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INDC International Nuclear Data Committee

IFRC Subcommittee on Atomic and Molecular Data for Fusion: Report on the Activities of the Atomic and Molecular Data Unit, June 2021 – May 2022

Prepared by

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ABSTRACT

The 23rd meeting of the Subcommittee on Atomic and Molecular Data of the International Fusion Research Council (IFRC) was held from 16 – 17 May 2022 as a hybrid event, with seven members attending in-person and four participants using video-conferencing software. This follows two shorter, virtual meetings in 2020 and 2021. Activities of the Atomic and Molecular Data Unit for the period June 2021 – May 2022 were reviewed and recommendations were made for continuing activities in 2022 – 2023 and for new projects in the 2024 – 2025 budget cycle. The proceedings, conclusions and recommendations of the Subcommittee meeting are briefly described in this report.

October 2022

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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.

As a result of disruption caused by the global COVID pandemic, the 22nd Meeting of the Subcommittee was held, in abbreviated form, as a virtual meeting from 14 – 15 June 2021 (https://amdis.iaea.org/meetings/ifrc-2020/), after an interim virtual meeting on 9 July 2020.

This report documents the hybrid meeting held from 16 – 17 May 2022 in-person at IAEA Headquarters in Vienna, Austria, and online for participants unable to travel. It provides a record of the projects and activities of the Atomic and Molecular Data (AMD) Unit since June 2021, and documents the recommendations made by the Subcommittee concerning planned activities for the next biennium (2024 – 2025).

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 planned 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 and other activities;

· A summary of planned activities for the current biennium, 2024 – 2025.

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

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

The Unit was granted a significant proportion of its unspent funds from 2020 in the form of a budget carry-over to 2021, and was able to appoint a one-year Special Service Agreement (SSA) consultant at the P3-level to work in the area of atomic and molecular data evaluation with a focus on providing improved data services. The appointed consultant, Dipti, took up the position in August 2021.

Two further home-based consultancies have been granted to work on:

(a) improving the software tools used by the Unit's database services website (pyvalem, django-pyref and django-valem): Martin Haničinec undertook this work for 60 days over the second half of 2021;
(b) preparing and entering data concerning collisional processes in the neutral beams of fusion devices into the CollisionDB database developed by Unit staff: Örs Asztalos (Budapest University of Technology and Economics) is currently engaged in this activity.

3. Coordinated Research Projects

F43022: Plasma-wall Interaction with Reduced-activation Steel Surfaces in Fusion Devices

Various kinds of reduced-activation steel are being considered as wall material for a fusion reactor, such as the planned DEMO demonstration power plant. However, not enough is known about plasma interaction, erosion and tritium retention in such steels. This CRP aims to enhance the knowledge base and develop new databases on the interaction of fusion plasma with the reduced-activation steel alloys that are being considered for constructing the plasma-facing components of a fusion reactor. It seeks to quantify the erosion due to exposure to plasma and to determine the retention and transport properties of tritium in the surface.

At the third Research Coordination Meeting (RCM), a further activity, the *Comparison Experiment for the Sputtering of Steel* (CESS), was initiated. This is being coordinated by Dr. habil. Wolfgang Jacob at the Max Planck Institute for Plasma Physics, Garching, Germany. Its aim is to compare sputtering yields in different experimental devices: as far as possible, identical samples (with comparable histories) will be exposed to deuterium plasma or ion irradiation under comparable exposure conditions and analysed by a range of techniques including (but not limited to) Mass loss, Scanning Electron Microscopy (SEM), and Thermal Desorption Spectroscopy (TDS). More details, including a list of participants, the distribution of steel samples and sample preparation techniques are available on the AMD Unit website at https://amdis.iaea.org/workshops/cess.

Despite the disruption caused by the COVID pandemic, data produced by the Steel Surfaces CRP has been deposited with the AMD Unit's hcdb database [1], and a paper concerning the CESS comparison exercise was published in *Nuclear Materials and Energy* [2]. Pending a decision about the conclusion of the CESS project, the CRP will be formally closed through the Agency's Research Contract Administration procedures in the coming year.

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

[2] R. Arredondo, M. Balden, T. Schwarz-Selinger, T. Höschen, T. Dürbeck, K. Hunger, K. Schlueter, A. Golubeva, P. Wang, D. Terentyev, W. Jacob, "Comparison experiment on the sputtering of EUROFER, RUSFER and CLAM steels by deuterium ions", *Nuclear Materials and Energy* **30**, 101118 (2022).

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

Neutral beam injection is a standard method used 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 aims to provide 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, D, T) neutral beams in the high temperature core plasma.

The first and second RCMs were held in Vienna in 2017 and 2019, respectively; the third meeting was due to be held in late 2020 but was postponed to November 2021 by the COVID pandemic. 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. The first took the form of a workshop, held at the Institute for Nuclear Research, Hungarian Academy of Sciences (ATOMKI) in Debrecen, Hungary from 26 – 28 August 2019. It was conceived in order to assess the sensitivity of predictions of hydrogen beam penetration and of beam emissions in relevant fusion plasma conditions to different modelling codes and uncertainties in atomic data. Test cases were shared in advance with the eight participating research groups, which involved H, D, He, and (optionally) Li and Na, at beam energies of 30, 100 and 1000 keV and plasma conditions representative of those present in fusion devices. The results were compared at the August workshop, with most participants presenting remotely. This work was presented at the 47th EPS (virtual) Conference on Plasma Physics (21 – 25 June 2021) and an article is in preparation for submission to *Journal of Physics B*. More details are available at https://amdis.iaea.org/workshops/neutral-beam-penetration-and-photoemission.

The second code comparison activity was initiated at the second RCM in February 2019; over the course of the year, participants have been producing calculated, state-resolved cross sections for the process $Be^{4+} + H(nl)$ using the following computational methods:

- Semi-classical Molecular Orbital (SC MO) close-coupling
- Classical Trajectory Monte Carlo (CTMC)
- Semi-classical Basis Generator Method (BGM) close-coupling
- Convergent Close-Coupling (CCC)
- Semi-classical Atomic Orbital (SC AO) close-coupling

Three projectile energies: 20, 100 and 500 keV/u were considered, chosen to be of relevance to fusion plasmas and overlap the typical validity range of the selected theoretical methods. The hydrogen target is considered in the ground state (1s) and excited states 2s, $2p_m$ ($m = 0$, ±1). The aim is to produce and compare data for a collision system in order to evaluate and assess these methods and to estimate the typical accuracy of the calculated cross sections for:

- Total electron capture
- Total ionization
- Total excitation
- State-selective processes (for the dominant channels).

The results of these calculations were discussed at the third RCM, which was held in virtual format from 24 – 26 November 2021 [1]. A final meeting, to make recommendations of data and to plan the CRP final report, will be held from 18 – 20 May 2022 [2]. More details are available at https://amdis.iaea.org/workshops/atomic-collisions-ccw.

Data resulting from the Neutral Beams CRP has been deposited in the AMD Unit's CollisionDB database [3].

[1] https://amdis.iaea.org/meetings/neutral-beams-rcm3/
[2] https://amdis.iaea.org/meetings/neutral-beams-cm/
[3] https://db-amdis.org/collisiondb/

F43024: Atomic Data for Vapour Shielding in Fusion Devices

This CRP focuses on the properties and creation of the vapour formed in front of plasma-facing components due to energetic plasma-wall interactions. In the course of fusion reactor operation, energy may be deposited onto the inner walls through small or large bursts known as edge-localized modes (ELMs), plasma transients and disruptions. These may lead to evaporation or ablation of the wall material, potentially causing significant damage to plasma-facing components and to the operation of plasma.

However, this evaporated, dense and expanding secondary plasma cloud, after forming in front of the surface, may have the ability to convert the continuous incoming fast particle kinetic energy from the main plasma into radiation energy, and gradient effects may cause this radiation to be directed away from the wall back into the plasma hence protecting the wall and its components. This conversion of energy into radiation largely directed away from the material wall is referred to as vapour shielding. Continuous vapour shielding has been demonstrated to reduce the heat flux to surfaces coated with liquid metals, such as lithium (Li) and tin (Sn), and their mixtures. Atomic data is needed to simulate the vapour shielding processes as well as to interpret spectroscopic measurements when vapour shielding is happening, either in transient or steady-state plasma conditions of a fusion device.

The participants in this CRP are engaged in the theory and modelling of plasma and vapour particle collisional processes, and of experiments of spectral line properties, vapour formation and spectral analyses. The CRP is organized to provide evaluated and recommended data for the principal atomic and molecular processes relevant to vapour formation, and data related to the elemental processes affecting the vapour shielding phenomenon. The primary emphasis is on interactions of hydrogen (H, D, T) with the liquid metal particles being ejected from Li and Sn targets. The 1st RCM was held from 13 – 15 March 2019 (as an in-person event), the 2nd RCM from 7 – 9 October 2020 (as a virtual event) and the third RCM will be held from 19 – 21 October 2022 (as a hybrid event).

Data produced as part of this CRP that have already been deposited in the AMD Unit's data libraries include:

Heavy particle collisional processes –

- $p + Be^{1,3+}$ and $p + Li$ (AOCC, MOCC)

- $p + H$ (CCC)

Electron-molecule collisional processes –

- $e + LiH$, $e + Li_2$

Plasma-liquid metal interactions (Molecular Dynamics, experiments) –

- $H + Li$ surface; $D + Li$ surface; $D_2 + Li$ surface

Information on this CRP's activities is found at https://amdis.iaea.org/CRP/vapour-shielding.

F43025: Hydrogen Permeation in Nuclear Materials

CRP on Hydrogen Permeation in Fusion Materials focuses on experiments, modelling and theory related to hydrogen permeation in fusion reactor first wall materials and components. At the time of writing, there are 20 participating research institutions from 15 Member States, with two more awaiting an exchange of signatures to formalize their participation. The first RCM of this CRP was held virtually from 23 – 27 November 2020 and attracted 51 participants from 15 Member States (including observers and co-workers of the CRP Principal Investigators). The second RCM is currently scheduled to take place from 22 – 24 Feb 2023 and will be organized as an in-person event. Two Technical Meetings related to this CRP have been held

1) Nuclear Fusion Fuel Permeation in Reactor First Wall Components, 4 – 6 October 2021, IAEA HQ, hybrid event

2) Effects of Hydrogen Supersaturation and Defect Stabilization in Nuclear Fusion Reactor Materials, 11 – 12 April 2022, Aix-en-Provence, France, in-person event

and their summaries are given in Section 5 of this report.

Summary of the main topics of this CRP:

- To inventorize parameters affecting hydrogen permeation in fusion-related materials (CRP materials currently: W, Be, ferritic/martensitic steels, Cu, CuCrZr), including temperature, microstructure and irradiation-induced defects (elastic effects: lattice defects and collisional cascades; inelastic effects: neutron-induced transmutations and gas formation). As a novel feature, there is an ongoing round-robin activity with a limited availability to perform research with neutron-irradiated tungsten samples as provided within the CRP;

- To assemble, evaluate and recommend data needed for hydrogen permeation in fusion materials, particularly diffusivity, retention, solubility, recombination and dissociation coefficients of hydrogen on unirradiated and irradiated materials. Data obtained through fundamental first-principles calculations and through experiments;

- To increase the knowledge of the isotope effect on hydrogen diffusion and mobility;

- To decrease the uncertainties related to hydrogen mobility parameters affecting permeation;

- To analyse the influence of material defects and microstructure on permeation, including the evolution of defects and microstructure during permeation experiments;

- To better understand the effect of surface and sub-surface conditions on permeation;

- To perform coordinated experiments and simulations (DFT, KMC, Rate Theories, etc.) to improve the knowledge-base on hydrogen permeation processes with non-irradiated and irradiated material;

- To compare experimental facilities and techniques in hydrogen permeation.

Two experimental round-robin activities are ongoing as part of this CRP:

Hydrogen Gas-Driven Permeation in Fusion Materials (GDPFM)

This round-robin exercise focuses on gas-driven permeation (GDP) of deuterium in EUROFER97, which is a reduced activation ferritic/martensitic (RAFM) steel. The activity aims to cross-compare permeation results obtained in different GDP facilities by using identical RAFM samples. EUROFER97 studied is provided by IPP Garching (Germany), and samples have been polished, annealed and pre-characterised at Forschungszentrum Jülich (FZJ; Germany) prior to distribution to participating laboratories at CEA (France), NRC "Kurchatov Institute" (Russia), ASIPP (China) and CNEA (Argentina). The samples will be used for GDP studies between 30 ℃ and 550 ℃ in the upstream pressure range between 1 – 1000 mbar. This activity is coordinated by FZJ.

Hydrogen in Neutron-irradiated Materials (HNIM)

Neutron-irradiated samples have been provided by SCK•CEN (Belgium) originating two irradiation campaigns, covering a variety of dpa (up to 1 dpa) and temperatures (50 – 1200 ℃). Tungsten samples have already been produced in a campaign from 2017 – 2019. The planned 2021 campaign had to be moved to 2022 and the irradiations are expected to be carried out by the end of year. In the 2022 irradiation campaign various grades of tungsten, CuCrZr, Mo, Fe, and EUROFER 97 will be used. Permeation studies and the effect of the evolution of neutron-induced defects will be studied using (at least) the following experimental techniques: gas-driven permeation (GDP), plasma-driven permeation (PDP), Positron Anihilation Spectroscopy (PAS), thermal desorption spectrometry (TDS) and nuclear reaction analysis (NRA). The participants in this exercise, to whom irradiated samples will be distributed in 2023 are: Idaho National Lab (INL, USA) [subject to approval from the US Department of Energy to join the CRP], MEPhI (Russia), UKAEA (UK) and the University of Helsinki (Finland).

Information on this CRP's activities is found at https://amdis.iaea.org/CRP/hydrogen-permeation.

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 (formerly NFRI, Republic of Korea) and NIFS (Japan).

ALADDIN

ALADDIN (A Labelled Atomic Data INterface) is 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. This database and its online interface is currently being improved to integrate better with other resources and to improve the validation and provenance of its data.

Starting in Autumn 2021, the Unit's plasma collisional data is being migrated onto a new software platform, based around the standards developed through Consultancy Meetings and, in particular, the Technical Meeting held in November 2019 [1]. This has involved the release of CollisionDB [2], a service providing a searchable interface for accessing published (but not necessarily critically-assessed) data which, at the time of writing, holds around 100,000 records. The development version of ALADDIN2 contains, at the time of writing, around 16,000 data sets; the process of migrating data into this service from the original ALADDIN database has led to the identification of several errors, inconsistencies and duplicates, as well as ambiguous and poorly-cited data; resolving these issues is an ongoing project in the Unit.

[1] https://amdis.iaea.org/meetings/software-tools/
[2] A development version of the CollisionDB database is available at https://db-amdis.org/collisiondb/
[3] The ALADDIN2 database, which uses the same software and standards as the CollisionDB database is available, in development form at https://db-amdis.org/aladdin2/

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 over the last year and was deployed in May 2021. 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.

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 14382 simulations for eight different elemental materials in 814 GB of data, a significant increase on the 1532 simulations / 132 GB of data over the course of one year. 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/.

A home-based consultant was appointed in July 2021 for a period of 10 days to implement a data upload functionality into the CascadesDB database: a Representational state transfer (RESTful) interface enabling data providers to upload JSON documents representing metadata for their simulations which are translated into the internal, searchable representations of those metadata in the relational database management system (RDBMS) used.

A further 30-day consultancy implemented the CSaransh software[1] developed by the Bhabha Atomic Research Centre (BARC) to post-process molecular dynamics simulations of collision cascades. CSaransh provides the following functionality:

- Defect statistics;
- Defect locations, classification, clustering;
- Metadata validation;

- Comparisons between cascade simulations;
- Subcascade identification.

This software was demonstrated at the 7th Code Centres Network meeting in October 2021; it is publicly available at https://cascadesdb.org/csaransh.

[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, in particular   through a visit to Paris-Saclay by the Unit Head in October 2021 refined the data model for this resource and improved the metadata descriptions and formats used.

The Unit is in the process of searching for a home-based consultant to assist with populating DefectDB with DFT data from, in particular, EDF and CEA Paris-Saclay.

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 339 institutions, 218 keyword classifications and 772 people. Parts of the Clerval resource, particularly the list of fusion-relevant conferences and meetings[2] replace the defunct Knowledge Base wiki on the old website.

The AMD Unit also maintains a list of external databases in atomic and molecular physics [3] – at the time of writing 31 such resources are described and linked to on this page.

[1] https://amdis.iaea.org/clerval/
[2] https://amdis.iaea.org/clerval/events/
[3] https://amdis.iaea.org/clerval/databases/

Data Standards

The Technical Meeting *Standards and Software Tools for Atomic and Molecular Databases* held in November 2019 updated and expanded the classification of collisional processes in plasmas maintained by the AMD Unit at https://amdis.iaea.org/databases/processes. In the last

year there have been a few minor changes and corrections to this list, which is now at Version 2.4. The process codes were deployed in the AMBDAS database, as described above, and also in the Unit's CollisionDB and ALADDIN2 databases.

The AMD Unit remains an active participant in the Virtual Atomic and Molecular Data Centre (VAMDC) consortium[1]: AMBDAS is deployed as a node for its "portal" of searchable databases, and work within the Unit on the PyValem Python package[2] is carried out in consultation and cooperation with the VAMDC. This software package enables the manipulation and validation of chemical formulas and species states for analysis and storage in databases.

[1] http://www.vamdc.org/
[2] https://github.com/xnx/pyvalem

5. Technical Meetings

Data Centres Network

The biennial meeting of Data Centres Network (DCN) has taken place since 1977 and has been coordinated and hosted by the AMD Unit of the IAEA. 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. It has been agreed within the DCN that IAEA should give priority to the collection and compilation of evaluated atomic collision data. This international atomic and molecular data programme provides information for the use of the global nuclear fusion research community on critically reviewed data on atomic and ionic collision processes as well as data on plasma-surface interactions important to fusion research, which could be used as a common database by fusion laboratories globally. The DCN plays an important role in setting priorities and recommending experts for data evaluation and validation.

Due to the Covid-19 pandemic, the 26th biennial meeting of the DCN was held virtually from 1 - 3 September 2021. Discussions were held on the following topics:

- Status and recent developments of data centres in the last two years (Oct. 2019 – Sep. 2021);

- Future prospects of data centre activities;

- Cooperation in the maintenance of bibliographical databases;

- Requirements for the generation, validation, and compilation of A+M /PMI (Plasma material interaction) data for fusion applications;

- Priorities for database development;

- Uncertainty quantification of fundamental data for fusion plasmas and proposed new meetings.

Detailed information can be found from the 26th DCN meeting webpage at https://amdis.iaea.org/meetings/dcn-26/ .

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. The CCN was initiated as the "A+M Computer Code Network" in a Technical Meeting held at IAEA Headquarters in 2005, with 11 participating research groups; since then the Network has become a Technical Meeting Series on computational aspects of fundamental data for fusion energy research, with no fixed membership or advisory committee. 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 7th meeting of the CCN was held, in virtual format from 18 – 20 October 2021 and continued the theme of the previous meeting in considering the ongoing development and promotion of data resources for radiation-induced damage in nuclear materials. Discussion focussed on the IAEA databases CascadesDB and DefectDB, described above.

These two databases are intended as part of a more broad-ranging suite of databases for fusion and fission material science with the following goals:

- To include experimental measurements and observations, particularly on steel (microscopy, XRD, positron emission, etc.)
- A fully-described set of DFT simulations and predictions of defect formation and behaviour, particularly in Fe.
- To expose an Application Programming Interface (API) so that data can be retrieved automatically from the database and included in computational workflows. This would allow, for example, cascade simulations to be input into hybrid models which use additional data and modelling to predict embrittlement of reactor structural components.
- To facilitate machine learning on large data sets, where available.
- To assess uncertainty propagation and estimation.

Global Network for the Atomic and Molecular Physics of Plasmas (GNAMPP)

The Global Network for the Atomic and Molecular Physics of Plasmas (GNAMPP) is a consortium of research groups working in the area of fundamental atomic and molecular physics

relevant to plasma processes. Its focus is on promoting collaboration and communication between experimentalists and theoreticians to improve the quality and completeness of data used in modelling and interpreting fusion plasmas. The Network provides a forum for the evaluation, validation and dissemination of data, the benchmarking of relevant modelling codes and the formulation of research guidelines and priorities.

The second GNAMPP meeting was held, in virtual format, from 6 – 9 December 2021. 68 participants from 21 Member States attended online; the focus of the event was aspects of the collisional-radiative properties of tungsten and hydrogen in the edge plasma of fusion devices, following on from a Technical Meeting on this subject held in spring 2021 [1].

The GNAMPP website is https://amdis.iaea.org/GNAMPP/, and provides profiles and contact details of research groups in the Network. Details of the second meeting are available from https://amdis.iaea.org/meetings/gnampp-2/.

At the time of writing there are three Working Groups concerned with tungsten and hydrogen in edge plasmas and five collaborations within GNAMPP, also described on the website [2].

[1]https://amdis.iaea.org/meetings/tm-tungsten-hydrogen/
[2] https://amdis.iaea.org/GNAMPP/collaborations/

Technical Meeting on Nuclear Fusion Fuel Permeation in Reactor First Wall Components

This meeting was held from 4 – 6 October 2021, in hybrid format. 54 participants representing 15 Member States discussed processes taking place in the fusion reactor wall materials with respect to permeation, retention, diffusion, trapping, de- and retrapping and surface recombination of hydrogen isotopes in order to assess the underlying mechanisms and parameters for containing and isolating the radioactive T fuel of a fusion reactor from the surrounding components. Of particular concern is the trapping and retention of T inside the reactor wall materials (the so-called *in-vessel term*), and the possibility of T diffusing through the material finding its way into the coolant liquid of the reactor components (the *ex-vessel term*), where it would pose a potentially serious environmental hazard when escaped in the coolant system and beyond. Study of hydrogen permeation in the first wall plasma-facing materials is further complicated by the elevated temperatures present under normal operation of a reactor and the anticipated damage they will suffer due to plasma-surface interactions and irradiation-induced damage by the flux of energetic 14 MeV neutrons produced in the D-T fusion reactions.

Objectives of this meeting were

- to review parameters affecting hydrogen permeation in fusion-related materials, including temperature, microstructure and irradiation-induced defects (neutron transmutation products; neutron and ion-induced lattice damage);

- to increase the knowledge of the isotope effect on hydrogen diffusion;

- to decrease the uncertainties related to diffusion, solubility and trapping parameters affecting permeation;

- to expand the knowledge-base concerning the influence of material microstructure on permeation, including the evolution of microstructure during permeation experiments;

- to assess and, as far as possible quantify, the effect of surface and sub-surface conditions on permeation;

- to review the status of coordinated experiments and other activities related to CRP on Hydrogen Permeation.

Further meeting information is found at https://amdis.iaea.org/meetings/hydrogen-permeation/.

This Technical Meeting is closely related to IAEA's ongoing CRP on Hydrogen Permeation in Fusion Materials (https://amdis.iaea.org/CRP/hydrogen-permeation). The CRP participants attending this meeting provided a brief progress report on their activities and the status of CRP-related round-robin activities were reviewed.

Technical Meeting on the Effects of Hydrogen Supersaturation and Defect Stabilization in Nuclear Fusion Reactor Materials

The event was organized as an in-person event from 11 – 12 April 2022 in Aix-en-Provence, France. 20 experts representing 5 Member States and one international organization (ITER) were invited to discuss and review current understanding on the physical processes related to effects and formation of

1) hydrogen (H/D/T) supersaturated layers in fusion reactor wall materials at subthreshold displacement energies and the effect of surface roughness to the supersaturated layer formation;

2) vacancy-type defect stabilization by hydrogen (H/D/T) in fusion reactor materials under neutron and heavy ion bombardment at energies above displacement threshold;

and to make conclusions and recommendations on:

- significance of these effects to material behaviour under fusion conditions;

- data needs for filling the knowledge gaps, e.g. define defects for systematic DFT/MD calculations;

- future activities with multi-scale calculations.

The meeting invitees represented experts of these phenomena (hydrogen supersaturation and defect stabilization by hydrogen) studied both experimentally and computationally. The key areas on hydrogen supersaturation and defect stabilization in fusion reactor materials and their

implications to the operation of a fusion reactor were identified. The importance of the topic for the fusion community was acknowledged and it was decided to pursue for a scientific publication of the meeting outcome and recommendations for future work. It was concluded that a follow-up meeting could take place within the Working Group 3 (Surface Effects) of the Global Network for Atomic and Molecular Physics of Plasmas (GNAMPP; https://amdis.iaea.org/GNAMPP/collaborations/8) as a specific topic at one of its Technical Meetings.

Further meeting information found online at https://amdis.iaea.org/meetings/ssl-defects/.

6. ICTP Schools and Workshops

The IAEA organizes several Workshops 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 an annual event to provide training and information exchange for computational scientists working on models and data for atomic, molecular and materials processes relevant to fusion energy research.

The COVID pandemic led to the cancellation of a planned two-week Workshop on the topic of *Radiation Damage in Nuclear Materials: "From Bohr to Young"* – this event will be re-proposed as an Advanced School for inclusion in the 2023 calendar of ICTP events.

Two virtual Workshops were held in 2021 and are described below.

6.1 Atomistic Modelling of Radiation Damage in Nuclear Systems

This joint IAEA–ICTP Workshop, which was held online from 4 – 8 October 2021, was a 5-day series of lectures and computing practical exercises to help early-career researchers in developing a qualitative and quantitative understanding of the atomistic modelling of radiation damage on materials, both for existing fission and proposed fusion reactors.

Atomistic modelling is the simulation of the behaviour of complex systems by explicitly taking its smallest constituent parts into account. In the context of radiation damage in nuclear materials, these simulations involve the bulk and surface atoms of reactor components and their interactions with energetic neutrons and plasma particles in the form of free atoms, molecules and ions. The computational techniques employed include molecular dynamics, density functional theory, and a variety of Monte Carlo methods; this Workshop provides an introduction to some popular software used to implement these techniques, with practical sessions on the free packages LAMMPS and SDTrimSP.

The course directors were:

- Kalle Heinola (IAEA)
- Christian Hill (IAEA)

- Jean-Christophe Sublet (IAEA)
- Nicola Seriani (ICTP; local organiser)

26 participants from 15 Member States joined 11 lecturers and directors for a combination of lectures, posters (as short, contributed presentations) and practical sessions covering the following topics. 50% of the participants were female.

- Irradiated material: defect and cascade production;
- Damage dose-rate, energies, and atomic displacement;
- Neutron-induced material defect simulation;
- Theoretical modelling of radiation effects;
- Plasma-surface interaction: erosion and surface-evolution studies;
- Plasma opacity;
- Hydrogen isotope deposition, trapping and permeation in fusion-relevant materials.

More details are available at https://amdis.iaea.org/workshops/ictp-2021. The Workshop was well-received, as interpreted through the anonymous, online questionnaire that participants were invited to complete (Appendix C). 19 responses were received; the mean overall rating given was 8.58/10 ($\sigma = 1.31$).

The recordings of the lectures in this course were placed on the IAEA's Open Learning Management System and are available at https://elearning.iaea.org/m2/.

6.2 Atomic Processes in Plasmas: Data-Driven Research

This School assisted Ph.D. students and other early-stage career researchers to develop their quantitative understanding of the fundamental processes that produce the observed behaviour and properties of plasmas; through lectures and practical computing sessions they also gained skills in the application of modern data science techniques to the calculation and evaluation of data on these processes. Scientists in developing countries without extensive experimental research facilities particularly benefit from such training in modern, data-driven computational physics.

The course directors were:

- Christian Hill (IAEA)
- Ludmila Marian (IAEA)
- Hyun-Kyung Chung (Korea Institute of Fusion Energy, Republic of Korea)
- Manuel Bautista (Western Michigan University, USA)
- Yuri Ralchenko (National Institute of Standards and Technology, USA)
- Udo von Toussaint (Max Planck Institute for Plasma Physics, Garching, Germany)
- George Thompson (ICTP; local organiser)

22 participants from 12 Member States joined eight lecturers for a combination of lectures, posters (as short, contributed presentations) and practical sessions covering the following topics:

- Plasma emission modelling;
- Practical exercises using FLYCHK and the NIST LIBS database;
- The principles of Molecular Dynamics modelling;
- Bayesian Inference for the determination of plasma-material interaction parameters;
- Demonstration and practical exercises using LAMMPS;
- Accessing, assessing and exploiting online data resources;
- Managing atomic and molecular data;
- Linux command line usage; Using Python and the JupyterLab environment for research.

More details are available at https://amdis.iaea.org/workshops/ictp-2021b. This Workshop was also well-received, as interpreted through the anonymous questionnaire that participants completed (Appendix D). 10 responses were received; the mean overall rating given was 8.80/10 ($\sigma = 1.08$).

6.4 Virtual IAEA Workshop on Computational Nuclear Science and Engineering for Nuclear Technology and Applications

An IAEA-organized workshop "Computational Nuclear Science and Engineering for Nuclear Technology and Applications" was held as a virtual event from 12 – 16 July 2021. Computational science applied to the field of nuclear science, technology and applications, is tightly related to the study and implementation of numerical analysis, codes and data libraries to address complex physics and engineering problems. With the advancement of computational resources, scientists are required to adopt a variety of modern tools, including multi-physics and multi-scale approaches in various plasma codes, first-principles calculations, molecular dynamics and Monte Carlo simulations, rate theories, dislocation dynamics, coupled thermal hydraulics and neutronics, structural mechanics and finite element/difference/volume methodologies.

The event and its interdisciplinary programme of lectures provided students, young researchers, and young professionals with critical skills and tools in areas such as mathematical techniques for modelling and simulation of complex systems, high performance computing, and computational methods for processing and analysing large data sets, applied in nuclear science and engineering. It was attended by nearly 200 participants representing 46 Member States.

The workshop was organized as an IAEA interdepartmental event with directors from Department of Nuclear Sciences and Applications (Nuclear Data Section (NDS) and Physics) and from Department of Nuclear Energy (Nuclear Power Technology Development Section (NENP)). The directors were:
- Matteo Barbarino (IAEA – Physics)
- Chirayu Batra (IAEA – NENP)
- Kalle Heinola (IAEA – NDS/AMD Unit)
- Jean-Christophe Sublet (IAEA – NDS/Nuclear Data Services Unit)

Topics covered included
- Computational methods for nuclear fusion science and for nuclear engineering;
- Probabilistic computational methods;
- High fidelity, high performance reactor modelling and simulation;

- Integrated multi-physics modelling for plasma science;
- Nuclear analysis in support for ITER design;
- Multi-physics and multi-scale methodologies;
- Open source data and codes for nuclear fusion science;
- Advanced computational methods for nuclear science and engineering.

Event agenda and details are found at https://conferences.iaea.org/event/255/ . Lecture materials and a quiz with multiple choice questions to each lecture are provided as a self-learning e-course material through CLP4NET found at https://elearning.iaea.org/m2/course/view.php?id=1074

The event served as a short introduction to an extended School/Workshop that took place in 2022 as an in-person event organized through IAEA-ICTP.

6.5 Joint IAEA-ICTP Advanced School/Workshop on Computational Nuclear Science and Engineering

The IAEA-ICTP "Advanced School/Workshop on Computational Nuclear Science and Engineering" was held as a hybrid event from 23 – 27 May 2022. The event was a follow-up school to the virtual "IAEA Workshop on Computational Nuclear Science and Engineering for Nuclear Technology and Applications" organized in July 2021 (see details in Section 6.4).

The event provided critical skills tools for students, young researchers, and young professionals in areas such as mathematical and computational techniques for modelling and simulation of complex nuclear systems, high performance computing, and computational methods for processing and analyzing large data sets, applied in nuclear science and engineering. The school had nearly 170 participants of which 25 attended the event in person. The event agenda comprised of lectures, poster sessions and hands-on workshops. Participants represented 47 Member States.

The school was organized as an IAEA interdepartmental event with directors from Department of Nuclear Sciences and Applications (Nuclear Data Section (NDS) and Physics) and from Department of Nuclear Energy (Nuclear Power Technology Development Section (NENP)). The directors were:
- Matteo Barbarino (IAEA – Physics)
- Chirayu Batra (IAEA – NENP)
- Kalle Heinola (IAEA – NDS/AMD Unit)
- Jean-Christophe Sublet (IAEA – NDS/Nuclear Data)
- Nicola Seriani (ICTP; local organizer)

Main topics of the school were:
- Tools for computational nuclear science and engineering
- Fundamentals of nuclear observable challenges
- Advanced modelling and simulation methodologies (nuclear fusion and nuclear engineering)
- Open source data and codes for plasma/fusion/fission science and engineering
- Advanced computational methods

Detailed information and downloadable material of the event is found at https://in-dico.ictp.it/event/9798/ .

7. Women in Fusion Network

In May 2021, the Fusion Energy Conference (FEC2020) held a side event webinar "Women in Fusion" to discuss gender equality and women empowerment in nuclear fusion. Discussion highlighted that the fusion community did not have a structured and permanent group dedicated to the promotion of women in the field, prompting the members of the discussion panel to create Women in Fusion (WiF) group. A series of meetings for organizing WiF were held virtually from October 2021 onwards by the founding members: IAEA, ITER, Fusion for Energy (F4E), General Atomics (GA) and EUROfusion. The 1st WiF Steering Committee (SC) was organized at ITER Headquarters from 24 – 25 May 2022. In this meeting, the SC members discussed e.g. the creation and public launch of the WiF website, development of research in gender equity for fusion and key activities supporting the organization's near-term objectives. From IAEA, Sehila Gonzáles de Vicente (Physics Section) was elected as the chair of WiF and Kalle Heinola (NDS/AMD Unit) as the scientific secretary.

WiF is a global and independent group, with strong support from its founding members. The goal of WiF is to be a platform for highlighting and encouraging the role of women in the fusion energy field, providing a tool for networking, and developing the needed evidence to shape policies around gender equity in fusion as the main focus, and in STEM in general. Initiated by a collaboration of founding members, WiF aims to collaborate with members and organizations around the world to ensure that women fusioneers have a platform for support and community building.

The Women in Fusion website was launched on 20th July 2022 at https://www.womeninfusion.org.

8. Unit Website

Developments

The Atomic and Molecular Data Unit has continued to maintain and develop its new website to communicate its work and provide details to meeting and project participants. The official URL is https://amdis.iaea.org/ and a new 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 available. As discussed above, the migration of ALADDIN onto a new platform is under way.

Statistics

The original website, https://www-amdis.iaea.org/, received 52,000 page views by 19,000 users over the time period May 2021 – April 2022, as compared with 35,000 page views by 12,000 users in the previous year. It is noted that the top 10 countries visiting the site are all members of the ITER consortium.

9. Duty Travel

Duty Travel by AMD Unit staff members continues to be disrupted by restrictions imposed by Member States on international travel, and by internal IAEA policies limiting such trips to a maximum of one per quarter. The following trips were made over the period June 2021 – May 2022.

Christian Hill, 10 – 14 October 2021, to CEA Paris-Saclay to work on development of the DefectDB database with DFT experts.

Christian Hill, 15 – 19 March 2022, Participation and invited oral presentation at the CECAM Workshop on Multiscale Modelling of Irradiation-Driven Processes for Emerging Technologies, at the École Polytechnique Fédérale de Lausanne (EPFL), Lausanne, Switzerland.

Christian Hill, 26 April – 1 May 2022, Consultation and development work on software for standardising atomic and molecular data formats for plasma collisional processes relevant to machine learning applications at University College London, UK.

Kalle Heinola, 11 – 12 April 2022, Scientific Secretary at "IAEA Technical Meeting on the Effects of Hydrogen Supersaturation and Defect Stabilization in Nuclear Fusion Reactor Materials", Aix-en-Provence, France

Kalle Heinola, 24 – 25 May 2022, 1st Steering Committee meeting of Women in Fusion group, ITER Headquarters, France

10. Publications

Scientific Articles

- A. Hollingsworth, M.-F. Barthe, M. Yu. Lavrentiev, P. M. Derlet, S. L. Dudarev, D. R. Mason, Z. Hu, P. Desgardin, J. Hess, S. Davies, B. Thomas, H. Salter, E. F. J. Shelton, K. Heinola, K. Mizohata, A. De Backer, A. Baron-Wiechec, I. Jepu, Y. Zayachuk, A. Widdowson, E. Meslin and A. Morellec, "Comparative study of deuterium retention and vacancy content of self-ion irradiated tungsten*", J. Nucl. Mat.* **558**, 153373 (2022).

- O. Lindblom, T. Ahlgren, K. Heinola, "Molecular dynamics simulations of hydrogen isotope exchange in tungsten vacancies", *Nucl. Mater. Energy* **29**, 101099 (2021).

- A. Widdowson, J. P. Coad, Y. Zayachuk, E. Alves, N. Catarino, V. Corregidor, M. Mayer, S. Krat, J. Likonen, K. Mizohata, C. Rowley, M. Zlobinski, M. Rubel, D. Douai, K. Heinola, T. Wauters, L. Dittrich, S. Moon, P. Petersson, A. Baron-Wiechec, L. Avotina, "Evaluation of tritium retention in plasma-facing components during JET tritium operations", *Phys. Scripta* **96**, 124075 (2021).

- S. Krat, M. Mayer, J. P. Coad, C. P. Lungu, K. Heinola, A. Baron-Wiechec, I. Jepu, A. Widdowson, "Comparison of JET inner wall erosion in the first three ITER-Like Wall campaigns", *Nucl. Mater. Energy* **29**, 101072 (2021).

- Tommy Ahlgren and Kalle Heinola, "Improvements to the Sink Strength Theory Used in Multi-Scale Rate Equation Simulations of Defects in Solids", *Materials* **13**, 2621 (2020).

- G. De Temmerman, K. Heinola, D. Borodin, S. Brezinsek, R. P. Doerner, M. Rubel, E. Fortuna-Zalesna, C. Linsmeier, D. Nishijima, K. Nordlund, M. Probst, J. Romazanov, E. Safi, T. Schwarz-Selinger, A. Widdowson, B. J. Braams, H.-K. Chung, C. Hill, "Data on erosion and hydrogen fuel retention in Beryllium plasma-facing materials", *Nucl. Mater. Energy* **27**, 100994 (2021).

- H. Ganser, C. Hill, J. H. George, J. M. Brown, M. Jackson, "Re-investigation of the infrared spectrum of the NCN radical by laser magnetic resonance spectroscopy", *Journal of Molecular Spectroscopy* **382**, 111547 (2021).

- V. Laporta, R. Agnello, G. Fubiani, I.Furno, C. Hill, D. Reiter, F. Taccogna, "Vibrational excitation and dissociation of deuterium molecule by electron impact", *Plasma Physics and Controlled Fusion* **63**, 085006 (2021).

INDC Reports

Dipti, K. Heinola, C. Hill, 26th Meeting of the A+M Data Centres Network: Summary Report of an IAEA Technical Meeting, 1 – 3 September 2021 (virtual event), *INDC(NDS) Report* 838 (2021) [https://nds.iaea.org/publications/indc/indc-nds-0838/]

K. Heinola, Hydrogen Permeation in Fusion Relevant Materials: Summary report of the First Research Coordination Meeting, 23 – 27 November 2020 (virtual event), *INDC(NDS) Report* 842 (2022) [https://nds.iaea.org/publications/indc/indc-nds-0842/]

C. Hill and K. Heinola, IFRC Subcommittee on Atomic and Molecular Data for Fusion: Report on the Activities of the Atomic and Molecular Data Unit, May 2018 – June 2021, *INDC(NDS) Report* 843 (2022) [https://nds.iaea.org/publications/indc/indc-nds-0843/]

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 (hybrid event), *INDC(NDS) Report* 854 (2022) [https://nds.iaea.org/publications/indc/indc-nds-0854/]

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://nds.iaea.org/publications/indc/indc-nds-0855/]

11. Cooperations and Other Activities

- The Practical Arrangements between the IAEA and the Korea Institute of Fusion Energy (KFE), formerly named the National Fusion Research Institute (NFRI), for cooperation in the area of atomic, molecular and plasma-material interaction data relevant to fusion have been successfully renewed and re-signed by the DDG-NE and President of KFE, and remain valid until 3 September 2024.

- The AMD Unit entered into a cooperation agreement with the organisers of the 6th Spectral Lineshapes in Plasmas (SLSP) Workshop, which will be held in Hyères, France from 17 – 21 October 2019 [1]. The Unit Head joined the Scientific Organising Committee for this event.

- 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 at Forschungszentrum Jülich, Germany from 8 – 10 June 2021 [2]. Unit Staff member Kalle Heinola joined the Scientific Organising Committee of the event.

- Kalle Heinola is a member of International Program Committee of the International Workshop on Hydrogen Isotopes in Fusion Reactor Materials (HWS) [3, 4], a satellite event to the biennial Conference on Plasma-Surface Interaction in Controlled Fusion Devices (PSI); the event will be held from 20 – 22 June, in virtual format.

- Christian Hill is a member of the International Organizing Committee of the International Conference on Atomic and Molecular Data and their Applications (ICAMDATA) [5], to be held in Bari, Italy from 25 – 29 September 2022.

- Christian Hill is chair of the Atomic Processes in Plasmas Conference (APiP) [6, 7] conference, to be held at the IAEA as a Technical Meeting from 15 – 19 May 2023 (postponed from 2021).

[1] https://plasma-gate.weizmann.ac.il/projects/slsp/slsp6/

[2] https://amdis.iaea.org/workshops/mod-pmi-2021

[3] https://www.psi2022.kr/abstract/abstract_04.html

[4] https://hydrogen.onuniverse.com/

[5] https://www.icamdata2022.it/

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

[7] https://conferences.iaea.org/event/238/

12. Future Meetings in the Present Biennium

Third RCM of the Vapour Shielding CRP

The final RCM of CRP F43024: Atomic Data for Vapour Shielding in Fusion Devices is planned for October 2022. The CRP participants will meet at IAEA Headquarters to review the data produced during the project, which will be distributed through the AMD Unit's website services, and to plan the writing of a final report.

The Third RCM will also review the prospects for a Code Comparison Workshop exercise on calculations of atomic data for edge plasma modelling, and consider prospects for future work on these topics.

First RCM of the Injected Impurities CRP

The First RCM of CRP F43026: Atomic Data for Injected Impurities in Fusion Plasmas is planned as an in-person meeting for November 2022, following a Consultancy Meeting to set the scope of the CRP to be held from 7 – 8 June 2022. Following the selection of participants and exchange of Research Contracts and Agreements, the meeting will serve as a forum to introduce work plans, build collaborations, and initiate network activities such as code comparison activities and knowledge-exchange.

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 it is intended that the event should be held as a Technical Meeting, jointly with the 27th meeting of the Data Centres Network from 15 – 19 May 2023. The organising committee is chaired by the AMD Unit Head.

The committee members are:

- 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 topics sessions proposed so far 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

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

The 2nd Technical Meeting on the CR Properties of Tungsten and Hydrogen in Edge Plasmas is planned to take place from 19 – 23 June 2023 at the IAEA HQ. The meeting will comprise of sessions reviewing the outcome and status of the three Working Groups established at the 1st Technical Meeting on CR Properties of Tungsten and Hydrogen:

- Working Group 1: A+M data recommendation and validation

- Working Group 2: Plasma experiments and comparison activities with CR models

   o Working Group 2a: W and hydrogen experiments with fusion and linear plasma devices

   o Working Group 2b: Photon opacity models in CR models

- Working Group 3: Plasma-surface process properties, trends and underlying effects.

The meeting will bring together experimentalists operating magnetic confinement devices and linear plasma devices, and computational researchers performing plasma simulations, CR modelling and fundamental plasma particle interaction calculations. Main topics include: W ejection rates from the source/wall surface and the resulted W charge states (q+), electronic recombination with W^{q+}, electron-induced excitation and ionization of W^{q+}, charge-exchange processes of W^{q+} with hydrogenic plasma species, formation and experimental observations of

WH$_x$ molecules, hydrogen isotope effects, divertor spectroscopic issues, effect of opacity and opacity modelling.

Eighth Technical Meeting on the Code Centres Network

The 8th Meeting of the Code Centres Network will take place in 2023 (dates to be confirmed, but likely to be in the autumn). Due to budgetary constraints imposed by the Director General's Office, it is likely that this meeting will be chosen to be held in virtual format, as in 2021. The meeting will focus on the simulation and analysis of radiation damage in fusion-relevant materials through computational techniques such as molecular dynamics (in the study of collision cascades and plasma-surface interactions) and density functional theory (DFT) (in the study of the energetics and evolution of radiation-induced defects in these materials).

Of growing importance in the field is the simulation of high-dose damage (as is anticipated in ITER and any viable nuclear fusion power plant) and the study of high-entropy alloys (HEAs) as candidate materials for the first wall of a fusion reactor. On this topic, the AMD Unit is currently advising the work of a post-doctoral researcher, Dhanshree Pandrey, at the ICTP carrying out DFT calculations of defects in low-activation HEAs. Ms Pandrey will report on her work at the CCN meeting.

First RCM of the Edge Plasmas CRP

The First RCM of CRP F43027: Formation and Properties of Molecules in Edge Plasmas is planned as an in-person meeting for summer 2023, following a Consultancy Meeting to set the scope of the CRP to be held in late 2022 or early 2023. The goal of the 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.

At the first Research Coordination Meeting of the CRP, participants will introduce their research and work plans, coordinate collaborative research work and set objectives for code comparison and benchmarking activities.

13. Proposed Coordinated Research Projects for the 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).

The summary of the proposed Task within the budget plan 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).

Continuation CRP on Hydrogen Permeation

A new CRP continuing the work 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 and that concerning Steel Surfaces (F43022) – TDS, sputtering, gas-driven permeation) – this new project would seek to at least start work (and community-building) on the effect of temperature and electric field gradients on hydrogen permeation in hydrogen in materials. This topic is 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 them out.

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

These CRPs will be proposed to the relevant Committee for Coordinated Research Activities (CCRA) with a view to holding their first Research Coordination Meetings in the 2024-25 biennium after Consultancy Meetings to address more specifically their scope, participation and expected outputs.

14. Proposed Technical Meetings for the Biennium 2024–25

Decennial Meeting, 2024

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 proposed meeting in 2024 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.

Some concern was raised by Subcommittee members about the lack of commonality between the fusion research communities focusing on plasma collisional / plasma-surface interaction data and in-material radiation-damage; it was agreed that the meeting should be concerned principally with the former topic.

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. Talks with the University of Helsinki to hold the meeting in Finland through a Host Government Arrangement are at an early stage.

[1] https://www-amdis.iaea.org/meetings/AMPMI14/

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:

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.

3rd Technical Meeting of the Global Network for the Atomic and Molecular Physics of Plasmas: this new Network is a consortium of research groups working in the area of fundamental atomic and molecular physics relevant to plasma processes. In addition to smaller ongoing collaborations, three Working Groups have been formed within the Network in connection with a Technical Meeting Series on Tungsten and Hydrogen in Edge Plasmas; meetings in connection with this topic, to coordinate work within the Network, are planned for 2024 and 2025.

IFRC Subcommittee Meeting

24th 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 2024, to allow for planning for the 2026-27 biennium by September 2024. 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 if possible.

15. 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.

The Subcommittee proposed to update its Methods of Work document as described in Appendix A; the key changes are summarised below.

- A removal of abbreviations to improve clarity;

- The removal of gendered pronouns: "Chairman" to be replaced by "Chair", "he" to be replaced by "they" throughout;

- Subcommittee Meeting minutes are to be made available on the AMD Unit's website but no longer required to be distributed in hard copy to the directors of fusion laboratories in Member States.

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, with the changes proposed at the meeting in 2022 indicated.

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, Molecular and Plasma-Material Interaction 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

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Appendix C: IAEA–ICTP Workshop on Atomistic Modelling of Radiation Damage in Nuclear Systems

The organisers of the 2021 Joint IAEA–ICTP Workshop on Atomistic Modelling of Radiation Damage in Nuclear Systems, which was held online from 4 – 8 October 2021, invited participants to complete an anonymous online questionnaire to gain feedback on the event; the results are given in this appendix.

2021 Joint ICTP-IAEA Workshop on Atomistic Modelling of Radiation Damage in Nuclear Systems

Summary of 19 responses.

What best describes your academic position?

Graduate Student	☐☐☐☐☐☐☐☐☐☐☐	11
Post-doc	☐☐☐☐☐	5
Career Scientist	☐	1

Which describes your research best?

Theory	☐☐☐☐☐☐☐☐☐☐	10
Experiment	☐☐☐☐☐☐☐☐☐	9

Which *operating system* do you use most?

Windows	☐☐☐☐☐☐☐☐☐☐☐	11
macOS	☐☐☐	3
Linux / Unix	☐☐☐☐☐	5
Other		0

How would you rate the Workshop, overall?

mean = 8.58 (1.31)

1		0
2		0
3		0
4		0
5	☐	1
6		0
7	☐☐	2
8	☐☐☐☐☐☐	6
9	☐☐☐☐	4
10	☐☐☐☐☐☐	6

How useful was the School to you, overall?

mean = 4.21 (0.52)

Not useful at all		0
A bit useful		0
Satisfactory	☐	1
Good	☐☐☐☐☐☐☐☐☐☐☐☐☐	13
Fantastic	☐☐☐☐☐	5

How did you find out about this School?

Through colleague / supervisor	☐☐☐☐☐☐☐☐☐☐☐	11

Through a mailing list (e.g. Molecular Dynamics mailing list)		0
Through the ICTP website	☐☐☐☐	4
Through the IAEA website	☐☐☐	3
Other (see below)		0

How did you find out about this School (other)?

Excellent workshop with good exposure to different modelling methods.

Some of the lectures were a bit hard for me but still, it was great to meet scientists who do interesting work.

ICTP WEBSITE

Through this workshop

Through friends and mates

How many lectures did you attend?

mean = 3.53 (0.75)

0 – 2		0
3 – 4	☐☐☐	3
5 – 6	☐☐☐	3
7 – 8	☐☐☐☐☐☐☐☐☐☐☐☐☐	13

How did you find the *level of difficulty* of the lectures?

mean = 3.16 (0.36)

Far too easy		0
A bit too easy		0
Just right	☐☐☐☐☐☐☐☐☐☐☐☐☐☐☐☐	16
A bit too hard	☐☐☐	3
Impossible to follow!		0

How *useful* did you find the lectures?

mean = 4.05 (0.60)

Not at all useful		0
Not very useful		0
Useful	☐☐☐	3
Very useful	☐☐☐☐☐☐☐☐☐☐☐☐	12
Exceptionally useful!	☐☐☐☐	4

How *useful* did you find the Computing Practicals?

mean = 3.63 (0.87)

Not at all useful		0
Not very useful	☐☐	2
Useful	☐☐☐☐☐☐	6

Very useful	□□□□□□□□	8
Exceptionally useful!	□□□	3

How did you find the *level of difficulty* of the computing practicals?

mean = 3.11 (0.64)

Far too easy	0	
A bit too easy	□□□	3
Just right	□□□□□□□□□□□	11
A bit too hard	□□□□□	5
Impossible to follow!	0	

How did you find the *video conferencing resources* (sound/video quality, chat functionality, etc.)

mean = 4.42 (0.67)

Awful	0	
Bad	0	
Average	□□	2
Good	□□□□□□□	7
Excellent	□□□□□□□□□□	10

What did you like most about the Workshop?

Hard to pick but all session were perfect for me

Lecture presentations

As an experimental researcher, this workshop enabled me to think about simulations. It allowed me to understand how simulations work and gave me a chance to listen to some good lectures.

All the lectures and tutorial workshops.

Computing practicals were so improving and motivating. Due to my lack of experience on Jupyter, it was a little hard to follow. Sharing the screen worked great for me. Running the first MD calculation was a good step for me as a prospective scientist.

Breadth of the topics addressed.

The schedule time was good and programs were implemented on time. The meeting was well managed and there was intimacy between the organizers and speakers.

Hands on tutorials

Educational content Friendly and patient presenters prompt answering of participants questions

The presentations were very well done and clear

I really enjoyed all lectures (especially the lecture of D. Mason)– very informative.

An opportunity to meet experts on the specific topic.

The lectures

1. The explanation of interatomic potentials and hardening of the potentials 2. Practical exercise to perform MD simulation of LAMMPS. 3. Data extraction from atomic data.

The lecturers were friendly and the feedback from them was warmly

What did you NOT like about the Workshop? Please be open and honest.

None

For an experimental person, like I am, the lectures were a bit difficult to understand but to someone who is into computational work this workshop is very well organised. Now I can look for collaborations for simulations and speak in their terms.

Just it was online.

Noting bad to say. Because of my lack of experience with computational methods practical sessions have been hard for me to follow. Special thanks to Christian Hill for showing the process on screen. Providing a DEMO and instructions sheet may be useful for participants on my level of knowledge.

Nothing major comes to mind. Perhaps that for both practicals we ended up watching a shared screen. For lack of computational power (LAMMPS) and because many people had troubles with SDTrimSP. Not sure how I would remedy this though, there's not much one can do in such a short time when it comes to hands on exercises.

The speed and accent of some speakers was not good for me and it was effective in understanding the content. It was my first time attending an online foreign workshop, and sometimes I missed the concept.

absence of emails of presenters for follow up and correspondence.

The practices were short and in my opinion I would have liked them to be more complete, but I understand the objective of the workshop.

Some short coffee breaks (even for online Workshop) would be very useful.

First of all, I think the workshop can be more interactive and informative if it was conducted on-site not virtual. Participants did not have a time to make network with colleague researchers. (I know it is because Covid, though.) About the practical session, I think this one could be improved if the organisers post slides prior to the session so that participants can try some on their own. The gap among participants exists and that was a big hurdle to smoothly conduct practical session.

The practical sessions

I did not like the SDTRIM practicals as the lecture before said it is not a very useful software. I found this particular practical session a bit confusing in parts.

The timing for each section was very short

Please write any further comments you would like to add below.

Overall, it was a well organised workshop.

I would like to thank ICTP for the most wonderful conference. It was a fruitful and amazing time for me.

It is the first workshop I have participated in. I am sort of proud and excited about being a part of the organization. Thank you for the great lectures and practice opportunities.

I wish we had access to the recorded speeches. Im Ph.D student and the first question doesn't have this option. I miss the last part (Q & A session) because something happened to me and I force to leave workshop.

fantastic workshop. this was the workshop i needed to give me perspective in the field. especially as i want to do more research in this field of nuclear materials

Thank you for allowing me to participate and I would like to be able to be there next year

Wish the opportunity like this one comes again soon..! Thank you for all the organisers and lecturers.

No

Overall it was an excellent workshop. The other drawback which I felt is that they may have included a session on DFT calculations and a practical on VASP rather than SDTRIM.

Thanks for giving me the opportunity to be part of this workshop. Hoping to be part of the next workshop.

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Appendix D: IAEA–ICTP Workshop on Atomic Processes in Plasmas: Data-Driven Research

The organisers of the 2021 Joint IAEA–ICTP Workshop on Atomic Processes in Plasmas: Data-Driven Research, which was held online from 13 – 17 December 2021, invited participants to complete an anonymous online questionnaire to gain feedback on the event; the results are given in this appendix.

2021 Joint ICTP-IAEA Workshop on Data-Driven Research on Plasmas

Summary of 10 responses.

What best describes your academic position?

Graduate Student	☐☐☐☐☐☐☐	7
Post-doc	☐	1
Career Scientist	☐☐	2

Which describes your research best?

Theory	☐☐☐☐☐☐	6
Experiment	☐☐☐☐	4

Which *operating system* do you use most?

Windows	☐☐☐☐☐☐☐	7
macOS		0
Linux / Unix	☐☐☐	3
Other		0

How would you rate the Workshop, overall?

mean = 8.80 (1.08)

1		0
2		0
3		0
4		0
5		0
6		0
7	☐	1
8	☐☐☐☐	4
9	☐	1
10	☐☐☐☐	4

How useful was the School to you, overall?

mean = 4.10 (0.83)

Not useful at all		0
A bit useful	☐	1
Satisfactory		0
Good	☐☐☐☐☐☐	6
Fantastic	☐☐☐	3

How did you find out about this School?

Through colleague / supervisor	☐☐☐☐☐☐☐	7

Through a mailing list (e.g. Molecular Dynamics mailing list)	0
Through the ICTP website	☐☐☐ 3
Through the IAEA website	0
Other (see below)	0

How did you find out about this School (other)?

It is very knowlegable

How many lectures did you attend?

mean = 3.70 (0.46)

0 – 2	0
3 – 4	0
5 – 6	☐☐☐ 3
7 – 8	☐☐☐☐☐☐☐ 7

How *useful* did you find the lectures?

mean = 4.00 (0.45)

Not at all useful	0
Not very useful	0
Useful	☐ 1
Very useful	☐☐☐☐☐☐☐☐ 8
Exceptionally useful!	☐ 1

How did you find the *level of difficulty* of the lectures?

mean = 3.30 (0.64)

Far too easy	0
A bit too easy	☐ 1
Just right	☐☐☐☐☐ 5
A bit too hard	☐☐☐☐ 4
Impossible to follow!	0

How *useful* did you find the Computing Practical?

mean = 3.80 (0.40)

Not at all useful	0
Not very useful	0
Useful	☐☐ 2
Very useful	☐☐☐☐☐☐☐☐ 8
Exceptionally useful!	0

How did you find the *level of difficulty* of the computing practicals?

mean = 3.00 (0.63)

Far too easy	0
A bit too easy	☐☐ 2
Just right	☐☐☐☐☐ 6
A bit too hard	☐☐ 2
Impossible to follow!	0

How did you find the *video conferencing resources* (sound/video quality, chat functionality, etc.)

mean = 4.30 (0.64)

Awful	0
Bad	0
Average	☐ 1
Good	☐☐☐☐☐ 5
Excellent	☐☐☐☐ 4

What did you like most about the Workshop?

Pretty interesting mix of topics, competent speakers

Overall, I do like all the workshop.

Thanks for the opportunity., I loved and interestingly learned the LIBS or LIPS based plasmas process and their plasma parameters evaluation. Respectively, the laser plasma and the thin-films formation. Election density, temperature calculations., Stark broading concept etc. I am also working for LIPS based nanostructures and their growth mechanism.

Professional and patient directors and speakers

I liked the range of topics, they were all interesting and relevant. The timetable was also perfect: not too long and not too brief. I'm also pleased that the poster session went ahead.

Lecture on Plasma emission modelling and the computing practical on LAMMPS. Recordings will be made available.

Workshop arrangement was very nice and the lectures from various experienced professors are very useful.

I like that a Jupyter environment with LAMMPS has been prepared for us.

What did you NOT like about the Workshop? Please be open and honest.

Nothing bad.

No specific, but I feel and felt for my part., I am unable to follow complete the mathematical calculation by using the computer simulations. Kindly, need some time to explore. Due to time constraints., I unde6. The situation.

There was no bad point

With the poster session, it was difficult to ask questions and have an open chat with the presenters. Obviously this is challenging to perform over Zoom but it was a shame to miss out on this networking opportunity.

Some lectures were too specific, where a birds eye view would be more useful. Presenting style can be improved, to make it more engaging to listen.

It's is totally on applications like software developments and uses of them. It's difficult to understand in one lecture but the good thing is you provides us the recording of the lectures which will be very helpful.

I expected more exercises on LAMMPS and Bayesian optimization.

Please write any further comments you would like to add below.

It would be helpful to split the individual hands-on exercises into two parts with a day in between. In the first part the principles and simple examples should be introduced, augmented with simple 'do-it-yourself'-tasks which could/should be tried offline before the second part. In the second part the arising questions could then be answered and (if time permits) then more advanced examples introduced. If one had a little bit time play with the tools the aspects of the more advanced samples are easier to digest.

I hope all lectures will be recorded.

It's very good arrangement, in future user (participants) need to interact by virtually with the expertise in the mathematical calculation/modelling/simulations. I wish to follow and keen to participate, present my field of research future upcoming workshop or seminar or short term courses. Thanking you Sincerely yours Dr. E. Manikandan, PhD., https://www.scopus.com/authid/detail.uri?authorId=35185347200

Maybe it would be ideal to survey participants before the start of the conference to ascertain the ability level and therefore help the speakers to pitch lectures at the appropriate level. It would be nice if the speakers had separate 'bullet points'/takeaways for people that use that system often vs those that may never need to use it but want to know briefly what they can use it for.

Very happy for giving me the opportunity to attend the workshop.

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