

Current Activities of IAEA A+M Unit

H.-K. Chung

Atomic and Molecular Data Unit, Nuclear Data Section
Division of Physical and Chemical Sciences

24th Data Centre Network (DCN) Meeting, September 4-6, 2017

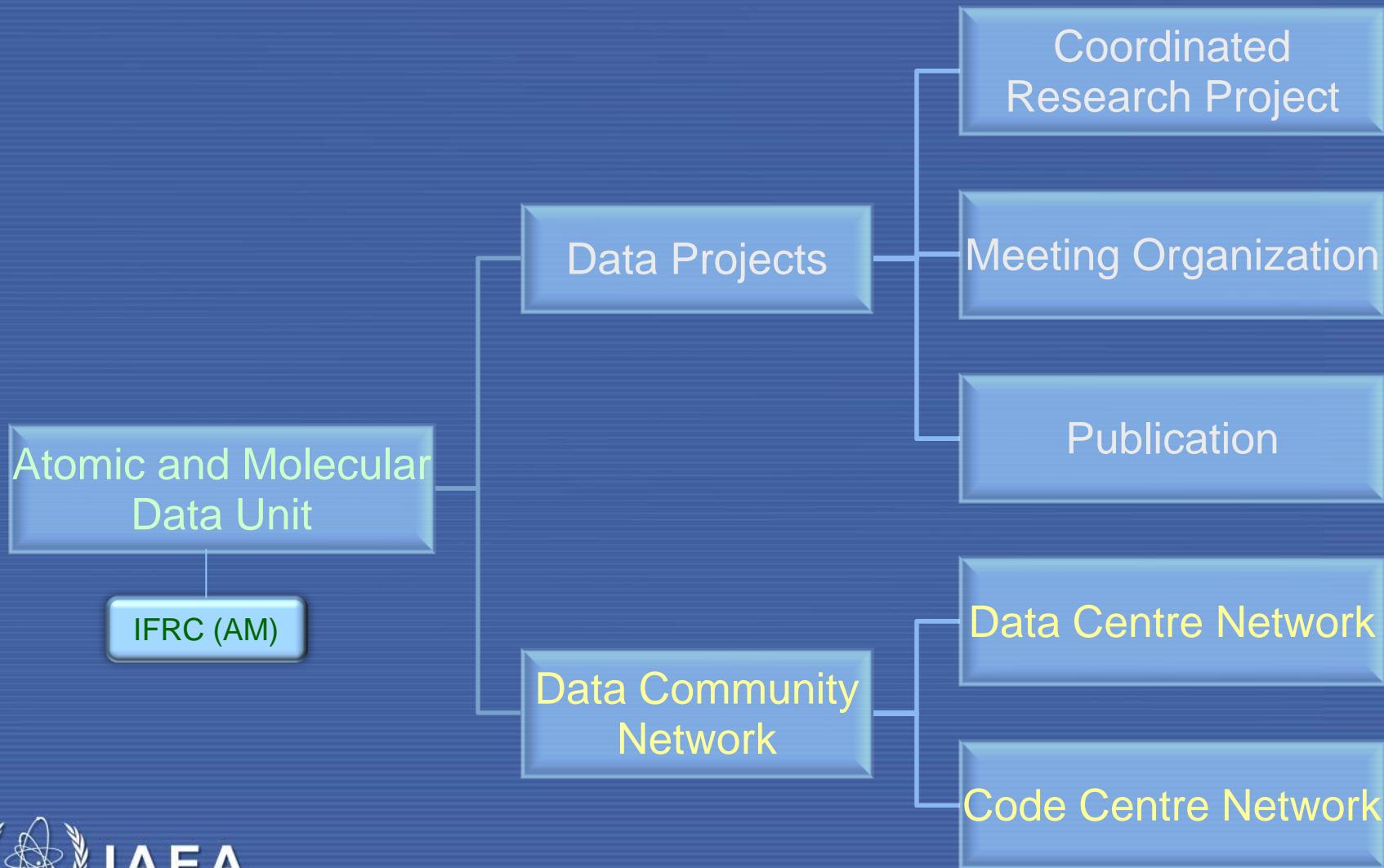


Unit Staff Changes

- Unit Head, Bas Braams retired in November 2016
- Hyun Chung became the Unit Head since December 2016 and will leave the Agency by the end of September 2017 due to the rotation policy.
- Christian Hill will be a new Unit Head from October 1st 2017.
- The recruitment of a P3 position of atomic physicist is in progress and will be complete no sooner than January 2018.

Atomic and Molecular Data Unit

Activities



Coordinated Research Projects

Data Generation and Exchange

CRP: Coordinated Research Project

- Main mechanism by which the AMD Unit encourages new research
- Unique Opportunity for Comprehensive and Synergistic Collaboration

Joint research on Atomic, Molecular & Plasma Surface Interaction Data for fusion:

- Representatives from 10 to 15 institutes world-wide
- Duration 3-4 years; 3 Research Coordination Meetings (RCM)

Objectives: To define and to coordinate international research on:

- Generation, compilation and evaluation of data
- Establishment of databases
- Development of new techniques

Outputs:

- Publications, Meeting Presentations and Reports
- Final Reports in “Atomic and Plasma-Material Interaction Data for Fusion” (APID); more recently in a journal (JPICS, Atoms)
- Data and Results in ALADDIN Numerical Database and Knowledge Base

Past, Present and Future CRPs

<http://www-amdis.iaea.org/CRP>

2008-2012: Characterization of Size, Composition and Origins of Dust in Fusion Devices

2009-2013: Light Element Atom, Molecule and Radical Behaviour in the Divertor and Edge Plasma Regions

2010-2014: Spectroscopic and Collisional Data for W from 1 eV to 20 keV

2011-2016: Data for kinetic modelling of molecules of H and He and their isotopes in fusion plasma

2012-2016: Erosion and Tritium Retention for Beryllium Plasma-Facing Materials

2013-2017: Plasma-Wall Interactions with Irradiated Tungsten and Tungsten Alloys in Fusion Devices

2015-2019: Plasma-wall Interaction with Reduced-activation Steel Surfaces in Fusion Devices

2016-2020: Data for Atomic Processes of Neutral Beams in Fusion Plasma

CRP on A+M Data for State-Resolved Modelling of H, He and their Isotopes in Fusion Plasma (2011-2016)

Objectives

- Species H, H⁺, H₂, H₂⁺, H₃⁺, He, He⁺, He₂⁺, HeH⁺, He₂⁺, H⁻ and isotopic variants; isotope effects are important; He is newly important
- Aim to be comprehensive for volume processes among the mentioned species and e-, hν
- Predominantly theoretical; some experiment

Data needs

- State-resolved cross-sections for kinetic modelling
- Electron-impact, radiative and photon-induced, and heavy particle collision processes

Participants

| | |
|---------------|------------------------------------|
| R. CELIBERTO | Polytechnic of Bari, Italy |
| U. FANTZ | MPI for Plasma Physics, Garching |
| C. JUNGEN | Laboratoire Aimé Cotton du CNRS |
| I. SCHNEIDER | Université Le Havre |
| V. KOKOOULINE | University of Central Florida |
| P. KRSTIC | Oak Ridge National Laboratory |
| X. MA | Chinese Academy of Sciences |
| O. MOTAPON | University of Douala, Cameroon |
| A. OREL | University of California at Davis |
| D. REITER | Forschungszentrum Jülich |
| K. SAWADA | Shinshu University |
| X. URBAIN | Catholic University of Louvain |
| J.-S. YOON | National Fusion Research Institute |

Research Coordination Meetings

First RCM: 10-12 August 2011

Second RCM: 3-5 July 2013

Third RCM: 14-16 March 2016

Final Report Atoms Journal

CRP on Erosion and Tritium Retention in Beryllium Plasma Facing Components (2012-2016)

Objectives

The key processes to be studied are physical and chemical sputtering by H, He and Be, which release beryllium impurities into the plasma, trapping and reflection of hydrogen (H, D, T) on beryllium surfaces, the transport of hydrogen in beryllium and means to extract trapped tritium.

Data needs

- Data for routine interaction of H/He and impurity ions with Be surface, and in transient events (melting, ablation)
- Most important projectiles: H, D, T, He, Be, C, N, O, Ne and Ar
- Data of mixed materials, especially, Be-(H,D,T,He), Be-C, Be-N, Be-O and ternary and higher mixtures

Participants

| | |
|---------------|---------------------------|
| R. DOERNER/ | PISCES Lab, UCSD |
| D. NISHIJIMA | |
| D. BORODIN | Forschungszentrum Jülich: |
| M. PROBST | University of Innsbruck: |
| S. IRLE/ | Nagoya University: |
| H. NAKAMURA | |
| K. NORDLUND/ | University of Helsinki |
| C. BJÖRKAS | |
| Ch. LINSMEIER | Forschungszentrum Jülich |
| W. JACOB | IPP, Garching |

Final Report in Preparation

Research Coordination Meetings

First RCM, 26-28 Sep 2012

Second RCM, 18-20 Aug 2014

Third RCM, 15-17 Jun 2016

CRP on Plasma-Wall Interaction with Irradiated Tungsten and Tungsten Alloys in Fusion Devices

Objectives

To support assessment of the prospects for tungsten-based plasma-facing materials in a fusion reactor environment

Data needs

Effects of neutron irradiation and charged particle surrogate irradiation on the microstructure of tungsten-based materials.

Relation between tungsten microstructure after irradiation and plasma-material interaction properties for erosion, tritium retention and tritium migration.

Synthesize information, extrapolate to fusion neutron fluence, and provide best expert estimates and uncertainties for tritium retention and transport

Research Coordination Meetings

First RCM, 26-28 November 2013

Second RCM, 8-11 September 2015

Third RCM, June 27-30, 2017



IAEA

Participants

- G. H. Lu et al., Beihang University, Beijing.
C. Liu, X. Wu et al., ISSP-CAS, Hefei.
G. Luo, C. Zhang et al., IPP-CAS, Hefei.
M. Barthe, C. Becquart et al., CNRS.
C. Grisolia, B. Rousseau et al., CEA.
M. Mayer, T. Schwarz-Selinger et al., IPP Garching.
B. Unterberg, J. Linke, Forschungszentrum Jülich.
S. Deshpande, P. M. Raole et al., IPR, Gandhinagar.
A. Hasegawa et al., Tohoku University.
Y. Hatano, Y. Oya et al., Toyama University.
M. Sakamoto, H. Watanabe et al., U. of Tsukuba.
T. Oda, H. Shim et al., Seoul National University.
Y. Gasparyan, A. Pisarev et al., MEPhI, Moscow.
B. Khrripunov, A. Ryazanov et al., Kurchatov Ins
S. Markelj et al., Josef Stefan Institute, Ljubljana.
S. Dudarev et al., CCFE, Abingdon.
B. D. Wirth et al., U. of Tennessee, Knoxville.
J. Allain, D. Ruzic et al., University of Illinois.
M. Shimada, B. Merrill et al., Idaho National Lab.

CRP on Plasma-wall Interaction with Reduced-activation Steel Surfaces in Fusion Devices

Background

- Main wall in DEMO or in a reactor will not be beryllium (too high erosion); tungsten is also unattractive (radiation issues). Some kind of low-activation steel looks attractive for the main wall, but more data are needed to assess just where it could be used.
- Special issue with steel: the alloy could be “self-passivating” with respect to erosion.

CRP Topics and Objectives

- Develop information about the microstructure of steel surfaces exposed to fusion neutrons and energetic plasma particles.
- Develop information about the relation between steel microstructure after irradiation and properties for erosion, tritium migration and ways to extract trapped tritium.
- To synthesize new information and provide best expert estimates and uncertainties for plasma-material interaction properties for steel surfaces in a fusion reactor environment.

Participants

- Peng Wang, Lanzhou Institute of Chemical Physics
- W. Jacob and T. Schwarz-Selinger, IPP Garching
- Y. Hirooka and N. Ashikawa, NIFS
- A. Golubeva and A. Spitsyn, Kurchatov Institute
- R. Doerner and D. Nishijima, UCSD PISCES Lab
- V. Maklai and I. Garkusha, IPP Kharkov
- D. Terentyev and L. Malerba, SCK-CEN

Meeting Plan

- **First RCM:** 9-11 December 2015
- **Second RCM:** 16-18 October 2017

CRP on Data for Charge Transfer Processes Related to Neutral Beams in Fusion Plasma

Objectives

Provide evaluated and recommended data for the principal atomic processes of heating and diagnostic neutral beams in fusion plasma.

Data needs

- Data for beam penetration, BES, MSE and CXRS/CHERS spectroscopy.
- Excitation and ionization in collisions between electrons and H/D/T neutrals.
- Excitation, ionization and charge transfer in collisions between hydrogen neutrals and fuel and selected impurity ions.
- (Lower priority:) collision processes in the hydrogen beam neutralizer; atomic processes of neutral beams of helium and lithium in fusion plasma.
- Electron energy from 100 eV to 100 keV, neutral energy from 1 keV to 1 MeV.

Participants

O. Marchuk, FZJ, Germany,
J. Ko, NFRI, Korea,
D. Stotler, PPPL, USA,
G. Pokol, Wigner Research Centre, Hungary,
M. O'Mullane, U of Strathclyde, UK,
A. Dubois, UPMC, France,
T. Kirchner, York University, Canada,
A. Kadyrov, Curtin University, Australia,
Y. Wu, IAPCM, China

Meeting schedule

- CM 17-18 March 2016
- First RCM 19-21 June 2017

CRP beyond 2018 (very tentative)

Procedure

- Preliminary proposal or proposals are submitted in the course of 2017-2018.
- Definitive proposal about 9 months before the intended start of the CRP
- Instead of a CRP we can choose to organize one or more technical meetings

Possible topic: Data for plasma interaction with liquid metal surfaces

- Most interest: Li, Ga, Sn
- Interest in plasma contamination and tritium retention
- Possible interest in related spectroscopy

Possible topic: Codes and data for vapour shielding in fusion plasma

- Relevant for disruptions, other pulsed heat load on walls
- Also relevant for pellet injection (D/T; impurity seeding)
- Classic problem of radiation transport
- Likely involvement from the WDM/HDM/ICF community

Meetings in 2015

<http://www-amdis.iaea.org/meetings/>

- The 3rd Spectral Line Shapes in Plasma Workshop
 - 2-6 March 2015, Marseille, France
- Joint ICTP-IAEA Advanced School and Workshop on Modern Methods in Plasma Spectroscopy
 - 16-27 March 2015, Trieste, Italy
- CM on "Guidelines for Uncertainty Quantification of theoretical atomic and molecular data"
 - June 22-23 2015, IAEA Headquarters, Vienna, Austria
- CM on " Evaluation and Uncertainty Assessment for Be, C, Ne Atomic Data"
 - July 13-15 2015, IAEA Headquarters, Vienna, Austria
- TM on "International Code Centres Network on Simulation of PMI Data"
 - July 29-31 2015, IAEA Headquarters, Vienna, Austria
- 2nd RCM on "PWI for Irradiated Tungsten and Tungsten Alloys in Fusion Devices"
 - September 8-11 2015, Seoul National University, Seoul, Korea
- Joint IAEA-KAERI CM on " Recommended Data for Processes of Tungsten Ions"
 - September 14-16 2015, Korea Atomic Energy Research Institute, Daejeon, Korea
- TM on "Technical Aspects of A & M Data Processing and Exchange, 23rd Meeting of the A & M Data Centres Network"
 - November 2-4 2015, IAEA Headquarters, Vienna, Austria
- **1st RCM on "Plasma Interaction with Reduced-Activation Steel Surfaces in Fusion Devices"**
 - December 9-11 2015, IAEA Headquarters, Vienna, Austria

Meetings in 2016

<http://www-amdis.iaea.org/meetings/>

- 3rd RCM on Atomic and Molecular Data for Hydrogen and Helium in Fusion Plasma
 - 14-16 March 2016, IAEA Headquarters, Vienna, Austria
- CM on data evaluation for heavy particle collision processes; CM on processes of neutral beams in fusion plasma
 - 17-18 March 2016, IAEA Headquarters, Vienna, Austria
- TM of the 20th IFRC Sub-committee on Atomic and Molecular Data for Fusion Research
 - 25-26 April 2016, IAEA Headquarters, Vienna, Austria
- 3rd RCM on Data for Erosion and Tritium Retention in Beryllium Plasma-Facing Materials
 - 15-17 June 2016, IAEA Headquarters, Vienna, Austria
- Joint ICTP-CAS-IAEA School and Workshop on Plasma-Material Interaction in Fusion Devices
 - 18-22 July 2016, Hefei, China
- CM on Developments in Data Exchange
 - 28-29 July 2016, IAEA Headquarters, Vienna, Austria
- TM on Uncertainty Assessment and Benchmark Experiments for Atomic and Molecular Data for Fusion Applications
 - 19-21 December 2016, IAEA Headquarters, Vienna, Austria

IAEA TM 2016 : Uncertainty Assessment and Benchmark Experiments for AM data

- December 21-23, 2016
- More than 50 Scientists from Plasma, Atomic, Molecular Physics Communities
- Meeting Objectives
 - Prioritization of A+M data needs for fusion applications.
 - Experimental methods and systems to benchmark theoretical A+M collision data.
 - Target uncertainties of A+M collision data for fusion applications.
 - Uncertainty quantification methods for theoretical A+M data.
 - Network of A+M physicists doing benchmark experiments and computations.



Meetings in 2017

<http://www-amdis.iaea.org/meetings/>

- Joint ICTP-IAEA School on Atomic Processes in Plasmas
 - 27 Feb – 3 March 2017, Trieste, Italy
- *The 4th Spectral Line Shapes in Plasma Workshop*
 - 20-24 March 2017, Baden, Austria
- *Third International Workshop on Models and Data for Plasma-Material Interaction in Fusion Devices (MoD-PMI 2017)*
 - 22-24 May 2017, Forschungszentrum Jülich, Jülich, Germany
- 1st RCM on Data for Atomic Processes of Neutral Beams in Fusion Plasma
 - 19-21 June, 2017, IAEA Headquarters, Vienna, Austria
- 3rd RCM on "PWI for Irradiated Tungsten and Tungsten Alloys in Fusion Devices"
 - 27-30 June 2017 , IAEA Headquarters, Vienna, Austria
- TM on "Technical Aspects of A & M Data Processing and Exchange, 23rd Meeting of the A & M Data Centres Network"
 - 4-6 September 2017, IAEA Headquarters, Vienna, Austria
- 2nd RCM on "Plasma Interaction with Reduced-Activation Steel Surfaces in Fusion Devices"
 - 16-18 October 2017, IAEA Headquarters, Vienna, Austria
- TM on "International Code Centres Network on Molecular Dynamics Data of Collisional Cascades after Irradiation""
 - 16-17 November 2017, IAEA Headquarters, Vienna, Austria

Joint ICTP-IAEA Advanced School and Workshop on Atomic Processes in Plasmas

Feb 27 – March 3, Trieste, Italy

56 participants from 19 MS (191 Applicants)

Objectives: provide lectures, computer code training and information exchange for young students and early career plasma physicists, plasma spectroscopists, users of atomic data for fusion, astrophysics and laser and plasma applications, and atomic and molecular physicists interested in plasma spectroscopy to expand their knowledge of plasma spectroscopy and atomic processes in plasmas.



Lectures:

Experimental Spectroscopy,
Atomic structure,
Radiation and autoionization,
Collision Physics,
Line intensities and CR modeling,
Radiation transport,
Line shapes

Codes:

GRASP/RATIP, FAC,
FLYCHK, CRETIN

Publications

<http://www-amdis.iaea.org/publications/>

- IAEA-INDC(NDS) Reports (<http://www-nds.iaea.org/publications/>)
 - Reports are published for every meeting
- International Bulletin on Atomic and Molecular Data for Fusion
 - Bibliographic Information on Atomic, Molecular and Plasma-Surface Interaction Data
 - Volume 70 (November 2016)
- Atomic and Plasma-Material Interaction data for Fusion (APID Series)
 - Data and papers related to results produced by CRPs and Consultants groups
 - All volumes are available on-line (<http://www-amdis.iaea.org/publications/APID/>)
Volume 17: CRP on “Atomic Data For Heavy Element Impurities in Fusion Reactors (in print)
APID/EP/1: CRP on “Light Element A & M and Radical Behaviour in the Divertor and Edge Plasma Regions”
- Special issues at Atoms Journals
 - CRP on Spectroscopic and Collisional Data for Tungsten from 1 eV to 20 keV:
[Atoms, Vol 3 \(2016\)](http://www.mdpi.com/journal/atoms/special_issues/fusion_plasma)
 - CRP on Atomic and Molecular Data for State-Resolved Modelling of Hydrogen and Helium and Their Isotopes in Fusion Plasma: Atoms Vol 4 (2016) and Vol 5 (2017)
http://www.mdpi.com/journal/atoms/special_issues/fusion_plasma

Atomic Molecular Data Information Services

<http://www-amdis.iaea.org>

International Atomic Energy Agency

Atomic Molecular Data Services

Provided by the Nuclear Data Section

Search Go

Databases » AMBDAS | ALADDIN | OPEN-ADAS | GENIE On-line Computing » HEAVY | AAEXCITE | RATES | LANL Codes | FLYCHK | FAC Data | GRASP2K

Atomic and Molecular Data Unit Activities

The Atomic and Molecular Data Unit operates within the Nuclear Data Section of the International Atomic Energy Agency, Vienna, Austria. The primary objective of the Atomic and Molecular Data Unit is to establish and maintain internationally recommended numerical databases on atomic and molecular collision and radiative processes, atomic and molecular structure characteristics, particle-solid surface interaction processes and physico-chemical and thermo-mechanical material properties for use in fusion energy research and other plasma science and technology applications.

Databases on Atomic and Molecular Data for Fusion.

[Atom,Molecule
Plasma-Surface
Data](#) [ALADDIN
Numerical
Database](#) [AMBDAS
Bibliographic
Database](#) [GENIE
Atomic Data
Search Engine](#) [OPEN ADAS
Database
Search](#) [Rovibronic
Energy levels
Triplet D₂](#) [FC Factors &
A-values of
H₂ & Isotopes](#)

Online Computing Capabilities

[Code
Centres
Portal](#) [LANL
Atomic
Physics](#) [FLYCHK
Non-LTE
Kinetics](#) [Heavy
Particles
Collisions](#) [Averaged
e- Impact
Cross-section](#) [Effective
e- Ionization
Rates](#) [ATOM-AKM
e - Collision
Data](#)

Knowledge Base for Atomic, Molecular and Plasma-Material Interaction Data for Fusion

Our Unit achieves its objectives by coordinating the activities of the **International Atomic and Molecular Data Center Network (DCN)** and **Code Center Network (CCN)**, initiation and conducting international **Coordinated Research Projects (CRP)**, organization of various types of **Expert's Meetings**, publication of **technical reports** on meetings and research activities and using other forms (research contracts, research agreements, consultancies) for stimulation of the generation, collection and critical assessment of the required atomic, molecular (A+M) and plasma-material interaction (PMI) data information.

The activity of Our Unit is supervised and biennially reviewed by the Subcommittee on Atomic and Molecular Data for Fusion of the International Fusion Research Council (IFRC A+M Subcommittee).

IAEA Nuclear Data Section

IAEA Meetings

Mar 20-24, 2017
The 4th Spectral Line Shapes in Plasma Workshop, Baden, Austria

May 22-24, 2017
Third International Workshop on Models and Data for Plasma-Material Interaction in Fusion Devices, Juelich, Germany

June 19-21, 2017
1st RCM of CRP on Data for Atomic Processes of Neutral Beams in Fusion Plasma

June 27-30, 2017
3rd RCM of CRP on Plasma-Wall Interaction for Irradiated Tungsten and Tungsten Alloys in Fusion Devices

Sep 4-6, 2017
24th Meeting of the Atomic and Molecular

AMO/PSI Meetings

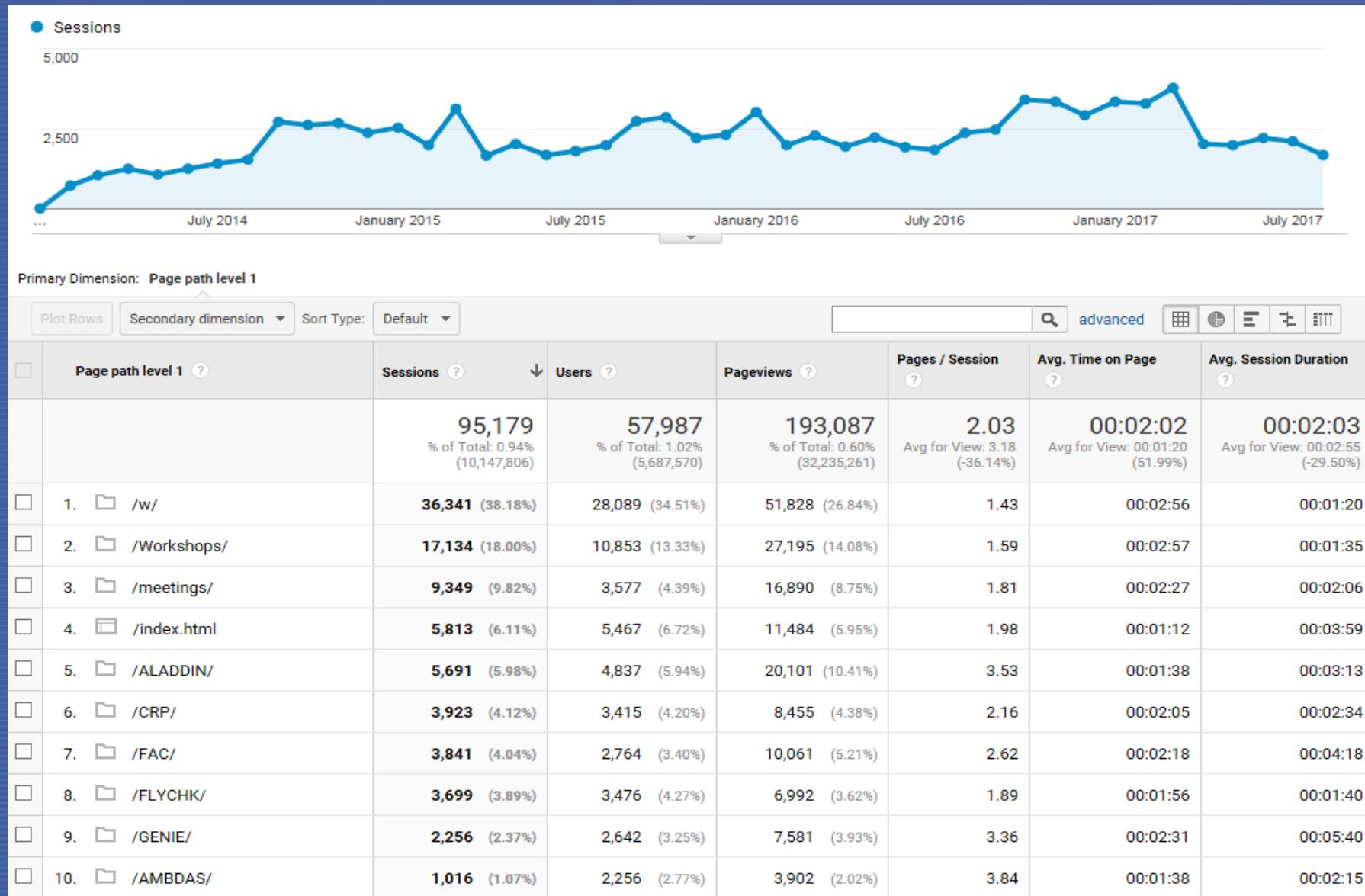
Apr 9-12, 2017:
International workshop on Warm Dense Matter

May 16-19, 2017: 16th International Conference on Plasma-Facing Materials and Components for Fusion Applications

Jun 5-9, 2017: 48th Annual Meeting of the APS Division of Atomic,Molecular and Optical Physics

Jul 23-25, 2017: 25th International Symposium on Ion Atom Collisions

More than 2000 Sessions per month



Nuclear data section leads the IAEA in web traffic (AMU on 6th)

NUCLEUS sites Jan 1, 2016 - Dec 31, 2016 ▾

Edit Email Export ▾ Add to Dashboard Shortcut This report is based on 9.11% of sessions. Learn more Greater precision ▾

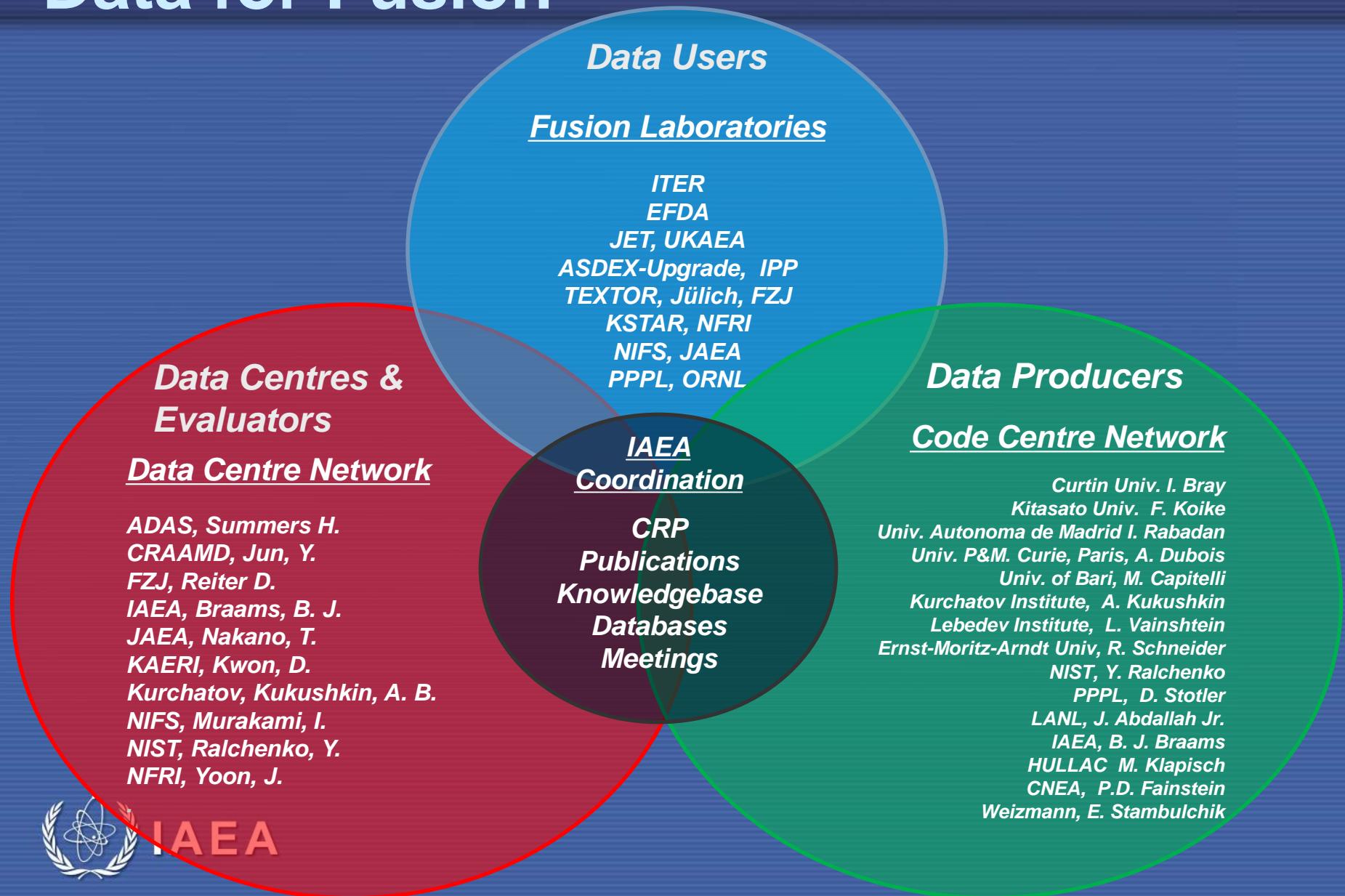
All Users 100.00% Pageviews + Add Segment

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| 1. www-ndc.iaea.org | NAPC/NDS | 1,567,327 (54.25%) | 443,209 (40.91%) | 00:07:05 | 201,614 (49.48%) | 78,271 (45.85%) | 92,406 (43.53%) |
| 2. conferences.iaea.org | MTCD | 536,724 (18.58%) | 317,451 (29.30%) | 00:07:51 | 64,190 (15.75%) | 17,044 (9.98%) | 25,264 (11.90%) |
| 3. www.nndc.bnl.gov | NAPC/NDS | 375,364 (12.99%) | 102,514 (9.46%) | 00:09:43 | 30,937 (7.59%) | 9,526 (5.58%) | 11,359 (5.35%) |
| 4. irs.iaea.org | NSNI | 135,624 (4.69%) | 40,979 (3.78%) | 00:09:22 | 5,410 (1.33%) | 88 (0.05%) | 3,051 (1.44%) |
| 5. inis.iaea.org | NE/NIS | 129,884 (4.50%) | 92,132 (8.50%) | 00:01:33 | 64,355 (15.79%) | 45,215 (26.48%) | 52,195 (24.59%) |
| 6. www-amdis.iaea.org | NAPC/NDS | 42,516 (1.47%) | 30,575 (2.82%) | 00:02:31 | 17,954 (4.41%) | 8,396 (4.92%) | 10,744 (5.06%) |
| 7. infcis.iaea.org | MTIT | 35,821 (1.24%) | 22,871 (2.11%) | 00:05:21 | 5,663 (1.39%) | 2,875 (1.68%) | 4,620 (2.18%) |
| 8. ola.iaea.org | OLA | 19,666 (0.68%) | 15,222 (1.40%) | 00:02:20 | 9,713 (2.38%) | 4,818 (2.82%) | 7,188 (3.39%) |
| 9. amdu1 | NAPC/NDS | 8,220 (0.28%) | 2,535 (0.23%) | 00:08:05 | 1,240 (0.30%) | 11 (0.01%) | 11 (0.01%) |
| 10. finas.iaea.org | NSNI | 7,013 (0.24%) | 2,513 (0.23%) | 00:10:53 | 241 (0.06%) | 0 (0.00%) | 187 (0.09%) |

Network Collaboration for AM/PSI Data for Fusion



IAEA

Data Centre Network (DCN) Activities

<http://www-amdis.iaea.org/DCN>

Domain : atomic and molecular (A+M), particle surface interaction (PSI) and bulk material properties (plasma-material interaction - PMI) data for fusion and other applications.

Established Program: Collection, Dissemination, Critical assessment (evaluation) and generation of A+M, PSI (PMI) data

- ALADDIN: Numerical database
- AMBDAS: Bibliographic database
- GENIE: Search Engine
- XSAMS: XML Schema for A+M/PSI Data
- New Databases for Plasma-Material Interaction

ALADDIN: Numerical Database

Data Dissemination <http://www-amdis.iaea.org/ALADDIN>



ALADDIN
Numerical database maintained by
the IAEA Nuclear Data Section A+M Data Unit

Atomic and Molecular Data

Electron Collisions
Photon Collisions
Heavy Particle Collisions

Particle-Surface Interactions

Erosion, Sputtering, Sublimation
Reflection
Trapping, Penetration

- Originally designed to host “evaluated and recommended” data only
- Currently a mix of evaluated data with CRP participants’ data
- Host evaluated and recommended data
 - Host Kyoto-JAEA database on heavy ion collisions (by Alex Imai)
- New Interface using GOOGLE free search forms is under development

AMBDAS:Bibliographic database

Data Dissemination <http://www-amdis.iaea.org/AMBDAS>

- Data Sources
 - AM/PSI Data entries relevant to fusion
 - Spectroscopic data from NIST (A. Kramida & J. Fuhr)
 - NFRI, NIFS, KAERI and IAEA collaboration for electron collisional data
 - Consultancies for plasma-material interaction data
- Data in the “International Bulletin on A & M Data for Fusion” available through AMBDAS
- New environment for bibliographical data collection
 - Web of Science
 - The SAO/NASA Astrophysics Data System

GENIE: Web search engine for atomic data

Data Exchange & Dissemination <http://www-amdis.iaea.org/GENIE>

Radiative properties – search on 9 databases

Collisional databases – search on 6 databases

Will work on the GENIE statistics outputs for collaborators

GENIE
A General Internet Search Engine for Atomic Data

Transition Probabilities
Wavelengths
Energy Levels

Ion: C IV

Enter wavelength in Å:
From to

| | | |
|--|-------------------------------------|-------------------|
| NIST Atomic Spectra Database | <input checked="" type="checkbox"/> | ? |
| Kurucz's CD-ROM 23 | <input checked="" type="checkbox"/> | ? |
| Atomic Line List v. 2.04 | <input checked="" type="checkbox"/> | ? |
| TOPbase (Opacity Project) | <input checked="" type="checkbox"/> | ? |
| Kelly Atomic Line Database | <input checked="" type="checkbox"/> | ? |
| MCHF/MCDHF Collection | <input checked="" type="checkbox"/> | ? |
| KAERI AMODS Spectral Lines | <input checked="" type="checkbox"/> | ? |
| CAMBD Atomic Spectra | <input checked="" type="checkbox"/> | ? |
| Spectr-W3 | <input checked="" type="checkbox"/> | ? |

[Go for A/E/lambda](#) [Reset](#)

Electron Impact Cross Sections
and/or Rate Coefficients

Ion: C 3+

Excitation [?](#)
 Ionization [?](#)
 Dielectronic recombination [?](#)

Cross sections [?](#) Rate coefficients [?](#)

| | | |
|---|-------------------------------------|-------------------|
| IAEA ALADDIN Database | <input checked="" type="checkbox"/> | ? |
| NIFS AMDIS Database | <input checked="" type="checkbox"/> | ? |
| CAMBD Collisional Processes | <input checked="" type="checkbox"/> | ? |
| NIST Atomic Cross Sections | <input checked="" type="checkbox"/> | ? |
| OPEN-ADAS | <input checked="" type="checkbox"/> | ? |
| Spectr-W3 | <input checked="" type="checkbox"/> | ? |

[Go for sigma/R](#) [Reset](#)



XSAMS: XML Schema for A+M/PSI Data

Data Exchange <http://www-amdis.iaea.org/xsams>

- Sep 2009: [First release version 0.1 of the schema](#)
- Mar 2010: [XSAMS Meeting in NIFS, Japan](#)
- Nov 2010: [XSAMS Meeting at IAEA](#)
- Jan 2011: [Version 0.1.1 \(bug fixes\)](#)
[Source forge project](#) <http://sourceforge.net/projects/xsams/>
- Oct 2011: [XSAMS Meeting at NIST](#)
- Feb 2012: [XSAMS Meeting with VAMDC, University of Vienna](#)

VAMDC continues to develop XSAMS??

Technical Discussions on XSAMS for DCN databases

Plasma-Material Interaction Databases

DFT database (Oda)

Click on the links inside the tabbed menu:

W Be C

Tungsten

Z=74

W W-H W-H-He W-N

Click on the links inside the tabbed menu:

W Be C

W-H

contents

Potential Model First-principles calculation

MD database (Dudarev, Sand)

November 16-17, 2017

TM of the code centre network on
molecular dynamics data of collisional
cascades after irradiation

- ★ Atomic coordinates in ASCII readable text file
 - Possible additional information: velocities, potential energy,...
- ★ Simple format: XYZ file

```
601526
Frame number 11687 40002. fs boxsize 212.068400 212.068400 212.068400
W -103.659726 79.923029 -103.661777 -8.900047
W -103.660175 79.923225 -100.496878 -8.900130
W -103.659834 79.922949 -97.330699 -8.900268
W -103.660790 79.923151 -94.167560 -8.898738
W -103.660363 79.922767 -91.003001 -8.900769
W -103.659343 79.923741 -87.837000 -8.899446
W -103.659576 79.923071 -84.671184 -8.900672
W -103.659617 79.923131 -81.507449 -8.900600
W -103.660214 79.922650 -78.343085 -8.900321
W -103.659035 79.923771 -75.177067 -8.900647
W -103.660728 79.923978 -72.012728 -8.899717
W -103.658488 79.923953 -68.845823 -8.900009
W -103.660177 79.924804 -65.681139 -8.902425
W -103.660350 79.924767 -62.515246 -8.900812
W -103.659859 79.923857 -59.350034 -8.900000
W -103.660107 79.923761 -56.185375 -8.900831
```

Code Centre Network (CCN)

<http://www-amdis.iaea.org/CCN>

Joint effort to gather and provide access to any information relevant for modellers in fusion plasma science

Purpose

To provide solutions to anyone willing AM/PSI data which can not be easily accessed on the web or which simply do not exist.

Tools

Online computing

Downloadable codes

Direct contacts with the CCN for any expertise

IAEA Activities

Organization of meetings and workshops for code developers

Dissemination of community available codes and code results

Online computing capabilities

Code Centre Network (CCN) Meetings

<http://www-amdis.iaea.org/CCN>

- The 3rd CCN Meeting in May 2013:
 - Uncertainty estimates of theoretical atomic and molecular data
- The 4th CCN Meeting in July 2015:
 - Uncertainty estimates of plasma-material interaction data
- The 5th CCN Meeting in November 2017:
 - Database on Molecular Dynamics Simulations of Collisional Cascades after Irradiation
- Code comparison workshops
 - Spectral Line Shapes in Plasmas Code Comparison Workshops (2012, 2013, 2015, 2017)
 - Third International Workshop on Models and Data for Plasma-Material Interaction in Fusion Devices (MoD-PMI 2017)
 - Code Comparison Workshop on Electron Dynamics in Atomic Collisions (2018)
 - Code Comparison Workshop on Neutral Beam Penetration, Beam Emissions and Beam-based Diagnostics (2018)
 - Code Comparison Workshop on Reaction-Diffusion Code (2018)

IAEA Online Codes and Code Results

- Average Approximation <http://www-amdis.iaea.org/AAEXCITE/>
 - Electron impact excitation cross sections for any ion and configuration
- Heavy particle collisions <http://www-amdis.iaea.org/HEAVY/>
 - Excitation, ionization and charge exchange for bare nucleus on hydrogenic target
- Effective Ionization/Recombination Rates <http://www-amdis.iaea.org/RATES/>
 - Level population distributions and radiative power rates from CR modeling
- LANL atomic data from CRP <http://www-amdis.iaea.org/LANL/>
 - Si, Cl, Ar ions (~ 2 GB)
- FAC atomic physics codes and atomic data <http://www-amdis.iaea.org/FAC/>
 - He – Si atoms (~ 30 GB)
- GRASP2K code distribution <https://int-amdis.iaea.org/GRASP2K>
- FLYCHK Collisional-Radiative code results <http://www-amdis.iaea.org/FLYCHK>
 - Charge state distributions and radiative loss rates for Z=1-79 for Te=0.5 eV- 100 keV

Knowledge Base: Inputs only from IAEA

page discussion view source history

Main Page

Knowledge Base for Atomic, Molecular and Plasma-Material Interaction Data For Fusion

Introduction

Atomic, molecular and plasma-material interaction processes play an important role in the energy balance, confinement and stability of a thermonuclear plasma. The primary goal of this Knowledge base is to identify the needs in the atomic, molecular and plasma-surface interaction data sets for fusion research, both magnetic confinement fusion [and inertial confinement fusion studies](#), to provide a direct link to the relevant data sources and present more information on the available data sets.

Data Needs

Magnetic Confinement Fusion

- [Introduction](#)
- [Spectroscopic Data](#)
- [Collisional Data for Edge Studies](#)
- [Collisional Data for Neutral-Beam Heating](#)
- [Radiative Plasma Cooling](#)
- [Plasma-Wall Interaction](#)
- [Material Properties](#)

Atomic Data

- [Atom-Electron Collisions](#)
- [Atom-Heavy-particle Collisions](#)
- [Atomic Radiative Properties](#)

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 - 2.2 Atomic Data
 - 2.3 Molecular Data
 - 2.4 Plasma-Material Interaction Data
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 - 3.2 Online Databases
 - 3.3 Data Centers
 - 3.4 Code Centers Network
- 4 Data Exchange
 - 4.1 Data Exchange Forum
- 5 Special Topics
 - 5.1 IAEA Coordinated Research Projects (CRP)
 - 5.2 IAEA Workshops
 - 5.3 NLTE Kinetics Code Comparison Workshops
 - 5.4 Meetings on A+M+PMI/PSI Processes and Data
 - 5.5 ITPA (International Tokamak Physics Activity)
 - 5.6 European Fusion Development Agreement (EFDA)
- 6 Fusion Research
 - 6.1 Magnetic Confinement Fusion Research
 - 6.2 Inertial Confinement Fusion Research

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Researchers in Atomic and Molecular Collision Experiments

Atom Collisions

- Institut fuer Atom- und Molekuelphysik, Justus-Liebig-Universitaet Alfred Müller, Stefan Schippers, E. Salzborn, ionization and recombination of ions
- University Wisconsin, USA C.C.Lin, J.B. Boffard, Excitation of neutral atoms, optical excitation functions
- Tsinghua Univ, Beijing, China Yi-Kang Pu, Excitation of neutral atoms, plasma methods to measure excitation of atoms
- Rice Univ., USA R. Stebbings, Single and multiple ionization of neutral atoms, Parallel plate capacitor method
- [1] R. S. Freund, Single and multiple ionization of neutral atoms, neutralized ion beam crossed with electron beam
- QUB Belfast B. Gilbody, M. Shah, J. Geddes, Single and multiple ionization of neutral atoms, vapor and gaseous effusive beams crossed with electron beam
- Innsbruck, Austria Tilmann D. Märk,
- LLNL EBIT, USA Peter Beiersdorfer, Electron-Ion collisions in plasmas, EBIT
- Fudan University, China Y. Zhou, Electron-Ion collisions in plasmas, EBIT
- Heidelberg EBIT, Germany Jose Crespo, Electron-Ion collisions in plasmas, EBIT
- Tokyo EBIT, Japan Nobuyuki Nakamura, Electron-Ion collisions in plasmas, EBIT
- Belfast EBIT, UK F. Currell, Electron-Ion collisions in plasmas, EBIT
- [1] G. H. Dunn, D. H. Crandall, R. A. Phaneuf, J. Kohl, Excitation of ions
- CEA Caen, France B. Huber, Excitation of ions
- JPL Pasadena, USA A. Chutjian, Excitation of ions
- QUB, UK J. Greenwood, I. Williams, Excitation of ions
- ORNL, USA M. Bannister, Excitation of ions
- [1] R. A. Phaneuf, M. Bannister, N. Djuric, Electron-Ion interacting beams experiments, Ionization of ions
- Auburn Univ, USA M. Fogle, Electron-Ion interacting beams experiments, Ionization and Recombination of ions
- Columbia Univ M. Hahn, D. Savin, Electron-Ion interacting beams experiments, Ionization and recombination of ions
- Univ. Catholique de Louvain, Belgium F. Brouillard, P. Defrance, D. Belic, Electron-Ion interacting beams experiments, Ionization of ions
- Stockholm University, Sweden R. Schuch, Electron-Ion interacting beams experiments, Recombination of ions
- GSI-Helmholtzzentrum fur Schwerionenforschung, Germany M. Lestinski, C. Brandau, Electron-Ion interacting beams experiments, Recombination of ions
- CAS, Lanzhou Xinwen. Ma, recombination of ions, HIRFL storage rings
- [1] H. Griem, H.-J. Kunze, M. Bitter (spectroscopy), Electron-Ion collisions in plasmas

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Molecule Collisions

- [Atomic and Molecular Physics Laboratories, Australian National University \(ANU\)](#) Stephen Buckman
- [University of Fribourg, Switzerland](#) Michael Allan, Electron Atom/Molecule collisions, DEA studies, biomolecules, elastic scattering and excitation, absolute values
- [Cal. State University Fullerton, USA](#) Morty Khakoo, Electron atom/molecule collisions, Elastic scattering, Electronic and vibrational excitation
- [Flinders University, Australia](#) Michael Brunger, Electron atom/molecule collisions, Elastic scattering, Electronic and vibrational excitation
- [CSIC Madrid, Spain](#) Gustavo Garcia, Electron atom/molecule scattering, total cross sections, energy loss
- [Open University, UK](#) Sam Eden
- [Maynouth, Ireland](#) Peter Van Der Burgt
- [IoP, Belgrade, Serbia](#) Zoran Petrovic, Electron transport, cross section sets, reaction rates, atoms and molecules
- [TATA, Mumbai, India](#) E. Krishnakumar, DEA measurements, velocity map imaging
- [Reyjavik, Iceland](#) Oddur Ingolfsson, DEA, biomolecules
- [Choong-Buk University, Korea](#) Hyuk Cho, Elastic scattering measurements
- [Mexico City, Mexico](#) Jaime Urquijo, Transport (swarm) measurements, atoms, and molecules
- [Sophia University, Tokyo, Japan](#) Masamitsu Hoshino, Elastic scattering and excitation measurements
- [Tokyo Institute of Tech. Japan](#) Kitajima, High resolution total cross section measurements
- [Aarhus University, Denmark](#) Lars Henrik Andersen, Nykola Jones, High resolution total cross section measurements
- [Innsbuck, Austria](#) Paul Schieir, Stefan Denifl, DEA, biomolecules
- [Sherbrooke, Canada](#) Leon Sanche, DEA, biomolecules
- [LBNL California](#) Ali Belkacem, Dan Slaughter, DEA, molecules
- [Juiz de Fof a, Brazil](#) Christina Lopes, Elastic and total cross sections, atoms/molecules
- [Sao Carlos, Brazil](#) Gustavo Homem, Developing new lab
- [University Wisconsin, USA](#) John Boffard, Electronic excitation
- [Lisbon, Portugal](#) Paulo Limao-Vieira, Charge transfer collisions, biomolecules
- [MPI Heidelberg, Stored and Cooled Ions, Germany](#) Alex Dorn, Electron impact ionization
- [MPI Heidelberg, Quantum dynamics and Control, Germany](#) A. Wolf, Collisions involving molecular ions
- [U Nebraska, USA](#) Tim Gay, Polarised electron experiments (amongst others)
- [Univ. Federale de Rio de Janeiro](#) E. C. Montenegro, electron (molecule/atom) collisions



Technical Discussions

- Funding for A+M data relevant to Fusion Applications
- Data Evaluation Activities
- Maintenance of Bibliographical Data on Collisional Processes
- Implementation of XSAMS and VAMDC node software
- Priority List of A+M/PSI data for Fusion
- Database Development
- Outreach to A+M/PMI scientists outside our community
- Outreach to Plasma scientists for A+M/PMI data awareness