

Databases and Coordinated Research Projects in the IAEA Atomic and Molecular Data Unit

B. J. Braams and H.-K. Chung

2011 ADAS Workshop

Auburn University, 6-8 October 2011



IAEA

International Atomic Energy Agency

Overview of A+M Data Unit Activities

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

International Atomic Energy Agency
Atomic Molecular Data Services
Provided by the Nuclear Data Section

IAEA.org | NDS Mission | About Us

Search Go

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

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
- 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), an advisory body to the Agency's Director General.

IAEA Nuclear Data Section

- IAEA-NDS Mission, Staff and more
- Nuclear Data Services
- Meetings Workshops
- Newsletters
- Coordinated Research Projects
- Nuclear Reaction Data Center Network
- Nuclear Structure & Decay Data Network
- Technical Reports, TECDOCs
- INDC-NDS Reports
- Computer Codes

IAEA Meetings

- May 23-25, 2011 2nd RCM of CRP on Light Element Atom, Molecule and Radical Behaviour in the Divertor and Edge Plasma Regions
- Aug 10-12, 2011 1st RCM of CRP on Atomic and Molecular Data for State-Resolved Modelling of Hydrogen and Helium and Their Isotopes in Fusion Plasma
- Sep 7-9, 2011 21st Meeting of the Atomic and Molecular Data Centres Network
- Oct 3-5, 2011 Consultants Meeting on XML Schema for Atoms, Molecules and Solids (XSAMS)
- Nov 30 - Dec 7

AMO/PSI Meetings

- Jun 05-08, 2011: International Workshop on Warm Dense Matter, Pacific Grove, California
- Jun 13-17, 2011: 42nd Annual Meeting of the APS DAMOP, Atlanta, GA
- Jul 19-22, 2011: Atomic Processes in Plasmas, Belfast, UK
- Jul 27-Aug 2,

Data Centres Network (DCN)

- The DCN includes 12 national data centres or related activities:

Terms of Reference:

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

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

- The DCN activities are coordinated by the IAEA A+M Data Unit and periodically reviewed (every two years) by IFRC A+M Subcommittee.
- Key issues for DCN presently: maintenance of bibliographical database, coordination of data validation (data evaluation) work, development of “data needs” document, extension of knowledge base (wiki) effort.

Code Centres Network (CCN)

- New effort (since 2008) to provide access to A+M codes relevant for fusion plasma modelling
- An IAEA web page provides summaries of the code capabilities and links to Centre web pages
- Some on-line code capabilities; other CCN partners provide contact information
- Flexible group of participants; we intend to use CCN as an umbrella for other code activities

CCN Participants

- CCC & RCCC, Curtin University, Australia, I. Bray
- CR Model, Kitasato University, Japan, F. Koike
- MELDF*-TCAM, QUAN, EIKON, CTMC, Universidad Autonoma de Madrid, Spain, I. Rabadan
- CDW and VPN, University P. & M. Curie, France, Alain Dubois; Centro Atomico Bariloche CNEA, Argentina, P.D. Fainstein
- Molecular cross Sections, SI calculations, University of Bari, Italy, M. Capitelli
- CR Models, Kurchatov Institute, Russian Federation, A. Kukushkin
- ATOM, ATOM-AKM, GKU, Lebedev Institute, Russian Federation, L. Vainshtein
- HYDKIN, Forschungszentrum Juelich, Germany, D. Reiter
- MCHF, GRASP2K, FLYCHK, NOMAD, National Institute for Standards and Technology, USA, Yuri Ralchenko
- DEGAS databases, Princeton Plasma Physics Laboratory, USA, D. Stotler
- LANL Codes, Los Alamos National Laboratory, USA, J. Abdallah, Jr.
- HULLAC code, ETHZ, Switzerland, M. Klapisch
- SDTRIM-SP, IPP Greifswald, Germany, R. Schneider
- AMD Services, International Atomic Energy Agency, H.-K. Chung

XML Schema for Atoms, Molecules and Solids (XSAMS)

- Project initiated in October 2003 during the DCN meeting
 - Working group composed of NIST, ORNL, IAEA, Obs Paris-Meudon
 - 2008: collaboration from Russia: Russian Federal Nuclear Centre (VNIITF)
 - 2009: VAMDC (Virtual Atomic and Molecular Data Centre, July 2009)
- Regular Consultants' Meetings organized by A+M Data Unit
- Presentations at ICAMDATA in October 2008, China
- Release of XSAMS version 0.1, 22 September 2009
- XSAMS has been adopted by VAMDC for their databases (24 teams)
- Present development of XSAMS is led by VAMDC
- Recent additions: Line shapes, Molecular spectroscopy, PAH
- Adoption of XSAMS version 1.0, 4 October 2011

Numerical database ALADDIN

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

ALADDIN

Atomic and Molecular Data

Electron Collisions
Heavy Particle Collisions

Particle-Surface Interactions

Erosion, Sputtering, Sublimation
Reflection
Trapping, Penetration

Note

Data presented here are IAEA recommended at their time of compilation. Data are mostly compiled from the [IAEA APID series](#), published results of [Co-ordinated research projects \(CRP\)](#) and from consultancies inside the IAEA Atomic and Molecular Data Unit.

The Author's Units for heavy particle collision cross-sections from 3 publications (NUC-FUS-SUPP/87 (1987), ORNL-6090 (1987), ORNL-6086 (1990)) were given incorrectly in ALADDIN as eV. The correct Author's Units are eV/amu. This was fixed on 2010-Feb-10.

[Dictionary](#) [Glossary](#) [Comments](#) [AMBDAS](#) [A+M Data Unit](#) [IAEA](#)

Atomic data from FLYCHK

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

FLYCHK: Generalized Model of Atomic Processes In Plasmas

On-line Capability of NLTE kinetics Code

The FLYCHK code provides a simple and general modeling capability to generate atomic level populations and charge state distributions for low-Z to mid-Z elements under NLTE(Non-Local Thermodynamic Equilibrium) conditions. The code is currently available at the [password-protected NIST website](#). For more information on details, validity and limitations of the code, please click [the FLYCHK information page](#).

Steady-State Charge State Distributions

Average charge states $\langle Z \rangle$ of atoms from Z=1 (Hydrogen) to Z=79 (Gold) are calculated by FLYCHK code and plotted over a wide range of plasma conditions. The calculation is done for the steady-state plasmas with electron temperatures from 0.5 eV to 100 keV and electron densities from 10^{12} cm^{-3} to 10^{24} cm^{-3} . Click the element in the periodic table and a page will appear with the information on $\langle Z \rangle$, Charge State Distribution and Total Radiative Power Loss Rates of the element.

Rate Coefficients at Coronal Equilibrium for Plasma Modeling Applications

To help plasma modeling applications, Rate coefficients of Direct Ionization, Excitation-Autoionization, Radiative Recombination and Dielectronic Recombination at coronal conditions are generated for a wide range of plasma temperatures from 0.5 eV to 100 keV. Also available are the Radiative Loss rates per Charge State, both Line radiation and Recombination radiation. They are available at the same page as Charge state distributions. The details of the methods are found at [the FLYCHK Rates information page](#).

1	H
3	4
Li	Be
11	12

Charge State Distributions up to Gold (Z<80)

Radiative power loss rates up to Gold (Z<80)

Electron temperature: 0.5 eV to 100 keV

Electron density: $1\text{E}12 - 1\text{E}24 \text{ cm}^{-3}$

[click here for limitations of FLYCHK results](#)

					2
					He
5	6	7	8	9	10
B	C	N	O	F	Ne
13	14	15	16	17	18

Bibliographical database AMBDAS

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

AMBDAS

Atomic and Molecular Bibliographic Data System

Search

Clear

Available Reactant/Surface Codes	Reactant Code	Ion Charge
? Reactant 1	<input type="text"/> H, Na, H ₂ O, HF	<input type="text"/> 2, 26, -1
Reactant 2	<input type="text"/> H, Na, H ₂ O, HF	<input type="text"/>
? Isoelectr. Sequence	<input type="text"/> H, Be, Ca	
? Surface	<input type="text"/> Mg, Ag ₂ O, Metal	

Examples are given in green

Attention: the codes are case-sensitive, i.e., 'HF' is Hafnium and 'HF' is Hydrogen-Fluorine

Category	Process
Structure and Spectra	---- Structure and Spectra ----
Photon Collisions	Line Shapes and Shifts
Electron Collisions	Structure, Spectra
Heavy Particles Collisions	Interatomic Potentials
Surface Interactions	Polarizabilities, Electric moments
Beam Heating and Fueling of Plasmas	Energy Levels, Wavelengths

Bibliography

? Author's name	<input type="text"/> Mott, N*Mott, *stein*	2 nd author's name	<input type="text"/>
? Keywords/Patterns	<input type="text"/> res*nance, *electron impact*	Exp vs Theory	<input type="text"/>
Years	<input type="text"/> -- <input type="text"/> 98, 1998, 02, 2002	Reference Type	<input type="text"/>

Sort by Year: | Abstract/Comment: | Search Case Sensitive: The maximal allowed number of references is 200.

Database search engine GENIE

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

GENIE

A General Internet Search Engine for Atomic Data

<p>Transition Probabilities Wavelengths Energy Levels</p> <p>Ion: C IV</p> <p>Enter wavelength in Å: From 1 to 10000</p> <table border="1"><tr><td>NIST Atomic Spectra Database</td><td><input checked="" type="checkbox"/></td><td><input type="checkbox"/></td></tr><tr><td>Kurucz's CD-ROM 23</td><td><input checked="" type="checkbox"/></td><td><input type="checkbox"/></td></tr><tr><td>Atomic Line List v.2.04</td><td><input checked="" type="checkbox"/></td><td><input type="checkbox"/></td></tr><tr><td>TOPbase (Opacity Project)</td><td><input checked="" type="checkbox"/></td><td><input type="checkbox"/></td></tr><tr><td>Kelly Atomic Line Database</td><td><input checked="" type="checkbox"/></td><td><input type="checkbox"/></td></tr><tr><td>MCHF/MCDHF Collection</td><td><input checked="" type="checkbox"/></td><td><input type="checkbox"/></td></tr><tr><td>KAERI AMODS Spectral Lines</td><td><input checked="" type="checkbox"/></td><td><input type="checkbox"/></td></tr><tr><td>CAMBD Atomic Spectra</td><td><input checked="" type="checkbox"/></td><td><input type="checkbox"/></td></tr><tr><td>Spectr-W3</td><td><input checked="" type="checkbox"/></td><td><input type="checkbox"/></td></tr></table> <p><input type="button" value="Go for A/E/lambda"/> <input type="button" value="Reset"/></p>	NIST Atomic Spectra Database	<input checked="" type="checkbox"/>	<input type="checkbox"/>	Kurucz's CD-ROM 23	<input checked="" type="checkbox"/>	<input type="checkbox"/>	Atomic Line List v.2.04	<input checked="" type="checkbox"/>	<input type="checkbox"/>	TOPbase (Opacity Project)	<input checked="" type="checkbox"/>	<input type="checkbox"/>	Kelly Atomic Line Database	<input checked="" type="checkbox"/>	<input type="checkbox"/>	MCHF/MCDHF Collection	<input checked="" type="checkbox"/>	<input type="checkbox"/>	KAERI AMODS Spectral Lines	<input checked="" type="checkbox"/>	<input type="checkbox"/>	CAMBD Atomic Spectra	<input checked="" type="checkbox"/>	<input type="checkbox"/>	Spectr-W3	<input checked="" type="checkbox"/>	<input type="checkbox"/>		<p>Electron Impact Cross Sections and/or Rate Coefficients</p> <p>Ion: C 3+</p> <table border="1"><tr><td><input checked="" type="radio"/> Excitation</td><td><input type="checkbox"/></td></tr><tr><td><input type="radio"/> Ionization</td><td><input checked="" type="checkbox"/></td></tr><tr><td><input type="radio"/> Dielectronic recombination</td><td><input checked="" type="checkbox"/></td></tr></table> <table border="1"><tr><td>IAEA ALADDIN Database</td><td><input checked="" type="checkbox"/></td><td><input type="checkbox"/></td></tr><tr><td>NIFS AMDIS Database</td><td><input checked="" type="checkbox"/></td><td><input type="checkbox"/></td></tr><tr><td>CAMBD Collisional Processes</td><td><input checked="" type="checkbox"/></td><td><input type="checkbox"/></td></tr><tr><td>NIST Atomic Cross Sections</td><td><input checked="" type="checkbox"/></td><td><input type="checkbox"/></td></tr><tr><td>OPEN-ADAS</td><td><input checked="" type="checkbox"/></td><td><input type="checkbox"/></td></tr><tr><td>Spectr-W3</td><td><input checked="" type="checkbox"/></td><td><input type="checkbox"/></td></tr></table> <p><input type="button" value="Go for sigma/R"/> <input type="button" value="Reset"/></p>	<input checked="" type="radio"/> Excitation	<input type="checkbox"/>	<input type="radio"/> Ionization	<input checked="" type="checkbox"/>	<input type="radio"/> Dielectronic recombination	<input checked="" type="checkbox"/>	IAEA ALADDIN Database	<input checked="" type="checkbox"/>	<input type="checkbox"/>	NIFS AMDIS Database	<input checked="" type="checkbox"/>	<input type="checkbox"/>	CAMBD Collisional Processes	<input checked="" type="checkbox"/>	<input type="checkbox"/>	NIST Atomic Cross Sections	<input checked="" type="checkbox"/>	<input type="checkbox"/>	OPEN-ADAS	<input checked="" type="checkbox"/>	<input type="checkbox"/>	Spectr-W3	<input checked="" type="checkbox"/>	<input type="checkbox"/>
NIST Atomic Spectra Database	<input checked="" type="checkbox"/>	<input type="checkbox"/>																																																			
Kurucz's CD-ROM 23	<input checked="" type="checkbox"/>	<input type="checkbox"/>																																																			
Atomic Line List v.2.04	<input checked="" type="checkbox"/>	<input type="checkbox"/>																																																			
TOPbase (Opacity Project)	<input checked="" type="checkbox"/>	<input type="checkbox"/>																																																			
Kelly Atomic Line Database	<input checked="" type="checkbox"/>	<input type="checkbox"/>																																																			
MCHF/MCDHF Collection	<input checked="" type="checkbox"/>	<input type="checkbox"/>																																																			
KAERI AMODS Spectral Lines	<input checked="" type="checkbox"/>	<input type="checkbox"/>																																																			
CAMBD Atomic Spectra	<input checked="" type="checkbox"/>	<input type="checkbox"/>																																																			
Spectr-W3	<input checked="" type="checkbox"/>	<input type="checkbox"/>																																																			
<input checked="" type="radio"/> Excitation	<input type="checkbox"/>																																																				
<input type="radio"/> Ionization	<input checked="" type="checkbox"/>																																																				
<input type="radio"/> Dielectronic recombination	<input checked="" type="checkbox"/>																																																				
IAEA ALADDIN Database	<input checked="" type="checkbox"/>	<input type="checkbox"/>																																																			
NIFS AMDIS Database	<input checked="" type="checkbox"/>	<input type="checkbox"/>																																																			
CAMBD Collisional Processes	<input checked="" type="checkbox"/>	<input type="checkbox"/>																																																			
NIST Atomic Cross Sections	<input checked="" type="checkbox"/>	<input type="checkbox"/>																																																			
OPEN-ADAS	<input checked="" type="checkbox"/>	<input type="checkbox"/>																																																			
Spectr-W3	<input checked="" type="checkbox"/>	<input type="checkbox"/>																																																			

Knowledge Base (Wiki)

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

 [Log in](#)



[page](#) [discussion](#) [view source](#) [history](#)

Main Page

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

knowledge base

- [Main Page](#)
- [Data Needs](#)
- [Data Sources](#)
- [Data Exchange](#)
- [Special Topics](#)
- [Fusion Research](#)

navigation

- [IAEA AMD WEB](#)
- [IAEA CRP](#)
- [Community Forum](#)
- [Current events](#)
- [Recent changes](#)
- [Random page](#)
- [Help](#)

search

toolbox

- [What links here](#)
- [Related changes](#)

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](#)

Contents [hide]

- 1 [Introduction](#)
- 2 [Data Needs](#)
 - 2.1 [Magnetic Confinement Fusion](#)
 - 2.2 [Inertial Confinement Fusion](#)
 - 2.3 [Atomic Data](#)
 - 2.4 [Molecular Data](#)
 - 2.5 [Plasma-Material Interaction Data](#)
- 3 [Data Sources](#)
 - 3.1 [Online Databases](#)
 - 3.2 [Data Centers](#)
 - 3.3 [Code Centers](#)
- 4 [Data Exchange](#)
 - 4.1 [Data Producers Directory](#)
 - 4.2 [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 [ITPA Diagnostics Group](#)
 - 5.5 [European Fusion Development Agreement \(EFDA\)](#)



Wiki, cont'd... <http://www-amdis.iaea.org/w>

toolbox

- What links here
- Related changes
- Special pages
- Printable version
- Permanent link

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

Inertial Confinement Fusion

- Equation of State
- Opacity
- Stopping Power
- Non-LTE Kinetics

Atomic Data

- Atom-Electron Collisions
- Atom-Heavy-particle Collisions
- Atomic Radiative Properties

Molecular Data

- Molecular Potentials
- Detachment
- Dissociation
- Elastic Scattering

4.2 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 ITPA Diagnostics Group
 - 5.5 European Fusion Development Agreement (EFDA)
- 6 Fusion Research
 - 6.1 Magnetic Confinement Fusion Research
 - 6.2 Inertial Confinement Fusion Research

Data Exchange

Data Producers Directory

- Experimental Group
- Theoretical Group
- Who's Who in Atomic & Plasma Physics Database [↗](#)
maintained at the Weismann Institute of Science

Data Exchange Forum

- XSAMS
- ICAMDATA

Wiki, cont'd... <http://www-amdis.iaea.org/w>

- [Atomic Radiative Properties](#)

Molecular Data

- [Molecular Potentials](#)
- [Detachment](#)
- [Dissociation](#)
- [Elastic Scattering](#)
- [Molecule-Electron Collisions](#)
- [Molecule-Heavy-Particle Collisions](#)
- [Molecular Radiative Transitions](#)

Plasma-Material Interaction Data

- [Introduction](#)
- [Erosion](#)
- [Sputtering](#)
- [Sublimation](#)
- [Reflection](#)
- [Trapping](#)
- [Desorption](#)
- [Particle Induced Electron Emission](#)
- [Wall Material Properties](#)
- [Penetration](#)
- [Dust](#)
- [Arcing](#)

Data Sources

Data Exchange Forum

- [XSAMS](#)
- [ICAMDATA](#)

Special Topics

IAEA Coordinated Research Projects (CRP)

The [Coordinated Research Projects \(CRPs\)](#) are normally three to five-year joint projects of a group of (10-15) laboratories, research teams or institutions, performing coordinated research to achieve certain well defined goal. The CRPs generally produce a significant amount of new data on the collision processes or structural properties of elements or materials relevant to fusion energy research, or perform detailed critical assessments of the existing data and selection of sets of "recommended" data (or best available at the time of assessment). The CRP results of adequate accuracy and completeness are stored in the IAEA numerical database [ALADDIN](#) and published in the IAEA publication "[Atomic and Plasma-Material Interaction Data for Fusion](#)": APID Series.

- [CRP\(2002-2006\): Tritium Inventory in Fusion Reactors](#)
- [CRP\(2004-2008\): Atomic and Molecular Data for Plasma Modelling](#)

Wiki, cont'd... <http://www-amdis.iaea.org/w>

Data Sources

Online Databases

Bibliographic Database

- [AMBDAS](#) [↗](#) IAEA AMD Unit
- [Atomic Spectra Bibliographic Databases](#) [↗](#) at NIST has three databases: Bibliographic Database on Atomic Transition Probabilities, Bibliographic Database on Atomic Spectral Line Broadening and Shifts and Bibliographic Database on Atomic Energy Levels and Spectra
- [CFADC Bibliography](#) [↗](#) The Controlled Fusion Atomic Data Center, Oak Ridge National Laboratory

Numerical Databases

- [ALADDIN](#) [↗](#) Atomic, Molecular and Plasma-Surface Interaction data
- [GENIE](#) [↗](#) Search Engine for numerical databases
- [NIST](#) [↗](#) NIST Atomic Spectra Database
- [NIST](#) [↗](#) NIST Molecular Spectroscopy database
- [MOLAT](#) Paris-Meudon Observatory
- [SPECTR-W³](#) Russian Federal Nuclear Center (RFNC-VNIITF)

Online Code Capabilities

- [FLYCHK](#) Generalized modeling capability of atomic processes

- [CRP\(2004-2008\)](#): Atomic and Molecular Data for Plasma Modelling
- [CRP\(2005-2009\)](#): Atomic Data for Heavy Element Impurities in Fusion Reactors
- [CRP\(2007-2011\)](#): Data for Surface Composition Dynamics Relevant to Erosion Processes
- [CRP\(2008-2012\)](#): Characterization of Size, Composition and Origins of Dust in Fusion Devices
- [CRP\(2009-2013\)](#): Light Element Atom, Molecule and Radical Behaviour in the Divertor and Edge Plasma Regions
- [CRP\(2010-2014\)](#): Spectroscopic and Collisional Data for W from 1 eV to 20 keV
- [CRP\(2011-2015\)](#): Atomic and Molecular Data for State-Resolved Modelling of Hydrogen and Helium and Their Isotopes in Fusion Plasma

IAEA Workshops

- [Workshop on A+M Data for fusion Energy Research ICTP Trieste, 2009](#) [↗](#)
- [Workshop on A+M Data for fusion Energy Research ICTP Trieste, 2006](#) [↗](#)
- [Workshop on A+M Data for fusion Energy Research ICTP Trieste, 2003](#) [↗](#)

NLTE Kinetics Code Comparison Workshops

- [Background](#)
- [Workshop Results](#)

Wiki, cont'd... <http://www-amdis.iaea.org/w>

■ [MOLAT](#) Paris-Meudon Observatory

- [SPECTR-W³](#) Russian Federal Nuclear Center (RFNC-VNIITF)

Online Code Capabilities

- [FLYCHK](#) Generalized modeling capability of atomic processes in plasmas

Data Centers

- [Atomic Data and Analysis Structure ADAS](#), UK
- [Oak Ridge National Laboratory CFADC](#), ORNL, USA
- [China Research Association of Atomic and Molecular Data CRAAMD](#) China
- [ENEA](#) ENEA, Italy
- [GAPHYOR LPGP](#) LPGP, France
- [IAEA, Atomic and Molecular Data Unit](#) Austria
- [Japan Atomic Energy Agency JAEA](#), Japan
- [Korea Atomic Energy Research Institute KAERI](#), Korea
- [Kurchatov Institute](#) Russia
- [Max-Planck-Institut für Plasmaphysik](#) Germany
- [National Institute for Fusion Science NIFS](#), Japan
- [National Institute of Standards and Technology NIST](#), USA
- [Virtual Atomic and Molecular Data Centre VAMDC](#), Europe
- [Russian Federal Nuclear Centre All-Russian Institute of Technical Physics RFNC-VNIITF](#), Russia

Code Centers

NLTE Kinetics Code Comparison Workshops

- [Background](#)
- [Workshop Results](#)

ITPA Diagnostics Group

- [Official Site to ITPA Diagnostics Group](#) 
- [Introduction to ITPA Diagnostics Special Working Group on First Wall Diagnostics](#)
- [Direct Link to Special Working Group on First Wall Diagnostics](#) 

European Fusion Development Agreement (EFDA)

- [Official Site: http://www.efda.org/](http://www.efda.org/) 
- [European Fusion Development Agreement](#)
- [EU Plasma Wall Interaction Task Force and Meetings](#)
- [Task Agreements on In-Vessel Dust and Tritium Management](#)

Fusion Research

Database issues

- ALADDIN: Provide only recommended data, or leave that evaluation outside ALADDIN? Recent DCN meeting showed new interest in data evaluation, esp. at NFRI.
- AMBDAS: Future maintenance of bibliography on collisional processes.
- GENIE: Good tool for a survey search, unified query language.
- XSAMS: Being implemented on many A+M databases for astrophysics and atmospheric science. Fusion?
- Knowledge Base (Wiki): Most accessed by far, flexible mechanism; content to grow.

CRP: Coordinated Research Project

Joint research on A+M/PMI topic for fusion:

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

Objectives:

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

Data and results:

- Journal publications
- Final reports in “Atomic and Plasma-Material Interaction Data for Fusion” (APID)
- Numerical data in ALADDIN
- Looking forward to results in Knowledge Base

Present and Planned CRPs

2007-2011: Data for Surface Composition Dynamics Relevant to Erosion Processes

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 Tungsten from 1 eV to 20 keV

2011-2015: Atomic and Molecular Data for State-Resolved Modelling of H and He and their Isotopes in Fusion Plasma

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

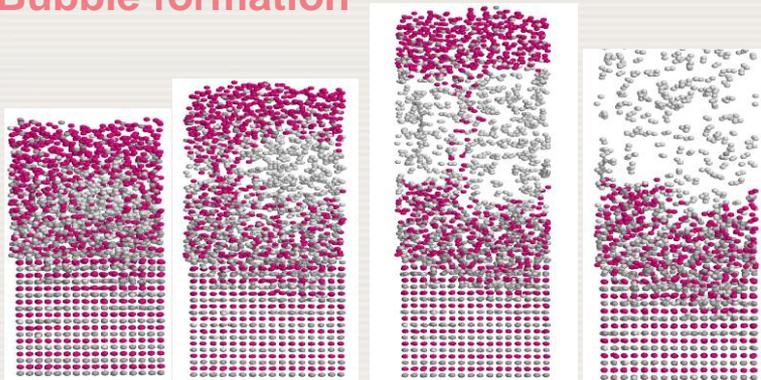
2013-2017 (tentative): Plasma Interaction with Irradiated Tungsten and Tungsten Alloys in Fusion Devices

CRP on Data for Surface Composition Dynamics Relevant to Erosion Processes (2007-2011)

Overall objective

- To better understand erosion processes and to find new methods to control erosion
- To collect and generate new data relevant to erosion dynamics in fusion reactors
- Investigated materials mainly the ones foreseen for ITER: C, W, Be

Bubble formation



100 eV 90% D +10% W on
W-terminated tungsten-carbide
Kai Nordlund, University of Helsinki

First outputs and outcomes

- Some new data included in ALADDIN
- New ALADDIN web interface for PSI

First RCM, 17-19 October 2007

Second RCM, 11-13 March 2009

Final RCM, 13-15 September 2010

CRP on Size, Composition and Origin of Dust in Tokomaks (2008-2012)

Objectives

- To determine the size, composition and origin of dust in tokamaks
- Understand dust transport
- Improve dust estimates
- Understand tritium retention in dust
- Investigate dust removal techniques
- Focus on dust from C, W and Be

First RCM: 10-12 December 2008

Second RCM: 21-23 June 2010

Third RCM: 30 Nov – 02 Dec 2011

Plans for a real dust database! (Effort centred at IPP Garching; based on automated analysis of 10s of thousands of individual dust images.)



Flaking of co-deposited layer on lower part of limiter, TFTR, Nov 1998

CRP on Light Element Atom, Molecule and Radical Behaviour in the Divertor and Edge Plasma Regions (2009-2013)

Objectives

To generate new data for radiative and collisional processes in ions of atoms and molecules of hydrogen, helium, lithium, beryllium, boron, carbon, nitrogen and oxygen at temperatures and densities typical of the edge and divertor region of fusion reactors

Data needs

- In diagnostics for plasma parameters such as temperature and density
- In plasma modelling
- Special focus on processes including ro-vibrational states of molecules
- Fine structure energy levels of molecules

First RCM: 18-20 November 2009

Second RCM: 23-25 May 2011

Third RCM: Q1 2013

CRP on Light Element Atom, Molecule and Radical Behaviour in the Divertor and Edge Plasma Regions (2009-2013)

Participants

Pierre DEFRANCE	UCL, Louvain-la-Neuve, Belgium
Dmitry FURSA/Igor BRAY	Curtin University of Technology, Perth, Australia
Ratko JANEV	Macedonian Academy of Sciences and Arts
Luis MENDEZ/Ismanuel RABADAN	UAM, Madrid, Spain
James MITCHELL	Université de Rennes I, France
Michael PINDZOLA/Teck LEE	Auburn University, AL, USA
David SCHULTZ	ORNL, USA
Hidekazu TAKAGI	Kitasato University, Sagamihara, Japan
Jianguo WANG	IAPCM, Beijing, China
Baoren WEI	Fudan University, Shanghai, China
Ioan SCHNEIDER	Université de Le Havre, France
Viorica STANCALIE	INFLPR, Romania

CRP on Spectroscopic and Collisional Properties of Tungsten from 1 eV to 20 keV

Concerned with W in all plasma regions, edge to core

- Electron-impact, radiative and photon-induced, and heavy particle collision processes
- Cross-sections for kinetic modelling
- Rate coefficients for macroscopic modelling
- Spectroscopic signatures for diagnostics
- Theory and experiment are both represented, with plenty of overlap among and between the two
- Aim to produce validated database for tungsten in plasma

First RCM: 13-15 December 2010

Second RCM: Q2 2012

Third RCM: Q4 2013; wrap-up in 2014

CRP on Spectroscopic and Collisional Properties of Tungsten from 1 eV to 20 keV

Participants

R. Srivastava, IIT Roorkee, India

A. Müller, University of Giessen, Germany

N. Nakamura, University of Electrocommunications, Japan

A. Ryabtsev/R. Kildiyarova, Russian Academy of Sciences, RF

W. Tchang-Brillet/A. Wyart, Observatoire de Paris, France

P. Beiersdorfer, Lawrence Livermore National Laboratory, USA

C.-Z. Dong, Northwest Normal University, China

F. Koike, Kitasato University, Japan

M. Trzhaskovskaya/V. Nikulin, St Petersburg Nuclear Physics Institute, RF

V. Lisitsa, Kurchatov Institute, RF

N. Badnell, University of Strathclyde, UK

J. Colgan, Los Alamos National Laboratory, USA

Yu. Ralchenko, National Institute of Standards and Technology, USA



CRP on Atomic and Molecular Data for State-Resolved Modelling of H and He and their Isotopes in Fusion Plasma

- Species H, H⁺, H₂, H₂⁺, H₃⁺, He, He⁺, He²⁺, HeH⁺, He₂⁺, H⁻ and isotopic variants; isotope effects are important; He is newly important
- Kinetic modelling: we want state-resolved cross-sections
- Aim to be comprehensive for volume processes among the mentioned species and e⁻, hv
- Predominantly theoretical; some experiment

First RCM: 10-12 August 2011

Second RCM: Q1 2013

Third RCM: Q3 2014; wrap-up in 2015.

CRP on Atomic and Molecular Data for State-Resolved Modelling of H and He and their Isotopes in Fusion Plasma

Participants

Roberto CELIBERTO and Mario CAPITELLI, Polytechnic of Bari, Italy

Ursel FANTZ and Dirk WÜNDERLICH, MPI for Plasma Physics, Garching

Christian JUNGEN, CNRS and U Paris-Sud, and Ioan SCHNEIDER, U Le Havre

Viatcheslav KOKOULINE and Talat RAHMAN, University of Central Florida

Predrag KRSTIC, Oak Ridge National Laboratory

Xinwen MA, Institute of Modern Physics, Chinese Academy of Sciences, Lanzhou

Ousmanou MOTAPON, University of Douala, Cameroon

Ann E. OREL, University of California at Davis

Detlev REITER, Forschungszentrum Jülich

Keiji SAWADA, Shinshu University, Japan

Xavier URBAIN and Pierre DEFRANCE, Catholic University of Louvain, Belgium

Jung-Sik YOON and Mi-Young SONG, National Fusion Research Institute, Korea



CRP on Erosion and Tritium Retention in Beryllium Plasma-Facing Materials

- Timely for input from JET ITER-Like Wall (ILW) and for planning for ITER.
- Focus on sputtering, reflection and trapping due to regular interaction of H/He and impurity ions with Be surface [*].
- Interested in mixed materials, esp. Be-C and Be-O.
- Mix of experiment and modelling.
- Schedule: RCMs in Q1 2012, Q4 2013, Q2 2015.
- [*] The Physics Section has a CRP on “Investigation of Materials under High Repetition and Intense Fusion Pulses” (2011-2016).

Planned CRP on plasma interaction with irradiated tungsten and tungsten alloys

- Strongly recommended by the IFRC subcommittee on A+M data as our second CRP for the 2012-2013 programme
- Tungsten alloys are foreseen for next step beyond ITER
- In any case, W transmutes to W-Re-Os
- Neutron irradiation causes voids and dislocations; changes PMI properties in ways that have not been much studied
- CRP on irradiated tungsten and tungsten alloys in 2013-2017 will support planning for DEMO

Summary of database work

Numerical database ALADDIN: Record of IAEA-sponsored work; we wish to broaden it. Data validation and recommendation issues.

Bibliographical database AMBDAS: Have been totally dependent on NIST and ORNL. Input to the collisions part is being revisited.

Database search engine GENIE: Valuable single query interface to multiple database

New knowledge base (wiki): The most visited part of our web site. Essentially single-person effort so far; we hope to broaden the effort.

Summary of CRP work

- CRPs are the main mechanism by which the A+M Data Unit encourages new research
- Recent budgets allow us to start about one new CRP per year
- Focus is on A+M and PMI data for Fusion
- Advice on topics from IFRC subcommittee is important
- Considerations for choice of topics:
 - ITER relevance is good, exclusively ITER not so good
 - Need to be able to assemble broad team
 - Must be active topic; we don't fund the research
 - We like focussed topic for best synergy