonian Academy of Sciences and Arts, North Macedonia	TC-AOCC on p + Li^+ and p + Sn^+
Predrag KRSTIĆ	Princeton Plasma Physics Laboratory, USA	Classical MD of Li surfaces with O and C impurities
Narendra SINGH	University of Delhi, India	Atomic data for Sn^{3-4+} and W^{11+}, W^{13+}
Francisco TABARÉS	Centro de Investigaciones Energeticas, Medioambientales y Tecnologicas (CIEMAT), Spain	LM (Li, Sn, LiSn) targets at TJ-11 (OLMAT project)
Ling LIU	Institute of Applied Physics and Computational Mathematics (IAPCM), China	AOCC and MOCC on p + Be and $Ne^{1,2+}$, $Ar^{1,2+}$

The following data were obtained and deposited with CollisionDB or the new pwiDB (plasma-wall interactions) as appropriate:

- Atomic data for Sn and W ions: $Sn^{3,4+}$, $Sn^{12–14+}$ and $W^{11–14+}$, W^{72+} (Flexible Atomic Code calculations)
- Heavy particle collisional processes: p + $Be^{1,3+}$ and p + Li (Atomic Orbital Close-Coupling (AOCC) and Molecular Orbital Close Coupling (MOCC) calculations)
- p + H collisonal processes (Wave-Packet Convergent Close-Coupling (WP-CCC))
- Electron-molecule collisions: e + LiH, e + Li_2 (Born-Bethe, T3M approximations)
- Hydrogen interaction with Li surfaces: H, D, D_2 → Li, LiH, LiD, LiO, Li_2O, LiOH (Molecular Dynamics)

32 articles arising from work carried out during the CRP have been published in the peer-reviewed literature; a full bibliography will be provided in the CRP final report (in preparation).

F43025: Hydrogen Permeation in Nuclear Materials

This CRP seeks to enhance the knowledge base and reduce uncertainties in data concerning the migration of hydrogen in component materials of relevance to nuclear fusion reactors. Materials of particular interest are tungsten; reduced-activation ferritic/martensitic steel (RAFM); materials used at interfaces and for piping, i.e. copper and the copper-based alloy CuCr1Zr0.1. Principal data needs are parameters affecting hydrogen transport in these materials, i.e. permeation, trapping, retention, and release (to be studied both experimentally and computationally through *ab initio* and multi-scale simulations); effect of neutron-induced damage and evolution of corresponding damage; component interfaces; and effect of surface chemistry, and surface evolution (e.g. through sputtering). As the CRP outcome there will be new detailed data relevant for the simulations and extrapolations of deuterium and tritium migration and transport in materials used in fusion reactor components. This data is planned to be published in the database *pwiDB*, which is dedicated to fusion data related to plasma-wall interaction processes.

There are 21 participating institutions from 15 Member States covering the following experimental and theoretical approaches:

- Gas-, ion- and plasma-driven permeation.
- Thermal Desorption Spectrometry (TDS), Nuclear Reaction Analysis (NRA), Positron Annihilation Spectroscopy (PAS), plasma devices, Scanning Electron Microscopy (SEM), Energy Dispersive X-ray Spectrometry (EDX), X-ray Photoelectron Spectroscopy (XPS), Glow Discharge Optical Emission Spectrometry (GDOES).
- Density Functional Theory (DFT), Molecular Dynamics (MD).
- Rate theory codes: Tritium Migration Analysis Program (TMAP), TESSIM (a diffusion trapping code), MHIMS (Migration of Hydrogen Isotopes in MaterialS).

Three RCMs and three Technical Meetings (TMs) are planned as part of this CRP:

- 23 – 25 Nov 2020: 1st RCM (online; 51 participants, 15 Member States);
- 4 – 6 Oct 2021: TM "Nuclear Fusion Fuel Permeation in Reactor First Wall Components" (hybrid event; 54 participants, 15 Members States);
- 11 – 12 April 2022: TM on "Effects of Hydrogen Supersaturation and Defect Stabilization in Nuclear Fusion Materials" (held in Aix-en-Provence, France; 17 experts, 6 Member States);
- 22 – 24 Feb 2023: 2nd RCM (IAEA HQ; 33 participants, 15 Member States);
- 3 – 5 Dec 2024 3rd RCM (IAEA HQ, scheduled);
- 2025, dates TBC (3rd Technical Meeting)

Subtask: Round-robin activity GDP for fusion materials (GDPFM)

The round-robin activity on gas-driven permeation (GDP) of hydrogen and deuterium in fusion plasma-facing materials is an outcome of the first RCM of this CRP in 2020. It focuses on GDP studies in EUROFER97 (batch #2), which is a reduced activation ferritic/martensitic (RAFM) steel. The activity aims to cross-compare permeation results obtained in different GDP facilities participating the CRP by using identically prepared RAFM samples. The EUROFER97 studied is provided by IPP Garching (Germany), and samples have been polished, annealed and pre-characterised at Forschungszentrum Jülich (FZJ; Germany) prior the distribution to participating laboratories. Currently there are three active participants: FZJ (Germany), CEA (France) and CNEA (Argentina). The GDP studies are carried out between 30 ºC and 550 ºC in the upstream pressure range between 10 – 1000 mbar and the experiments were done with samples with identical thicknesses and with and without Pd coating. This activity is coordinated by FZJ.

Subtask: Hydrogen in Neutron-irradiated Materials (HNIM)

This task studies the effect of neutron irradiation-induced defects on transport properties of hydrogen isotopes, including tritium, in fusion component materials. The activity comprises various studies on samples originating from two separate neutron irradiation campaigns at BR2 (Mol, Belgium). First campaign from 2017 – 2019 comprised of irradiations of various grades of tungsten and the samples were provided by SCK•CEN (Belgium). The second campaign was initially planned to take place in 2021 but, due to the COVID pandemic, had to be postponed first to 2022 and further to 2023. The campaign samples are provided by SCK-CEN (Belgium), UKAEA (UK) and MEPhI (Russia) and comprise of various grades of tungsten, CuCrZr, Mo, Fe, steels and EUROFER97 (batch #3). Irradiations were completed in end of 2023 and, at the time of writing, samples are about to be shipped to CRP participants at Idaho National Laboratory (USA), UKAEA (UK), MEPhI (Russia) and University of Helsinki (Finland).

The two irradiation campaigns cover a variety of dpa levels (up to 1 dpa) and irradiation temperatures (50 – 1200 °C). Permeation and the effect of defect evolution will be studied using (at least) the following experimental techniques: gas-driven permeation (GDP), plasma-driven permeation (PDP), Positron Annihilation Spectroscopy (PAS), thermal desorption spectrometry (TDS) and nuclear reaction analysis (NRA). The aim of the analyses is to characterize the resulted neutron damage in the samples and their effect to the diffusion and permeation of hydrogen species using deuterium and, notably, tritium isotopes. As the irradiation levels are expected to mainly comprise of single defects or small clusters, the qualitative and quantitative information on the damage evolution as a function of temperature plays a crucial role in understanding damage effects to fuel permeation and retention in the reactor armour and structural materials.

Participants and activities for the Hydrogen Permeation CRP

CSI	Institute and Member State	Activity
Tommy AHLGREN	University of Helsinki, Finland	Hydrogen Diffusion, Retention and Irradiation Induced Damade in Fusion-Relevant Materials
Pablo BRUZZONI	Comision Nacional de Energia Atomica (CNEA), Argentina	Study of Hydrogen Isotopes Permeation and Diffusion in F82H Ferritic-Matensitic Steel for Fusion Applications
Long CHEN	Beihang University, China	Deuterium Retention in Tungsten under Influences up to 10^{29} m^{-2}
Sergei DANILCHENKO	Institute of Applied Physics of National Academy of Sciences of Ukraine (NASU), Ukraine	Development of the X-Ray Diffraction (XRD) and Thermal Desorption Spectroscopy (TDS) Techniques for Investigation of Proton (Deuterium/Helium) Induced Near-Surface Effects

		in Fusion-Relevant Materials
Russell DOERNER / Anže ZALOŽNIK	University of California, San Diego, USA	Experimental Validation of H Permeability Models for Be, W and RAFM Steels
Yves FERRO	Aix Marseille Université - Laboratoire de Physique des Interactions Ioniques et Moléculaires - UMR 7345, France	Hydrogen Permeation through an Oxidized Tungsten Surface, at the Tungsten Copper Interface, and in Defective Beryllium
Christian CRISOLIA / Floriane MONTUPET-LE-BLOND	Commissariat a l'Energie Atomique et aux Energies Alternatives (CEA), France	Hydrogen Isotopes (Deuterium and Tritium) Permeation Studies in Fusion Materials
Anne HOUBEN	Forschungszentrum Jülich GmbH (FJZ), Germany	Hydrogen Permeation Studies on Fusion Materials and the Influence of Interfaces on the Permeation: Gas-driven Permeation Measurements on Bulk and Layered Substrates and Hydrogen Retention Studies
Wolfgang JACOB	Max-Planck-Gesellschaft zur Förderung der Wissenschaften e.V., Germany	Ion-Driven Permeation Experiments and Modelling
Mikhail LAVRENTIEV	UK Atomic Energy Authority, United Kingdom	Combined Experimental and Theoretical Studies of the Retention and Permeation of Hydrogen Isotopes in Fusion-Relevant Materials

Byeongchan LEE	Kyung Hee University, South Korea	Interatomic Potential Development for H Permeation in Critical Components
Qiao LI	Lanzhou Institute of Chemical Physics, China	Influence of the Permeation Barrier Oxide Layers on Hydrogen Permeation of W and RAFM Steel
Sabina MARKELJ	Jožef Stefan Institute, Slovenia	Experiments and Modelling of in Situ Uptake, Transport and Release Studies of Hydrogen Isotopes in Irradiated Tungsten
Ali MUSHARAF	Bhabha Atomic Research Centre, India	Atomistic Modeling of Permeation of Hydrogen Isotopes through Fe, W, Cu, and Cr
Olga OGORODNIKOVA	Moscow Engineering Physics Institute (MEPhI), Russia	Deuterium Retention and Permeation in W and Steels in the Presence of the Thermal Gradient, Ion-Induced Surface Modification and Defects
Yasuhisa OYA	Shizuoka University, Japan	Plasma Driven Permeation of Hydrogen Isotope for W
Daniel PRIMETZHOFER	Uppsala University, Sweden	Ion Beam Analyses of Materials Exposed to Hydrogen Isotopes (H,D,T) in Permeation Experiments: Surface Pre-Characterisation and Post-Exposure Depth Profiling of Isotopes in Steel, Tungsten, Cu-Cr-Zr

Masashi SHIMADA	Idaho National Laboratory (INL), USA	Plasma-and Gas-Driven Tritium Permeation in Fusion Materials
Dmitry TERENTYEV	Centre d'Etude de l'Energie Nucleaire -SCK.CEN, Belgium	Assessment of the Neutron Irradiation-Induced Microstructure of Fusion Materials in the Framework of Hydrogen Permeation
Brian WIRTH	University of Tennessee (UT), USA	Modeling and Experimental Investigation of Hydrogen Permeation in Fusion Materials
Haishan ZHOU	Chinese Academy of Sciences, China	Plasma-Driven Permeation of Hydrogen through Materials and Components

F43026: Atomic Data for Injected Impurities in Fusion Plasmas

Impurity ions are deliberately seeded into fusion plasmas for a variety of purposes. From the earliest days of magnetic-confinement fusion energy research, the spectra of light impurity ions, such as those of helium, lithium and carbon were used as a diagnostic tool to determine plasma properties. With the advent of very large-scale experimental devices such as ITER, impurity injection is increasingly being used to redistribute the power transported from the plasma core to the reactor wall in order to reduce the heat load on, and hence damage to, the plasma-facing reactor wall components. Furthermore, impurities such as nitrogen, neon and argon and have been used in such devices to improve plasma control by diminishing the amplitude of edge-localized modes (ELMs), plasma disruptions and other transient events that inhibit confinement and have the potential to cause serious damage to wall components.

In order to interpret and predict the behaviour and properties of impurities in fusion plasma, a significant amount of modelling, involving data on the collisional-radiative characteristics of the impurities and their environment is required. For a few species, high-quality data is available, but in many cases the currently-available data is incomplete, missing, or of uncertain quality.

This CRP will provide fundamental data for modelling the behaviour of first-row and noble gas atoms in edge and divertor plasmas for ELM and disruption mitigation and for plasma diagnostics, and establish a trusted repository of data concerning the collisional–radiative properties of plasma–impurity interactions to facilitate modelling of plasmas in magnetic confinement fusion devices.

The CRP was approved by a meeting of the Committee for Coordinated Research Activities (Nuclear Applications) (CCRA-NA) on 10 February 2022 and a Consultancy Meeting to plan the activity was held from 7 – 8 June 2022 [1]. Proposals for Research Agreements and Research Contracts were evaluated over the period to the end of 2022 and the first Research Coordination Meeting held virtually from 27 – 29 March 2023 [2]. The participating institutes, Chief Scientific Investigators (CSIs) and research areas are described in the table below.

The meeting noted the increased potential importance of boron as an plasma impurity because of its role as a hardener and getter for tungsten in the most recent proposals for the ITER first wall. This will be discussed at the next RCM of the CRP with a view to putting the generation and evaluation of data on boron and its ions as high-priority activities within the project.

[1] https://amdis.iaea.org/meetings/ii-cm/
[2] https://amdis.iaea.org/meetings/injected-impurities-rcm1/

Participants and activities for the Injected Impurities CRP

CSI	Institution and Member state	Topics
Haikel JELASSI	National Center of Nuclear Sciences and Technologies (CNSTN), Tunisia	Energy levels, oscillator strength, radiative rates, electron impact excitation and radiative recombination process of He-like, Li-like and Be-like Ne, Ar and N ions
Valdas JONAUSKAS	Vilnius University, Lithuania	Calculation of cross sections and rate coefficients for the ionization process for the N^{+}, N^{2+}, $Ne^{+?}$, Ne^{3*}, Ne^{**}, Ar^{3+}, Ar^{**} and ArS ions
Alisher KADYROV	Faculty of Science and Engineering, Curtin University, Australia	Interactions of C, N, O, Ne, Ar, W with H, D, T, He and H_2 (and isotopologues)
Xinwen MA	Institute of Modern Physics, Chinese Academy of Sciences (IMPCAS), China	Dielectronic recombination (DR) precision spectroscopy; DR measurement for the Ar^{9+} (F-like), Ar^{10+}, Ar^{11+}, Ar^{13+} ions.
Sebastián OTRANTO	Instituto de Física del Sur (IFISUR), Universidad Nacional del Sur (UNS), Argentina	State selective charge exchange processes between Ar and Ne ions with hydrogen (1s, 2s, 2p) by CTMC
Yuri RALCHENKO	National Institute of Standards and Technology, USA	Critical evaluation of atomic spectroscopic data for typical injected impurities in fusion plasmas (e.g., Ar, N, Ne)
Lalita SHARMA	Indian Institute of Technology, Roorkee, India	Atomic structures and electron impact excitation cross-sections of impurity ions (N, Ne, Ar, Kr, and Xe)
Nicolas SISOURAT	Laboratoire de Chimie Physique – Matière et Rayonnement (LCPMR), Sorbonne Université, France	Accurate cross sections for charge exchange between nitrogen ions and hydrogen atoms in a wide range of collision energies using MOCC, ASCC
Károly TŐKÉSI	Institute for Nuclear Research (ATOMKI), Hungary	Ionization, charge exchange and excitation cross sections in collision between Li, Na, He, Ne, Ar ions with ground and excited states hydrogen atoms ([Q]CTMC)

Participants and activities for the Injected Impurities CRP

Zhongshi YANG	Institute of Plasma Physics, Chinese Academy of Sciences (ASIPP), China	Impurity transport in edge plasma with Ar/Ne seeded radiative divertor operation on the EAST tokamak

F43027: The Formation and Properties of Molecules in Edge Plasmas

Molecules are known to play an important role in the physics of the edge regions of magnetically-confined plasmas. In the detached divertor region with high recycling, the isotopologues of hydrogen molecules can be present at relatively high concentrations: these molecules will undergo a variety of processes including vibrational excitation, dissociation and ionization through collisions with other energetic plasma particles.In addition, various other hydrogen-containing molecules form, directly or indirectly as a result of interactions of plasma particles with reactor surfaces: the impact and properties of species such as BeH and BeH^+ on, for example, impurity transport remains unquantified.

The goal of this CRP is to recommend fundamental data concerning the formation, spectroscopic properties and reactions of molecular species in the boundary plasmas of magnetic-confinement fusion devices; participants will be drawn from the fusion plasma modelling community and the network of computational and experimental plasma physicists working on the calculation and measurement of the collisional and spectroscopic properties of molecules under relevant conditions of temperature and density.

This CRP was approved by a meeting of the Committee for Coordinated Research Activities (Nuclear Applications) (CCRA-NA) on 20 June 2023 following a Consultancy Meeting to plan the activity held from 20 – 21 April 2023 [1]. Proposals for Research Agreements and Research Contracts were evaluated over the period to the end of 2023 and the first Research Coordination Meeting held at IAEA Headquarters from 6 – 8 December 2023 [2]. The participating institutes, CSIs and research areas are described in the table below.

- *Data for molecular hydrogen*: Plasma-molecular interactions can have a profound impact on detachment physics, interpretation of optical emission diagnostics and detachment control, particularly in strongly-baffled Alternative Divertor Configurations. Recent work showed the importance of such processes experimentally and has shown strong contrasts between experiments and simulation results, due to inaccuracies in the hydrogen molecular data used in exhaust simulations. To address these challenges, the rate data used in plasma-edge simulations requires revision. Within this CRP, UKAEA will perform an overview and assessment of currently used rate data; following this, recommendations will be made, in consultation with all CRP participants, concerning how the data can be revised with the aim of constructing a new, recommended data set, preferably with uncertainties, which can be validated through collisional-radiative modelling and post-processing of higher-level exhaust simulations.

- *Data for boron-containing species*: This planned collaboration between Forschungszentrum Jülich, Germany and the National Institute for Fusion Science, Japan will aim to validate the

Participants and activities for the Molecules in Edge Plasmas CRP

CSI	Institution and Member state	Topics
Ghassan ANTAR	American University of Beirut, Lebanon	Design and operation of a leak-detection system for the ITER vacuum vessel based on glow-discharge of water
Dmitriy BORODIN	Forschungszentrum Jülich, Germany	Improvement of the collisional-radiative model (CRM) in the EIRENE edge plasma code
Kalyan CHAKRABARTI	Scottish Church College, India	Collision cross secction calculations on two or more of the molecules/molecular ions: BH, LiH, BeH_2^+, BH+, BH_2, BH_2^+
Dmitry FURSA	Curtin University, Australia	MCCC calculations of electron-impact collisional cross sections for processes involving H_2, HeH^+, LiH, LiH^+, BH, and BH^+
Tomoko KAWATE	National Institute for Fusion Science, Japan	Molecular structure and electron-impact excitation/ionization cross section calculations for boron hydride molecules; analysis of LHD experimental activities.
Åsa LARSON	Stockholm University, Sweden	Calculation of electron scattering processes with molecular cations, such as dissociative recombination, rovibrational excitation/de-excitation and dissociative excitation can be studied
Nicolina POP	Politehnica University of Timișoara, Romania	Systematic calculations of dissociative recombination (DR), vibrational excitation (VE) and dissociative excitation (DE) cross sections and rate coefficients for electron impact on BeH+ and isotopologues; DR and RVE (rovibrational excitation) cross sections for H_2^+ , D_2^+, HD^+ , NH^+.
Ioan SCHNEIDER	Université le Havre Normandie, France	Multichannel Quantum Defect Theory applied to H_2^+, NeH^+ and BH^+.
Jonathan TENNYSON	University College London, UK	Spectroscopy and electron collision calculations for BH, BH^+, LiH, WH, OH, OH^+ and possibly NH, NH^+.
Kevin VERHAEGH	UKAEA, UK	Compilation and evaluation of data relevant to modelling the divertor regions of experimental magnetic-confinement fusion devices.

modelling of boron-containing molecules, ions and radicals, including BH and BH^+ using

data from the Large Helical Device (LHD) which has undergone boronization for wall-conditioning in several experimental campaigns. Because of programmatic priorities at NIFS, details of the activity will be established at the second RCM, likely to be held in 2025.

- *Data for water-derived species in glow discharges for leak detection*: The American University of Beirut (AUB), in collaboration with ITER, is exploring the concept of detecting and localizing leaks in the ITER vacuum vessel using a glow-discharge plasma. In practice, this requires spectral and collisional data for molecular and molecule ion fragments derived from H_2O. A collaboration between AUB and University College London has been initiated to provide these data for use in modelling activities.

[1] https://amdis.iaea.org/meetings/molecules-cm/
[2] https://amdis.iaea.org/meetings/edge-plasmas-rcm1/

4. Data Services

The AMD Unit maintains several databases of fundamental atomic and molecular data of relevance to nuclear fusion. They are updated by Unit staff, and through projects, *ad hoc* consultancies and arrangements with research institutes in several Member States, particularly NIST (USA), KFE (Republic of Korea) and NIFS (Japan).

ALADDIN and CollisionDB

ALADDIN (A Labelled Atomic Data INterface, [1]) has historically been the Unit's principal numerical database. It stores and maintains only recommended and critically assessed (evaluated) numerical databases of atomic and molecular (A+M) collisional and radiative properties (cross sections, spectroscopic data), plasma-surface interactions (PSI) processes (such as physical sputtering, erosion, etc.) and bulk material properties (e.g. thermomechanical properties, particle diffusion, retention, etc.) for nuclear fusion research.

Data are mostly compiled from the IAEA APID series, published results of Coordinated Research Projects (CRP) and from consultancies arranged by the Unit.

The ALADDIN database and its online interface have been improved to integrate better with other resources and with the removal of duplicated, ambiguous and incorrect data. The valid plasma collisional data are now part of CollisionDB [2], a online database and software platform initiated in Autumn 2021. CollisionDB provides a searchable interface for accessing published (but not necessarily critically-assessed) data which, at the time of writing, holds 122 568 records. Evaluated data, including data from ALADDIN are flagged as such in CollisionDB.

CollisionDB exposes an Application Programming Interface (API) and a Python library, PyCollisionDB [3] has been written to interact with this API. The project is described in detail in a recent publication in the journal *Atoms* [4].

[1] https://www-amdis.iaea.org/ALADDIN/
[2] https://amdis.iaea.org/db/collisiondb
[3] https://github.com/xnx/pycollisiondb
[4] C. Hill, Dipti, K. Heinola, M. Haničinec, CollisionDB: A new database of atomic and molecular collisional processes with an interactive API, *Atoms* **12**(4), 20 (2024). doi:https://doi.org/10.3390/atoms12040020

AMBDAS

AMBDAS (Atomic and Molecular Bibliographic Data System) is a bibliographic database of peer-reviewed articles presenting data on atomic, molecular and plasma-surface interactions for nuclear fusion research. Publications are searchable by reactant species (or surface), data category (collisional process, electronic structure property, plasma modelling application, spectral parameters, etc). Updates to the database occur at least twice a year, in particular with regular contributions from colleagues at NIST (atomic spectroscopy), KFE and NIFS (collisional processes).

A new online interface for AMBDAS, available at https://amdis.iaea.org/db/ambdas has been developed and, at the time of writing contains 52 331 records. As well as improving the search functionality, the references were reclassified according to the plasma processes identified in the Technical Meeting *Standards and Software Tools for Atomic and Molecular Databases* held at IAEA Headquarters in November 2019. These processes and the abbreviations used for them in AMBDAS are described at https://amdis.iaea.org/databases/processes. The latest edition of the standards document describing these classifications is version 2.5 (April 2024).

CascadesDB

The CascadesDB database project, which was initiated by the 5th Code Centres Network Meeting held in November 2017, is a repository of molecular dynamics simulations of collision cascades in materials of relevance to nuclear fusion energy research. At the time of writing it contains 17 024 simulations for eight different elemental materials approximately 1 TB of data. The data are described by a flexible and comprehensive metadata schema; the online, searchable interface can be queried by author, material, temperature and projectile or primary knock-on atom (PKA) energy, and returns links to compressed archives containing the simulation xyz

files and the associated metadata in HTML, XML, JSON and plain text formats. Further details are available at the URL https://cascadesdb.iaea.org/.

Future work on CascadesDB will improve and simplify the process for uploading new data sets and extend the CSaransh software [1], developed by the Bhabha Atomic Research Centre (BARC), to post-process molecular dynamics simulations of collision cascades in order to provide a machine-readable, statistical summary of the defect classification and distribution for each cascade simulation.

[1] https://github.com/haptork/csaransh

DefectDB

DefectDB is a database of density functional theory (DFT) calculations of radiation-induced defect structures in materials of interest to nuclear fusion and fission applications. A Consultancy Meeting, held in January 2020 at IAEA Headquarters with experts from CEA Paris-Saclay, developed the relational database model for this repository and deployed a prototype interface at https://db-amdis.org/defectdb; further development of this resource has been hampered by unsuccessful attempts to engage a consultant in the activity of uploading new data sets and by an apparent reluctance of some researchers with DFT data to share these data in a free, online database.

Clerval

Clerval [1] is a database of institutions and events of relevance to the use, calculation and measurement of atomic, molecular and plasma-material interaction data in nuclear fusion research. In addition to being a resource for the fusion community, it serves as part of the backend of the new AMD Unit website to assist with the management of meetings, CRPs and other projects. Institutions, events and people are associated with keywords which help organize content and facilitate searching. At the time of writing, Clerval contains 399 institutions, 964 people, 190 events (conferences, workshops and other meetings) and 33 external databases in atomic and molecular physics.

[1] https://amdis.iaea.org/clerval/

pwiDB: Plasma-Wall Interactions Database

In 2023 a new database resource, pwiDB [1], was initiated to store and distribute fundamental plasma-wall interaction data for fusion energy research. The database is divided into two parts, tentatively referred to as psiDB: plasma-surface interactions (including sputtering, retention

and reflection) and pmiDB: plasma-(bulk) material interactions (including diffusivity, solubility and permeation). The first of these contains data generated as part of CRP F43024: Vapour Shielding whilst the second has been populated from data provided by G. de Temmerman (formerly at ITER) and by M. Lavrentiev (UKAEA). At the time of writing, psiDB contains 25 datasets and pmiDB contains 287; for the most part this database was populated by the AMD Unit's consultant, Ms Benyahia.

Both databases provide online search functionality, full metadata exportable in JSON format and browser-based visualization tools.

[1] https://db-amdis.org/pwidb

5. Technical Meetings

Atomic Processes in Plasmas (APiP) (2023 Technical Meeting)

This biennial conference series originally planned to hold its 21st meeting in Vienna in the spring of 2021. The disruption caused by the COVID pandemic have led to its postponement, and was held as a Technical Meeting, jointly with the 27th meeting of the Data Centres Network from 15 – 19 May 2023. The organising committee was chaired by the AMD Unit Head. The website and meeting report are available on the Unit website [1].

The committee members were:

- Djamel Benredjem, Laboratoire Aimé-Cotton de l'université Paris-Sud, France
- Hyun-Kyung Chung, Korea Institute of Fusion Energy, Republic of Korea
- Christian Hill, International Atomic Energy Agency, Vienna, Austria
- Hae Ja Lee, Stanford Linear Accelerator, United States of America
- Oleksandr Marchuk, Forschungszentrum Jülich, Germany
- Taisuke Nagayama, Sandia National Laboratories, United States of America
- Nobuyuki Nakamura, University of Electro Communications, Japan
- Olivier Peyrusse, Lab. PIIM, Aix-Marseille Université, France
- Matthew Reinke, Oak Ridge National Laboratory, United States of America

The local organizers were:

- Christian Hill, International Atomic Energy Agency, Vienna, Austria
- Kalle Heinola, International Atomic Energy Agency, Vienna, Austria
- Dipti (consultant), International Atomic Energy Agency, Vienna, Austria
- Bastiaan Braams (consultant), International Atomic Energy Agency, Vienna, Austria

- Charisse Monfero (administrative assistant), International Atomic Energy Agency, Vienna, Austria
- Lidija Vrapcenjak (administrative assistant), International Atomic Energy Agency, Vienna, Austria

The topics sessions encompass a wide range of theoretical and experimental techniques relevant to the fundamental physics of plasmas:

- Magnetically-confined fusion plasmas
- Astrophysical and atmospheric plasmas
- Atomic and molecular data for plasma research
- Low-temperature plasmas
- X-ray sources
- Warm dense matter
- Medical applications of plasmas
- High energy-density plasmas
- Laser-plasma interactions
- Data resources for plasma modelling
- Plasma spectroscopy

In addition, there was a six-lecture series of tutorials which were recorded and the videos made available online at the meeting website [1]:

- *Atomic processes in plasmas*, Yuri Ralchenko (NIST, USA)
- *Atomic cross-section calculations*, Chris Fontes (LANL, USA) and Connor Ballance (QUB, UK)
- *FAC for intermediate users*, Ming Feng Gu (UC Berkeley, USA; Prism Computational Sciences Inc.)
- *Density effects on plasmas*, Stephanie Hansen (Sandia, USA)
- *Electron-molecule collisions*, Mourad Telmini (University of Tunis El Manar, Tunisia)
- *X-ray lasers*, Nina Rohringer (DESY, Germany)

[1] https://amdis.iaea.org/meetings/apip21/

Data Centres Network

The Data Centres Network (DCN) for atomic, molecular and plasma-material interaction (AMPMI) is a collection of 12 national data centres for the collection, critical assessment, evaluation and generation of fundamental AMPMI data for fusion applications. The biennial DCN meeting of has taken place since 1977 and has been coordinated and hosted by the AMD Unit.

The 27th DCN meeting in 2023 was organized as a parallel event with the 21st Atomic Processes in Plasmas (APiP) Conference. Both events took place in-person at the IAEA Headquarters. DCN meeting participants comprised of network members and three guest experts representing Oak Ridge National Laboratory (USA), Vilnius University (Lithuania) and Sorbonne Université (France).

The objectives of the DCN meeting are to exchange information regarding the activities of the data centres and to review their progress; to coordinate the work in the national data centres by assessing priorities in data evaluation and production, and to make plans for specific evaluations; to evaluate and revise procedures for collection and exchange of bibliographical and numerical data; and to review atomic and molecular data needs for nuclear fusion research. Discussions were held on the following topics:

- Status and recent developments of data centres in the last two years (Sep. 2021 – May 2023);
- Requirements for the generation, validation, and compilation of AMPMI data for fusion applications. Points of focus were on processes with tungsten, injected impurities (such as the X-point radiator gases) and boron;
- Applications of neural networks to determination of ion stopping powers in matter;
- Collisional-radiative (CR) models of H and D plasmas
- Measurements and calculations of S/XB ratio of sputtered W I species;
- Uncertainty quantification (UQ) of fundamental data for fusion plasmas and proposed new meetings. Continued discussion on the UQ workshop focusing to nitrogen as a studied system. Current DCN meeting had two presentations focusing nitrogen processes: e + N^{1-2+} ionization and cross sections for state-resolved H + N^{2-3+}.

Code Centres Network

The Code Centres Network (CCN), coordinated by the AMD Unit, is a joint effort to gather and provide access to any information relevant for modellers in fusion plasma science. Its focus is on the modelling and calculation of data that are difficult to measure experimentally. Every two years, AMD Unit staff identify an area with data needs within the scope of the the Network and invite qualified participants to contribute to addressing these needs.

The 8th meeting of the CCN was held, in virtual format from 15 – 17 November 2023 and discussed the current status and future administration of the Virtual Atomic and Molecular Data Centres Consortium (VAMDC), in particular with respect to sustainability and promoting FAIR data principles within consortium members.

The VAMDC aims to be an interoperable e-infrastructure that provides the international research community with access to a broad range of atomic and molecular data. The data format

proposed to facilitate this interoperability, the XML-based XSAMS format, was drafted in a Technical Meeting of the IAEA in 2003. In the subsequent two decades, however, JSON (JavaScript Object Notation) has overtaken XML as a more practical and efficient storage and interchange format. The meeting explored ways in which modern large language model (LLM) artificial intelligence tools can be leveraged to effect the conversion of existing data from XSAMS to JSON.

The online nature of the meeting meant that a large number of VAMDC stakeholders could participate and 34 representatives from 11 Member States contributed. The consortium currently links 39 databases, 25 of which were represented at the meeting. More details, including the meeting report, are available on the meeting website [1].

[1] https://amdis.iaea.org/meetings/ccn-8/

Technical Meeting on Collisional-Radiative Properties of Tungsten and Hydrogen in Edge Plasma of Fusion Devices

The 2nd Technical Meeting on CR properties of Tungsten and Hydrogen in Edge Plasmas was held from 28 November – 1 December 2023, at IAEA Headquarters [1,2]. This in-person event gathered 40 participants representing 17 Member States and ITER. In addition to sessions focusing on experiments and modelling of plasma processes in fusion devices there were sessions on fundamental and collisional-radiative modelling, and the programme included a special session on open issues in the new ITER operational baseline.

The meeting followed the outline and priorities set as an outcome from the 1st Technical Meeting on CR properties of Tungsten and Hydrogen held from 28 March – 1 April 2021. The three Working Groups (WGs) are those established after the 2021 meeting:

- WG 1: Atomic and Molecular Data Recommendation and Validation with CR Models for W and Hydrogen
- WG 2: Plasma Experiments and Comparison Activities with CR Models
    a) W and Hydrogen Experiments with Fusion Devices and Linear Plasma Devices
    b) The Inclusion of Reduced Photon Opacity Information in CR Models
- WG 3: Plasma-Surface Process Properties, Trends and Underlying Effects

Specific highlights from the discussions are as follows:

- Experimental data from the third D-T plasma operation campaign at JET tokamak (JET DT3) is unique and the first molecular spectra on the formation of TT and DT is available.

- The worlds largest stellarator, Wendelstein 7-X (W7-X), has made spectroscopic observation on the formation of H_2 molecules.
- Outlining ITER fusion data needs played key topic in the discussions: role of boronization in the plasma operation; formation of B and B-W layers and their impact on spectroscopy and the corresponding data needs; impurity injection optimization in full-W wall configuration to minimize the W source through sputtering processes; role of impacts from plasma edge-localized modes (ELMs) and charge exchange neutrals (CXNs) to W influx from the wall.
- Measurements of ground-state population of sputtered W species.
- Modelling of W metastables important as they can play a crucial role in quantifying the plasma W content; nature of W^{0-5+} states should be modelled; *e*-impact ionization cross sections to W^{7-10+} and W^{38-45+}.
- Ionisation of sputtered W^0 still a priority (modelling and experiments needed).
- Surface models for W sputtering; effect of the magnetic field *B* to W redeposition.
- CR modelling community has a great need for an extensive database of reaction probabilities. The error bas from CR modelling correlate directly with the quality of the input data.
- Successful progress have been done for a CR hybrid model for W^{20-35+}. The next step is a CR model for lower W^{q+} as these are greatly needed.
- The cross section data used in molecular convergent closed-coupling (MCCC) calculations for e + molecular hydrogen processes provides good results, but more molecular data is needed: e.g. molecular CX processes, hydrogen impact excitation and ionization, etc. In particular, input data for D_2 is essential.

[1] https://conferences.iaea.org/e/tm-W-H-2
[2] https://amdis.iaea.org/meetings/tm-tungsten-hydrogen-2/

6. Schools and Workshops

The IAEA organizes several Workshops, often in conjunction with the Abdus Salam International Centre for Theoretical Physics (ICTP) in Trieste, Italy; in recent years the AMD Unit has participated in this by running training and information exchange events for computational scientists working on models and data for atomic, molecular and materials processes relevant to fusion energy research.

A single ICTP Workshop was held in Trieste in 2024 and the AMD Unit cooperated in an externally-organised event in Valladolid in 2023 – these are described below.

6.1 International School on Atomic and Molecular Data Evaluation and Curation

This School was held from 22 – 25 October 2023 at the Faculty of Sciences at the University of Valladolid, Spain, in cooperation with the National Institute of Standards and Technology (NIST), USA and the IAEA. The 4-day event of lectures and computing practical exercises was designed to help early-career researchers develop their knowledge of good practices regarding critical compilation and treatment of atomic data and to provide networking and knowledge-exchanging activities. Specifically, the School objectives were:

- Training of data producers and future group leaders on critical compilation and curation of atomic data.
- Developing skills for atomic data description and classification (metadata descriptors, FAIR data principles and similar).
- Connecting the atomic data community with the NLTE atomic kinetics community to enhance communication.
- Establishment of collaborations and partnerships among participants.
- Networking, Knowledge Exchange and Capacity-building within the atomic data community.

More details are available at https://amdis.iaea.org/meetings/isamdec-1/.

6.2 Joint ICTP/IAEA School on Data for Modelling Atomic and Molecular Processes in Plasmas

This joint IAEA-ICTP Workshop was a 5-day series of lectures and computing practical exercises to help early-career plasma physicists develop an understanding of the techniques used to model and simulate the radiative and collisional properties of plasmas. The topics chosen are those relevant to the modelling and spectroscopic analysis of plasmas at the atomic level with applications to fusion, astrophysics and industry.

The course directors were:

- Christian Hill (IAEA)
- Kalle Heinola (IAEA)
- Dipti (IAEA)
- Yuri Ralchenko (National Institute of Standards and Technology, USA)
- Sebastiján Brezinsek, (Forschungszentrum Jülich, Germany)
- Sandro Scandolo (ICTP, local organizer)

53 participants from 20 Member States joined seven lecturers for a combination of lectures, posters (as short, contributed presentations) and practical sessions covering the following topics:

- Fundamental principles of spectroscopic diagnostics

- Advances in experimental plasma diagnostic techniques
- Calculations of atomic and molecular structure and properties
- Collisional-radiative modelling
- Online codes for the calculation of ionization distributions and spectra
- Spectroscopic characteristics of non-Maxwellian and highly transient plasmas
- Spectral line broadening
- Astrophysical spectroscopy
- Plasma opacity
- Principles of evaluation and uncertainty quantification of atomic and molecular data
- Data management and dissemination

More details are available at https://amdis.iaea.org/workshops/ictp-2024. This Workshop was also well-received, as interpreted through the anonymous questionnaire that participants completed. 28 responses were received; the mean overall rating given was 8.93/10 (σ = 1.12).

7. Women in Fusion Group

The Women in Fusion (WiF) group was launched in 2021 with the support from IAEA, ITER, Fusion for Energy (F4E), EUROfusion, General Atomics and Indian Youth Nuclear Society. WiF activities are managed through a Steering Committee, which comprises of its eight founding members. WiF is a global organization with an aim to act as platform and meeting point for national groups and other organizations and individuals. It encourages women working in fusion and supports women with various backgrounds. WiF promotes diversity in the fusion workforce, promotes women's contribution to the field of fusion and pursues to attract and retain talent and future generations in this field. IAEA supports WiF through activities by Kalle Heinola (AMD Unit), who takes part in the strategic and executive planning, event organization as well as provides technical coordination and assistance.

- The WiF webpage was launched in July 2022 [1].
- As of Jan 2023, WiF is a registered legal independent entity (NPO and NGO).
- WiF is free for its members. Currently it has more than 700 members covering Europe, North and South America, Africa, Asia and Oceania.
- WiF launched a global mentoring programme on 8 March 2023. Areas of mentoring include physics, engineering, administration and communications.
- During period 2022 – 2023:
    - WiF was a panel and seminar organizer/co-organizer in 11 international conferences and symposiums;
    - WiF organized five seminars.

[1] https://www.womeninfusion.org

8. Unit Website

Developments

The Atomic and Molecular Data Unit has continued to maintain and develop its website to communicate its work and provide details to meeting and project participants. The official URL is https://amdis.iaea.org/. The email address, fusion-data@iaea.org, provides a point of contact for Unit staff independent of any one individual. Some resources, particularly the ALADDIN and legacy AMBDAS databases remain on the older website, https://www-amdis.iaea.org/, which is still publicly available. As discussed above, the migration of the remaining plasma-surface interaction data from ALADDIN onto a new platform is under way.

Statistics

The Unit's website received 67 000 page views by 14 000 users over the time period May 2023 – June 2024, as compared with 52 000 page views by 9 500 users in the previous year. It is noted that the top 10 countries visiting the site are all members of the ITER consortium. In total, users from 163 countries have accessed the AMDIS web services.

9. Duty Travel

Duty Travel by AMD Unit staff members continues to be an important means of communicating our activities to the relevant communities and of meeting with CRP participants and other stakeholders between Technical and Research Coordination Meetings. The Duty Travel trips undertaken by Unit staff since the previous IFRC Subcommittee meeting are listed below.

- 23 – 25 August 2022, Meetings with LOC of IAEA Decennial Meeting on Fusion Data at University of Helsinki and VTT Technical Research Centre of Finland, Helsinki and Espoo, Finland (K. Heinola)
- 25 – 29 September 2022, *12th International Conference on Atomic and Molecular Data and their Applications (ICAMDATA)*, Bari, Italy: to act as co-director and panellist (C. Hill)
- 3 – 7 October 2022, *75th Annual Gaseous Electronics Conference*, Sendai, Japan: to give an invited presentation (C. Hill)
- 14 – 18 November 2022, Meetings with UKAEA, Culham, UK (K. Heinola)
- 5 – 10 December 2022, *43rd Annual Meeting of Fusion Power Associates & 2nd Steering Committee Meeting of Women in Fusion*, Washington, USA (K. Heinola)
- 31 January – 2 February 2023, Integration of the CollisionDB API with the Neutral Beam modelling code RENATE and expansion of the CollisionDB data sets on alkali atom processes, Budapest, Hungary (C. Hill and Dipti)
- 22 – 26 May 2023, *19th International Conference on Plasma-facing Components and Materials (PFMC)*, Bonn, Germany (K. Heinola)

- 29 – 31 May 2023, *6th International Workshop on Models and Data for Plasma-material Interactions in Fusion Devices (MoD-PMI)*, Aachen, Germany (K. Heinola)
- 25 July – 1 August 2023, *33rd Conference on Photonic, Electronic and Atomic Collisions (ICPEAC)*, Ottawa, Canada: to represent the AMD Unit and present (C. Hill)
- 5 – 7 September 2023, Database population of DefectDB, Aix Marseille University, Marseille, France (K. Heinola)
- 20 – 22 September 2023, Software infrastructure and population of the CascadesDB database, Helsinki, Finland (C. Hill)
- 15 October 2023, *62nd Meeting of the International Fusion Research Council (IFRC)*, London, UK (K. Heinola)
- 16 – 21 October 2023, *29th IAEA Fusion Energy Conference (FEC 2023)*, London, UK: to represent the AMD Unit (C. Hill and K. Heinola)
- 22 – 25 October 2023, *1st International School on Atomic and Molecular Data Evaluation and Curation*, Valladolid, Spain: to act as co-organizer and lecturer (C. Hill)
- 23 – 25 January 2024, *Annual Meeting of the Fusion Power Coordination Committee (FPCC) of International Energy Agency (IEA)*, Garching, Germany (K. Heinola)
- 28 – 29 February 2024, *JET Celebration Day*, UKAEA, Culham, UK (K. Heinola)
- 18 – 22 March 2024, *Joint ICTP-IAEA School on Data for Modelling Atomic and Molecular Processes in Plasmas*, Trieste, Italy: to act as director and lecturer (C. Hill)
- 13 – 17 May 2024, *26th International Conference of Plasma-surface Interactions (PSI)*, Marseille, France (K. Heinola)
- 21 – 23 May 2024, *Nordic Nuclear Forum 2024 & Meeting with the LOC of IAEA Decennial Meeting on Fusion Data*, Helsinki, Finland (K. Heinola)

10. Publications

Scientific Articles

- C. Hill, Dipti, K. Heinola, M. Haničinec, CollisionDB: A new database of atomic and molecular collisional processes with an interactive API, *Atoms* **12**(4), 20 (2024).
- A. Liski, …, K. Heinola, et al., Solubility of hydrogen in WMoTaNbV high-entropy alloy, *Materials* **17**, 2574 (2024).
- M. L. Dubernet, …, C. Hill et al., Atomic and Molecular Databases Open Science for a sustainable world, *Proceedings of the International Astronomical Union* **18**(S371), 72 (2024).
- Dipti, I. Bray, D. V. Fursa, C. Hill, Yu. Ralchenko, *Recommended electron-impact excitation and ionization cross sections for Be II, Atomic Data and Nuclear Data Tables* **156**, 101634 (2024).
- C. Hill et al., Atomic collisional data for neutral beam modeling in fusion plasmas, *Nuclear Fusion* **63**, 125001 (2023).

- A. Owens, T. He, M. Hanicinec, C. Hill, S. Mohr, J. Tennyson, LiDB: Database of molecular radiative lifetimes for plasma processes, *Plasma Sources Science and Technology* **32**, 085015 (2023).
- R. Anirudh, …, C. Hill et al., 2022 Review of Data-Driven Plasma Science, *IEEE Transactions on Plasma Science* **51**, 1750-1838 (2023).
- T. Vuoriheimo, …, K. Heinola et al., Hydrogen isotope exchange experiments in high entropy alloy WMoTaNbV, *Nuclear Materials and Energy* **34**, 101348 (2023).
- T. Vuoriheimo, …, K. Heinola et al., Deuterium retention in tungsten studied by sequential implantations at ELM-relevant energies, *Nuclear Materials and Energy* **34**, 101392 (2023).
- A. Liski, K. Heinola, et al., Irradiation damage independent deuterium retention in WMoTaNbV, *Materials* **15**, 7296 (2022).
- A. Hollingsworth, …, K. Heinola et al., Comparative study on deuterium retention and vacancy content of self-ion irradiated tungsten, *Journal of Nuclear Materials* **558**, 153373 (2022).

INDC Reports

Since the previous IFRC Subcommittee Meeting, the IAEA has become a member of the CrossRef open digital infrastructure organisation, enabling it to assign Digital Object Identifiers (DOIs) to its publications. The Nuclear Data Section and the Division of Conference and Document Services have collaborated to initiate the process of DOI assignment with publications of the International Nuclear Data Committee (INDC), including those reporting the proceedings of meetings held by the AMD Unit.

- C. Hill, Data for Atomic Processes of Neutral Beams in Fusion Plasma: Summary Report of the Third Research Coordination Meeting, 24 – 26 November 2021, *INDC(NDS) Report* 855 (2022) [https://doi.org/10.61092/iaea.twqe-92hz]
- C. Hill, Summary Report of a Consultancy Meeting in preparation of a Coordinated Research Project on Atomic Data for Injected Impurities in Fusion Plasmas, 7 – 8 June 2022, INDC(NDS) Report 854 (2022) [https://doi.org/10.61092/iaea.174s-13da]
- C. Hill, Virtual Atomic and Molecular Data Centres Consortium Annual Meeting; Summary Report of the 8th Biennial Technical Meeting of the Code Centres Network, 15 – 17 November 2023, INDC(NDC) Report 897 (2023) [https://doi.org/10.61092/iaea.s57n-ra6p]
- C. Hill, The Formation and Properties of Molecules in Edge Plasmas: Summary Report of the First Research Coordination Meeting, 6 – 8 December 2023, INDC(NDS) Report 896 (2023) [https://doi.org/10.61092/iaea.4w1d-eec2]
- C. Hill, 21st Atomic Processes in Plasmas Conference: Summary Report of the Technical Meeting, 15 – 19 May 2023, INDC(NDS) Report 881 (2023) [https://doi.org/10.61092/iaea.csbv-dg73]
- K. Heinola, Joint IAEA-FZJ Technical Meeting on the Collisional-Radiative Properties of Tungsten and Hydrogen in Edge Plasmas of Fusion Devices, 29 March – 1 April 2021, INDC(NDS) Report 848 (2023) [https://doi.org/10.61092/iaea.gt1c-hv9e]

- C. Hill, K. Heinola, IFRC Subcommittee on Atomic and Molecular Data for Fusion: Report on the Activities of the Atomic and Molecular Data Unit, June 2021 – May 2022, INDC(NDS)-861 (2022) [https://doi.org/10.61092/iaea.wmqh-17vn]

11. Cooperations and Other Activities

- The Practical Arrangements between the IAEA and the Korea Institute of Fusion Energy (KFE), for cooperation in the area of atomic, molecular and plasma-material interaction data relevant to fusion remain in place until 3 September 2024. The process to renew them for a further three years beyond this date has been initiated.

- K. Heinola was a member of International Program Committee of the International Workshop on Hydrogen Isotopes in Fusion Reactor Materials (HWS) [1, 2], a satellite event to the biennial Conference on Plasma-Surface Interaction in Controlled Fusion Devices (PSI); the event was held from 20 – 22 June 2022, in virtual format.

- C. Hill was a member of the International Organizing Committee of the International Conference on Atomic and Molecular Data and their Applications (ICAMDATA) [3], which was held in cooperation with the IAEA in Bari, Italy from 25 – 29 September 2022.

- The AMD Unit entered into a cooperation agreement with the International Workshop on Models and Data for Plasma-Material Interaction in Fusion Devices (MoD-PMI), held in Aachen, Germany from 29 – 31 May 2023 [4]. Unit Staff member K. Heinola joined the Scientific Organising Committee of the event.

- The AMD Unit entered into a cooperation agreement with the University of Valladolid concerning the organization of the 1st International School on Atomic and Molecular Data Evaluation and Curation (ICAMDEC), held in Valladolid, Spain from 22 – 25 October 2023 [5]. The Unit Head joined the Scientific Organising Committee as co-director for this event.

- The AMD Unit entered into a cooperation agreement with the organisers of the 7th Spectral Lineshapes in Plasmas (SLSP) Workshop, which will be held in Gran Canaria, Spain from 30 – 4 October 2024 [6]. The Unit Head joined the Scientific Organising Committee for this event.

- C. Hill is a member of the International Organizing Committee of the International Conference on Atomic and Molecular Data and their Applications (ICAMDATA) [7], which was held in cooperation with the IAEA at Northwest Normal University, Lanzhou, China from 22 – 26 September 2024.

[1] https://www.psi2022.kr/abstract/abstract_04.html
[2] https://hydrogen.onuniverse.com/

[3] https://www.icamdata2022.it/
[4] https://amdis.iaea.org/meetings/mod-pmi-2023/
[5] https://amdis.iaea.org/meetings/isamdec-1/
[6] https://plasma-gate.weizmann.ac.il/projects/slsp/slsp7/
[7] https://icamdata.nwnu.edu.cn/#/

12. Future Meetings and Workshops in the Present Biennium

Decennial IAEA Technical Meeting on Atomic, Molecular and Plasma-Interaction Data for Fusion Science and Technology

The AMD Unit has, historically, held a general Technical Meeting on atomic, molecular and plasma-material interaction data for fusion science and technology every 10 years, most recently in Korea in 2014 [1]. As with previous meetings, the upcoming meeting in 2024 [2] will aim to advance data-oriented research on these data that are important for fusion plasma simulation, fusion plasma diagnostics and fusion energy technology. As part of this goal, the meeting will promote collaboration among fusion energy researchers and researchers in atomic, molecular and materials science, raise awareness in the community of the continuing science needs for fusion and highlight the contributions that can be made by this community to fusion energy science and technology.

The meeting will feature invited and contributed oral presentations as well as a poster session. All talks are scheduled for 30 minutes including question time. The event was held from 15 – 19 July 2024 at the University of Helsinki, Finland through a Host Government Arrangement.

[1] https://amdis.iaea.org/meetings/decennial-2014/
[2] https://amdis.iaea.org/meetings/decennial-2024/

Second RCM of the Injected Impurities CRP

The Second RCM of CRP F43026: Atomic Data for Injected Impurities in Fusion Plasmas is planned as an in-person meeting to be held at IAEA Headquarters in December 2024. The meeting will establish participants' Workplans for the coming 18 months, review ongoing activities and make plans for collaborative activities including code comparison and fundamental data validation through collisional-radiative modelling.

Third RCM of the Hydrogen Permeation CRP

The Third RCM of CRP F43025: Hydrogen Permeation in Fusion-Relevant Materials is planned as an in-person meeting, to be held at IAEA Headquarters from 3 – 5 December 2024. The meeting will review participants' progress with their Workplans over the course of the CRP, review ongoing activities and make plans for concluding or extending the CRP to allow further work to be performed.

MoD-PMI 7: International Workshop on Models and Data for Plasma-Material Interaction in Fusion Devices

The seventh International Workshop on Models and Data for Plasma-Material Interaction in Fusion Devices (MoD-PMI 2025) will be organized from 26 – 28 May 2025 in cooperation with the International Atomic Energy Agency and hosted at IAEA HQ. The meeting brings together researchers from the areas of fusion energy and materials science to review advances, both experimental and in modelling, in the study and understanding of processes relevant to plasma-material interaction (PMI) relevant for fusion devices and reactors.

MoD-PMI is a satellite workshop for the International Conference in Plasma-Facing Materials and Components (PFMC). The 20th PFMC is organized from 19 – 23 May 2025 in Ljubljana, Slovenia [1]. Its topics of focus are as follows:

- Direct use of first-principle approaches to plasma-material interaction (DFT and beyond).
- Applications of multi-scale methodologies.
- Machine learning methods for materials data prediction.
- PMI and neutron irradiation effects to material surface composition, morphology and micro-structure evolution.
- Experimental PMI data for modelling: sputtering mechanisms, implantations, spectroscopy, microscopy, etc.

[1] https://pfmc20.com/

Technical Meetings

The following Technical Meetings are proposed to continue the biennial meeting series of the three Networks coordinated by the AMD Unit:

28th Technical Meeting of the Data Centres Network: this long-standing network of eleven data centres meets in odd-years and constitutes a standing Advisory Group for advising the Agency on the technical aspects of data exchange and processing. The 2025 meeting is anticipated to be held in the autumn.

9th Technical Meeting of the Code Centres Network: this meeting will also be held in 2025, on an aspect of modelling and calculation of data that are difficult to measure experimentally; as

in recent years it is anticipated that this Network Meeting will be concerned with the simulation of neutron-induced radiation damage in fusion-relevant materials.

Proposed Joint IAEA-ICTP-MAMBA School

The proposed 2-week school "Joint IAEA-ICTP-MAMBA School on Materials Irradiation: from Basics to Applications" is joint project by IAEA, ICTP and Horizon Europe project "MAMBA", a MSCA-SE consortium for staff exchanges between EU Member States and Associated Countries [1]. The School focuses to the fundamentals of irradiation, the effects of irradiation and its numerous applications. In addition to fusion applications, its topics cover various irradiation applications, from space electronics, radiation-resistant materials, accelerator technologies, nuclear decommissioning and quantum mechanics to multi-scale simulations and the safe analysis of heritage objects. The event aims to develop understanding of the basic experimental and theoretical physics in materials response to irradiation and further to provide advanced, state-of-the-art experimental and computational tools and their application to control and tailor the properties of materials exposed to irradiation.

At the time of writing, the decision for holding the school is pending.

[1] Horizon Europe "MAMBA", https://cordis.europa.eu/project/id/101131245.

13. Coordinated Research Projects starting in the present Biennium (2024–25)

Properties of Tungsten Ions in Fusion Plasmas

The ionization balance and spectroscopic and collisional properties of tungsten at temperatures between 1 keV and 10 keV are subject to large uncertainties and disagreements between theory and experiment. It is proposed that a new CRP to address data needs in this domain be initiated in the 2024 – 25 biennium. The last time the topic of tungsten ions in plasma was addressed was in CRP F41027: "Spectroscopic and Collisional Data for Tungsten from 1 eV to 20 keV" (2010 – 15) and progress in experimental and computational techniques motivates another project in the near future, particularly given the importance of this temperature range at the pedestal region of tokamak devices.

Initial consultation amongst the GNAMPP community will start in advance of planning the CRP, along with a review of the state-of-the-art in respect of dielectric recombination calculations and experiments (amongst others, research groups at Los Alamos National Laboratory, Aix-Marseille University and the Institute of Modern Physics / Chinese Academy of Sciences (IMP-CAS) are active in this area).

This CRP is also intended to complement the ongoing Technical Meeting series on tungsten and hydrogen in edge plasmas (which focuses on lower plasma temperatures). A consultancy meeting will be held at IAEA headquarters from 29 – 30 August 2024 to set the scope of the

CRP, identify potential participants, determine code comparison, benchmarking and evaluation activities, and establish outcomes, performance indicators and a timeframe for the project.

The summary of the proposed Task within the budget plan for the Division of Physical and Chemical Sciences in the Department of Nuclear Sciences and Applications (NAPC) for the coming biennium is as follows:

Task Name: *Properties of Tungsten Ions in Fusion Plasmas*

- **Task Number: CRP F43028**
- **Description:** The provision of evaluated data filling the gaps in existing data sets concerning tungsten ions in the plasmas of magnetic-confinement fusion energy devices.
- **Responsible Organisation:** NAPC-Atomic and Molecular Data Unit
- **Task Objective:** The establishment of a trusted repository of evaluated data concerning the collisional-radiative properties of tungsten ions in fusion energy devices.
- **Task Relevance to Projects Objective:** The data production and other activities undertaken over the course of this CRP will directly assist in the modelling of the behaviour of tungsten ions which enter the plasma in fusion devices through sputtering and erosion mechanisms.
- **Task Relationship with other Tasks:** This activity is most closely related to the Atomic and Molecular Data Unit's activities on data evaluation and storage (Task 2024.02), ongoing activities concerning processes in edge plasmas (Task 2024.08), and CRP Tasks F43025 (Hydrogen Permeation), F43026 (Injected Impurities) and F43027 (Molecules in Edge Plasmas).

14. Proposed Technical Meetings for the Biennium 2026–27

14.1 Network and other Technical Meetings

The following Technical Meetings are proposed to continue the biennial meeting series of the three Networks coordinated by the AMD Unit:

29th Technical Meeting of the Data Centres Network: this long-standing network of eleven data centres meets in odd-years and constitutes a standing Advisory Group for advising the Agency on the technical aspects of data exchange and processing. The 2027 meeting is anticipated to be held in the autumn.

10*th Technical Meeting of the Code Centres Network*: this meeting will also be held in 2027, on an aspect of modelling and calculation of data that are difficult to measure experimentally.

14.2 IFRC Subcommittee Meeting

25th Technical Meeting of the International Fusion Research Council Subcommittee on Atomic and Molecular Data for Fusion should be held at IAEA Headquarters in Vienna in May or

June 2026, to allow for planning for the 2028-29 biennium by September 2026. It was determined that a new member of the subcommittee from Ente per le Nuove Technologie l'Energia e l'Ambiente (ENEA), Italy, should be appointed, in accordance with the updated Terms of Reference (below and Appendix A), if possible. The Subcommittee should also seek to appoint new members from India and Spain, and a representative from the DIII-D National Fusion Facility in the US. Wolfgang Jacob announced his imminent retirement and his proposed replacement, Thomas Schwarz-Selinger, was endorsed by the Subcommittee.

15. Proposed Activities for the Biennium 2025–26

15.1 Extension of the Hydrogen Permeation CRP

The extension of the large, ongoing Hydrogen Permeation CRP (F43025) was proposed; in addition to various proposed round robin exercises that exceed the timescale of the current CRP – in particular, the analysis of hydrogen permeation in neutron-irradiated samples. Additionally, it was reported that INL and UKAEA are able to perform experiments on the neutron-irradiated samples using tritium. Given the four CRPs that would already be underway during the current biennium 2024-2025, this would obviate the need to initiate a new one. In practice, the extension could be requested of the CCRA-NA for one further Research Coordination Meeting (to be held in person).

It was also noted that results reported in the studies of hydrogen permeation should, as far as possible, be validated through experiments; this can be promoted within the CRP through benchmarking exercises and, for example, best-practice recommendations for calibration.

There was some further discussion on the effect of electric field gradients and temperature gradients (the Soret Effect) on hydrogen permeation in hydrogen in materials. This topic has essentially never been studied before but is anticipated to be of great importance to ITER for which it is not even known whether the net effect of such gradients is to push hydrogen isotopes into the wall or pull it out. However, little information is available in the literature on the effect of temperature gradient to the hydrogen transport in materials.

Possible new CRPs on tritium-breeding materials and interfaces between reactor materials were discussed but it was decided not to proceed with these in the coming biennium. A stronger case was made for a CRP on tungsten surfaces (sputtering, reflection and retention) and this proposal should be considered should the CCRA decide not to extend the Hydrogen Permeation CRP.

15.2 Collaboration with IEA

As one of the outcomes of the 1st Technical Meeting on Tungsten and Hydorgen in Edge Plasmas (28 March – 1 April 2021) was the establishment of Working Groups (see Section 5 of this report) focusing on tungsten processes and the proposal for the IAEA to seek collaboration with International Energy Agency (IEA) in the field of fundamental experimental research on atomic and molecular processes relevant for tungsten-based fusion machines.

The Fusion Power Coordination Committee (FPCC) of IEA supervises IEA Technology Collaboration Programmes (TCPs) for fusion. The TCP framework is a multilateral mechanism to provide a platform for IEA countries to work together to advance research, development and commercialization of energy technologies such as fusion. An overview of the eight fusion

TCPs is provided in Ref. [1]. The TCP on Plasma-Wall Interactions (PWI TCP) focuses on plasma physics, first wall materials and surface physics of plasma-facing components. The programme aims to study PWIs experimentally in dedicated linear plasma devices and high heat load test facilities. This network of PWI TCP contracting facilities comprises of plasma devices around the world. The aim of the IAEA-IEA collaboration is to establish scientific projects and joint research between IAEA/AMD Unit's networks [2,3] and the members of the PWI TCP facilities in the field edge plasma processes and PWIs. Proposed activities would be experimental validation of critical A+M and PSI processes used in CR modelling for W and hydrogen isotopes: i) atomic data; ii) molecules: rovibrationally resolved molecules, molecular processes such as molecule-assisted recombination (MAR), dissociation (MAD) and ionization (MAI); and iii) W sputtering yields (surface effects, such as roughness and hydrogen coverage; charge states of emitted W species; etc). Corresponding CR modelling would comprise of e.g. molecule modelling with EIRENE and W sputtering and emission modelling with ERO codes.

The IAEA-IEA collaboration proposal was presented at the IEA FPCC Annual Meeting (24 – 25 Jan 2024). It was endorsed by the Chair of the FPCC and approved by the Chair of the PWI TCP.

[1] https://www.iea.org/about/technology-collaboration/fusion-power
[2] IAEA WG2 "W and Hydrogen Experiments": https://amdis.iaea.org/GNAMPP/collaborations/7
[3] https://amdis.iaea.org/GNAMPP/

15.3 Database of Experimental Spectra from EBITs and Tokamaks

It was noted that a large amount of atomic spectral data exists from experimental devices including electron beam ion traps (EBITs) and tokamaks. However, these data are rarely made publicly available in a usable form and are often stored in a variety of formats unique to the operating laboratory. Furthermore, particularly in the case of tokamak spectra, the conditions (plasma density and temperature, etc.) may be distinct to a particular experimental run or discharge (shot) and may be measured along an inhomogeneous line-of-sight. Nonetheless, a curated database of such spectra would be a useful resource to help identify transitions, to validate and benchmark theoretical models and simulations of atomic processes in plasmas and to refine diagnostic tools. There is also an obvious cross-disciplinary application to the astrophysics community.

Furthermore, it is hoped that such a database could promote standardization of data formats and data sharing in the field and act as a reference repository for comparison and to aid with spectral assignment across devices and plasma conditions.

A break-out meeting is planned during the upcoming Decennial Meeting, to be followed by a further consultancy meeting if necessary, to initiate this activity by identifying potential data producers and to draft a data format and related tools for searching and visualizing experimental spectra.

A related activity relating specifically to the spectroscopy of boron and tungsten for ITER was discussed and a comparison Workshop, held at ITER, along the lines of the spectral lineshapes in plasmas (SLSP) workshop series should be considered: Unit staff will liaise with ITER over

the coming year to explore the possibility of holding such an event in 2026, with support from the IAEA.

16. IFRC Subcommittee Terms of Reference

The International Fusion Research Council Subcommittee on Atomic and Molecular Data for Fusion held its first meeting in January 1981 after its original Terms of Reference and Methods of Work were approved by the IAEA administration in December 1980. The Terms of Reference give the Subcommittee the authority to determine its own methods of work and since then minor changes have been made to this document, most recently in 2002.

At the 2022 meeting, the Subcommittee proposed to update its Methods of Work document as described in Appendix A of the report to that meeting [1]. The Unit Head presented the proposed changes at a meeting of the IFRC Committee in July 2022, which endorsed the new document with minor changes. Appendix A of this report reproduces the complete, approved Terms of Reference.

[1] C. Hill, K. Heinola, IFRC Subcommittee on Atomic and Molecular Data for Fusion: Report on the Activities of the Atomic and Molecular Data Unit, June 2021 – May 2022, INDC(NDS)-861 (2022) [https://doi.org/10.61092/iaea.wmqh-17vn]

Appendix A: Terms of Reference

The Terms of Reference guiding the scope, operation and membership of the IFRC Subcommittee on Atomic and Molecular Data for Fusion is given below.

TERMS OF REFERENCE

IFRC Subcommittee on Atomic and Plasma-Material Interaction Data for Fusion

The International Fusion Research Council (IFRC) Subcommittee on Atomic and Plasma Material Interaction Data for Fusion will serve as a continuing Subcommittee within the framework of the International Atomic Energy Agency. Its function will be to review periodically the planning and execution of the Agency's Atomic and Plasma-Material Interaction Data Programme for Fusion and to advise the Director General on its direction in accordance with the needs of fusion research and reactor design.

Composition: the Subcommittee shall be composed of fusion and atomic scientists nominated by IFRC.

Methods of Work: the Subcommittee shall determine its own methods of work. The IAEA Nuclear Data Section shall provide the secretariat services to the Subcommittee.

Meetings: the Subcommittee shall be convened at a frequency not exceeding two years, and shall normally meet at the IAEA Headquarters. The cost of participation of Subcommittee Members will be born by the Government or sponsoring institute of the member. No interpretation will be required.

METHODS OF WORK

IFRC Subcommittee on Atomic and Plasma-Material Interaction Data for Fusion

Under the Terms of Reference of the IFRC Subcommittee on Atomic and Plasma- Material Interaction Data for Fusion (hereinafter referred to as the Subcommittee), as approved by the IAEA Administration on .....1993, the Subcommittee is authorized to determine its own Methods of Work.

I. Scope and Responsibilities

In addition to the general functions of the Subcommittee, stated in the Terms of Reference, the Subcommittee shall

- regularly review the IAEA programme on Atomic, Molecular and Plasma-Material Interaction Data for Fusion;
- review Atomic, Molecular and Plasma-Material Interaction data needs and recommend their priorities;

- assist in specifying and planning topical data meetings and coordinated research programmes;
- assist in maintaining contacts between the IAEA Atomic and Molecular Data (AMD) Unit and the fusion community;
- assist in the coordination of data centres.

II. Organization

1. Chair: the Chair shall be a member of the Subcommittee and shall serve for two meetings. The Chair may be renominated by the Subcommittee. The responsibility of the Chair shall remain in effect between meetings and they shall be kept informed by the Subcommittee members and the Scientific Secretary of relevant activities and developments.

2. Vice-Chair: the Vice-Chair shall be a member of the Subcommittee and shall serve for two meetings.

3. Scientific Secretary: the Scientific Secretary shall be the Head of the AMD Unit of the IAEA Nuclear Data Section, and shall serve as a member of the Subcommittee.

4. Membership: the Subcommittee shall be composed of 12 – 14 scientists representing the diverse national (e.g., Universities, National Laboratories, etc.) and international (eg., EURATOM, ITER, etc.) organizations involved in fusion-related research activities. A member of the Subcommittee who is no longer able to fulfil their duties may be replaced by decision of the Chair, Vice-Chair and the Scientific Secretary. New members of the Subcommittee shall be proposed by the Chair and the Scientific Secretary to the Subcommittee members, for their approval. Suggestions for new members from outgoing, present and former members of the Subcommittee are welcomed. The membership of the Subcommittee shall be reported to the IFRC for endorsement.

III. Meetings

1. Preparation: the preparation of the meetings shall be done in a timely manner by the Scientific Secretary of the Subcommittee in collaboration with the incoming and outgoing Chair.

2. Frequency: the Subcommittee shall nominally meet every two years at the IAEA Headquarters.

3. Proceedings: the proceedings of the meetings shall be written by the Scientific Secretary and shall be issued as an IAEA report after having been approved by all Subcommittee members. The proceedings of every meeting shall be made available to the IFRC and INDC committees, and placed on the AMD Unit's website.

4. Observers: all meetings of the Subcommittee shall be open to Observers and Experts as defined by the IAEA's Guidelines for Technical Meetings.

Appendix B: Subcommittee Members

Hyun-Kyung CHUNG, Innovation Strategy Division, Korea Institute of Fusion Energy, 169-148 Gwahak-ro, Yuseong-gu, DAEJEON 34133, REPUBLIC OF KOREA

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Appendix C: Meeting Participants

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Appendix D: Agenda

IAEA Headquarters, Vienna, Austria: Meeting Room M0E07

Thursday, 6 June 2024

10:00 – 10:30	Melissa DENECKE (DIR-NAPC): Meeting Opening; Christian HILL and Kalle HEINOLA: Welcome, introduction of the participants, adoption of the agenda
10:30 – 11:00	**Christian HILL**, *IAEA, Austria* General report on activities
11:00 – 11:30	**Kalle HEINOLA**, *IAEA, Austria* Review of Vapour Shielding and Hydrogen Permeation CRPs
11:30 – 11:45	Coffee Break
11:45 – 12:15	**Christian HILL**, *IAEA, Austria* Review of Injected Impurities and Molecules in Edge Plasmas CRPs
12:15 – 12:45	**Kalle HEINOLA**, *IAEA, Austria* Review of Edge Plasmas Technical Meeting Series
12:45 – 13:00	**Christian HILL**, *IAEA, Austria* Activities of the DCN, CCN and GNAMPP Networks
13:00 – 14:00	Lunch
14:00 – 14:30	**Christian HILL**, *IAEA, Austria* Database activities in the AMD Unit
14:30 – 15:00	**Christian HILL**, *IAEA, Austria* Other AMD Unit activities
15:00 – 16:00	Discussion and Review of AMD Unit activities.
19:00 – 21:00	Social Dinner: Zur Alten Kaisermühle, Fischerstrand 21A, 1220 Wien.

Friday, 7 June 2024

09:30 – 10:00	**Christian HILL**, *IAEA, Austria* Future Events and Projects
10:00 – 10:30	General discussion: future CRP Proposals, Cooperations and Outreach
10:30 – 11:00	Coffee Break
11:00 – 12:00	General discussion: future data activities, Technical Meetings and staffing issues.
12:00 – 12:30	Any other business; meeting recommendations and conclusion.

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