

Database and Knowledge Base developments at IAEA A+M Unit

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Nuclear Data Section, Division of Physical and Chemical Sciences

June 22nd 2010

2nd RCM on Characterization of size, composition and origins of dust in fusion devices



IAEA

International Atomic Energy Agency

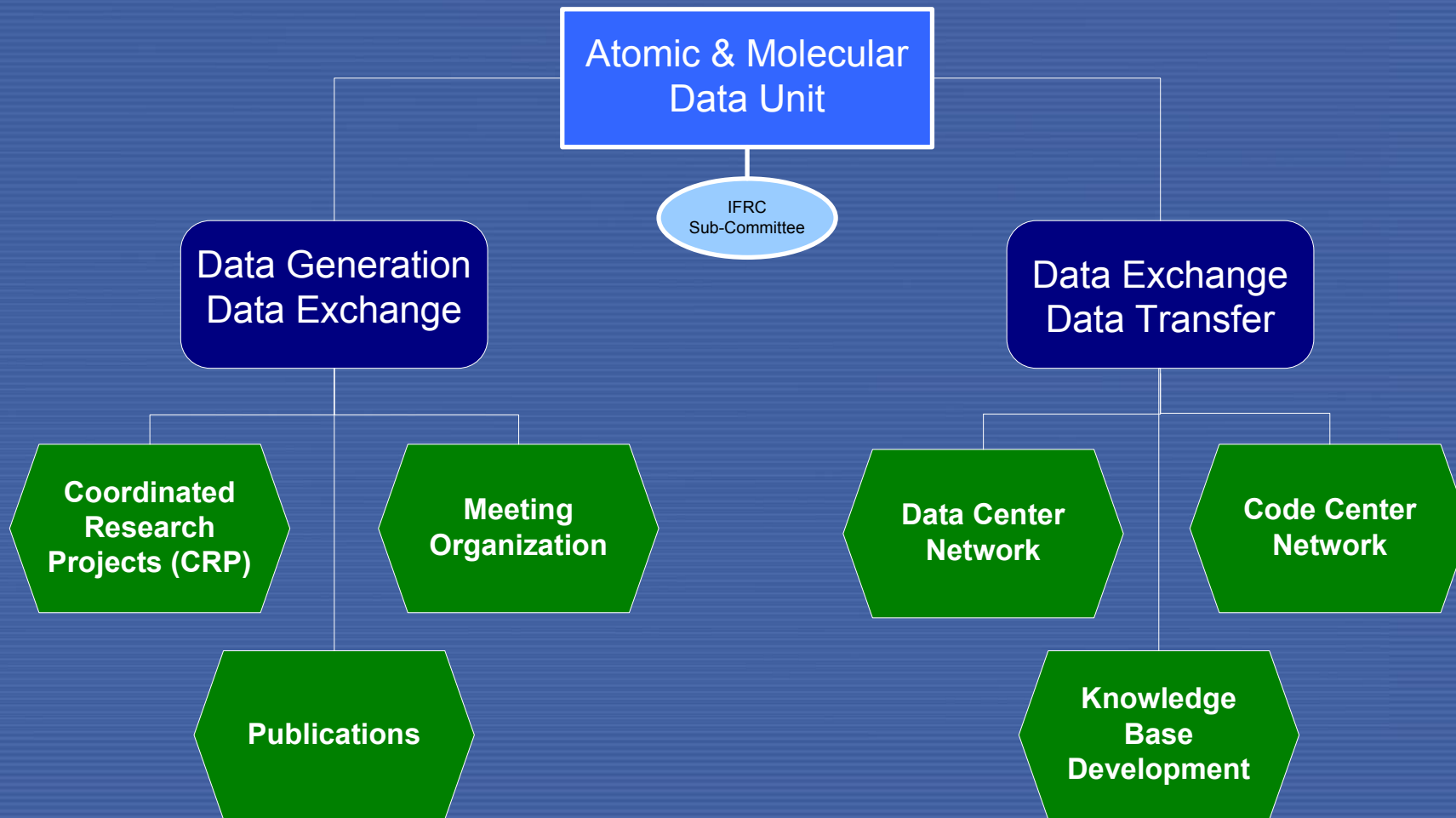
International Atomic Energy Agency (IAEA)

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

- Founded in 1957
- Vienna, Austria
- 151 Member States
(As of December 2009)
- 6 Departments
- 2200 Staff
- Regular Budget of US\$275M
- Additional ~ US\$80M for Technical Cooperation
- assists its Member States, in the context of social and economic goals, in planning for and using nuclear science and technology for various peaceful purposes, including the generation of electricity, and facilitates the transfer of such technology and knowledge in a sustainable manner to developing Member States;



A+M Data Unit Activities



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 A+M/PMI Data 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

Outputs:

- Publications, Meeting Presentations and Reports
- Final Reports in “Atomic and Plasma-Material Interaction Data for Fusion” (APID)
- Data and Results in ALADDIN Numerical Database and Knowledge Base



Past, Present and Future CRPs

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

2002-2006: Tritium Inventory in Fusion Reactors

2004-2008: Atomic and Molecular Data for Plasma Modelling

2005-2009: Atomic Data for Heavy Element Impurities in Fusion Reactors

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 W from 1 eV to 20 keV

2011-2015 (tentative): Data for kinetic modelling of molecules of H and He and their isotopes in fusion plasma

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

2013-2017 (tentative) Plasma-Wall Interaction of Tungsten and its Alloys in Fusion Devices

(More tentative) Data for kinetic modelling of hydrocarbon ions in fusion plasma

Meetings in 2010

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

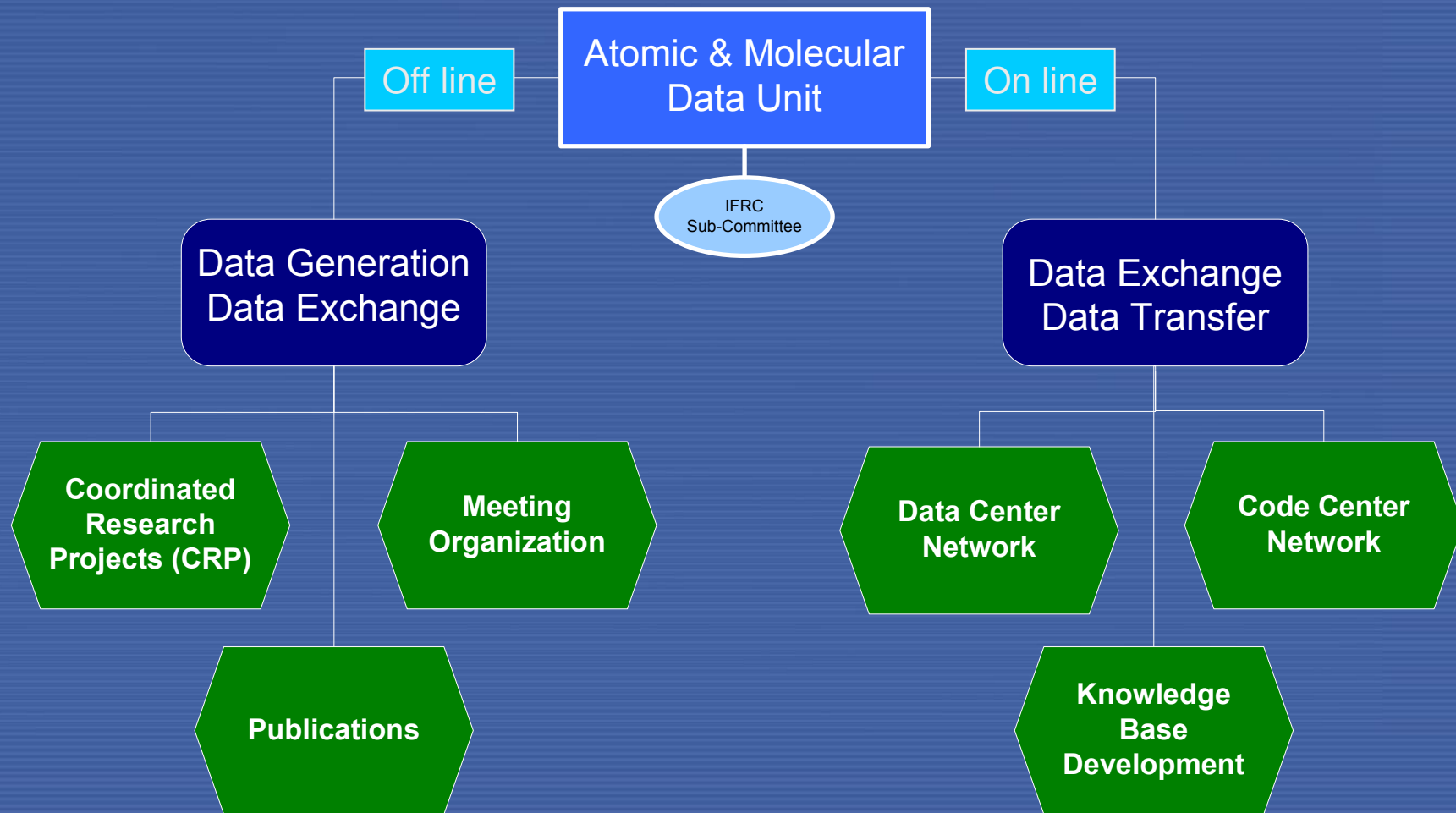
- CM on "XML Schema for Atomic and Molecular Data"(March 2010, NIFS)
- TM of the 17th IFRC Sub-committee on "Atomic and Molecular Data for Fusion Research" (April 2010)
- 2nd RCM on "Characterization of size, composition and origins of dust in fusion devices" (June 2010)
- 3rd RCM on "Data for Surface Composition Dynamics Relevant to Erosion Processes" (Sept. 2010)
- TM on "International Code Centres Network" (Sept. 2010)
- CM on "Database needs for plasma modelling" (Sept. 2010)
- CM on "XML Schema for Atomic and Molecular Data"(Nov. 2010)
- 1st RCM on "Spectroscopic and Collisional Data for Tungsten from 1 eV to 20 keV" (Dec. 2010)

Publications

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

- IAEA-INDC(NDS) Reports
 - Reports are published for every meeting and Consultant's visit
- International Bulletin on Atomic and Molecular Data for Fusion
 - Bibliographic Information on Atomic, Molecular and Plasma-Surface Interaction Data
 - Published once a year
 - Volume 67, December 2008
 - Volume 68, December 2009
- Atomic and Plasma-Material Interaction Data for Fusion (APID Series)
 - Data and papers related to results produced by CRPs and Consultants groups
 - Edition in preparation
 - Volume 15: CRP on "Tritium Inventory in Fusion Machines"
 - Volume 16: CRP on "Atomic and Molecular Data for Plasma Modelling"
 - Volume 17: CRP on "Atomic Data For Heavy Element Impurities in Fusion Reactors"

Online Activities: Data Transfer



Atomic Molecular Data Information Services

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

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

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Search

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

Overview of 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.

- **Overview on Databases on Atomic and Molecular Data for Fusion.**
 1. **ALADDIN**
 2. **AMBDAS**
 3. **GENIE**
 4. **OPEN-ADAS**
 5. **Rovibronic energy levels for triplet electronic states of molecular deuterium**
 6. **Franck-Condon Factors, Transition Probabilities and Radiative Lifetimes for Hydrogen Molecules and their Isotopomers**
- **Overview on Online Computing Capabilities**
 1. **Heavy Particles collisions**
 2. **Average Approximation**
 3. **Rate coefficients**
 4. **Los Alamos atomic physics codes**
 5. **FLYCHK**
- **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

March 24-26, 2010
Consultants Meeting on XML Schema for Atoms, Molecules and Solids (XSAMS)

April 27-28, 2010
Meeting of the International Fusion Research Council Subcommittee on Atomic and Molecular Data for Fusion

June 21-23, 2010
2nd RCM of CRP on "Characterization of Size, Composition and Origins of Dust in Fusion Devices"

September 13-15, 2010
3rd RCM of CRP on "Data for Surface Composition Dynamics Relevant to Erosion Processes"

September 27-28

AMO/PSI Meetings

May 16-20, 2010:
High Temperature Plasma Diagnostics, New Jersey, USA

May 24-28, 2010:
19th Plasma Surface Interaction, San Diego, USA

May 25-29, 2010:
41st Annual Meeting of the Division of Atomic Molecular and Optical Physics, APS

June 16-18, 2010:
11th HITRAN(High-resolution TRANsmision molecular absorption database) + 9th Atmospheric

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
- OPEN-ADAS: Numerical Database
- GENIE: Search Engine on Numerical Databases

ALADDIN: Numerical Database

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

- Atomic and Molecular Collisional Database
 - Heavy Particle Collisions / Electron Collisions / Photon Collisions
 - Search by Reactants, Products, Process, Data Types, Authors, Publication
- Plasma Surface Interaction Database
 - Reflection / Sputtering / Radiation Enhanced Sublimation / Penetration
 - Search by Projectile, Surface, Chemical Component, Data Type, Author, Publication
- Data developed through CRPs, TMs and CMs recommended by IFRC A+M
 - List of Publications (<http://www-amdis.iaea.org/ALADDIN/datalist.php>)

ALADDIN PSI Database

ALADDIN

Go to data selection Filter from selection Reset request

Process

Reflection
Chemical Sputtering
Physical Sputtering
Radiation Enhanced Sublimation
Penetration

Projectile

H
D
T
[3]He

Surface

Be
Graphite
α-Carbon
CFC

Chemical Component

Be
C
W
H

Data Description

Mean Penetration Depth vs. angle and energy
Sputtered energy and energy reflection coeff. vs. angle and energy
Sputtering yields and particle reflection coeff. vs. angle and energy
Sputtering yields vs. incident flux density

Data Type

Derived
Experimental
Theoretical

First Author	Publication	Date
Behrish R. Doerner R.P. Eckstein W. Haasz A.A.	IAEA-APID-7A (1998) IAEA-APID-7B (2001) INDC(NDS)-249 (1991) INDC(NDS)-287 (1993)	2007 2006 2005 2003

Go to data selection Filter from selection Reset request

[Dictionary](#) [Glossary](#) [Comments](#) [Home](#)

AMBDAS: Bibliographic database

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

- Data Source
 - Spectroscopic data from NIST (A. Kramida & J. Fuhr)
 - Collisional data from ORNL
 - Data entries relevant to fusion
 - Published in the International Bulletins #67 and #68 (in press)
- Version 3.1 (April 2010)
 - Search by Reactants, Process, Authors, Keywords, Year
 - Results with Author, Title, Reference and DOI (Digital Object Identifier) Link
 - CrossRef Query (<http://doi.crossref.org>) at \$500 / year fee
 - Out of 46878 reference data, 34420 data are linked to the full text of the electronic journal and 5115 data are linked to the abstract by the DOI link.
- All data in the International Bulletin available on Atomic and Molecular Data for Fusion through AMBDAS

AMBDAS Screen Shot

AMBDAS

Atomic and Molecular Bibliographical Database

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" value="W"/> 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	Inelastic Energy Losses
Photon Collisions	--- Surface Interactions ---
Electron Collisions	Accommodation
Heavy Particles Collisions	Adsorption, Desorption
Surface Interactions	Chemical Reactions
Beam Heating and Fueling of Plasmas	Desorption

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"	
Years	<input type="text"/> - <input type="text"/> 98, 1998, 02, 2002	Reference Type	<input type="text" value="-----"/> ▾

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



OPEN-ADAS

Data Dissemination <http://open.adas.ac.uk/>

- **ADAS** is an interconnected set of computer codes and data collections for modelling
 - Radiating properties of ions and atoms in plasmas for fusion and astrophysical application
 - Analysis and interpretation of spectral measurements
- **OPEN-ADAS** is a free web access to ADAS data
 - A joint development between the ADAS Project and the IAEA to provide access to fundamental and derived atomic data from the ADAS project and its related databases.
 - 124 registered users (89 from non-ADAS sites) as of 01/08/09

OPEN-ADAS
Atomic Data and Analysis Structure

OPEN-ADAS Version 1.0
[Report Error](#) | [Create Account](#) | [Log In](#)

Freeform search
Search by wavelength
Search by ion
Search by data class
Documentation
Download code
Terminology
Statistics
About ADAS
About OPEN-ADAS

OPEN-ADAS Freeform Search

For comments and questions see: [Contact Details](#)

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GENIE

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

Web search engine for atomic data

Radiative properties – search on 8 databases

Collisional databases – search on 4 databases

<p>Transition Probabilities Wavelengths Energy Levels</p> <p>Ion: <input type="text" value="C IV"/></p> <p>Enter wavelength in Å: From <input type="text" value="1"/> to <input type="text" value="10000"/></p> <table border="1"><tr><td>NIST Atomic Spectra Database</td><td><input checked="" type="checkbox"/></td><td><input type="button" value="?"/></td></tr><tr><td>Kurucz's CD-ROM 23</td><td><input checked="" type="checkbox"/></td><td><input type="button" value="?"/></td></tr><tr><td>Atomic Line List v.2.04</td><td><input checked="" type="checkbox"/></td><td><input type="button" value="?"/></td></tr><tr><td>TOPbase (Opacity Project)</td><td><input checked="" type="checkbox"/></td><td><input type="button" value="?"/></td></tr><tr><td>Kelly Atomic Line Database</td><td><input checked="" type="checkbox"/></td><td><input type="button" value="?"/></td></tr><tr><td>MCHF/MCDHF Collection</td><td><input checked="" type="checkbox"/></td><td><input type="button" value="?"/></td></tr><tr><td>KAERI AMODS Spectral Lines</td><td><input checked="" type="checkbox"/></td><td><input type="button" value="?"/></td></tr><tr><td>CAMBD Atomic Spectra</td><td><input checked="" type="checkbox"/></td><td><input type="button" value="?"/></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="button" value="?"/>	Kurucz's CD-ROM 23	<input checked="" type="checkbox"/>	<input type="button" value="?"/>	Atomic Line List v.2.04	<input checked="" type="checkbox"/>	<input type="button" value="?"/>	TOPbase (Opacity Project)	<input checked="" type="checkbox"/>	<input type="button" value="?"/>	Kelly Atomic Line Database	<input checked="" type="checkbox"/>	<input type="button" value="?"/>	MCHF/MCDHF Collection	<input checked="" type="checkbox"/>	<input type="button" value="?"/>	KAERI AMODS Spectral Lines	<input checked="" type="checkbox"/>	<input type="button" value="?"/>	CAMBD Atomic Spectra	<input checked="" type="checkbox"/>	<input type="button" value="?"/>		<p>Electron Impact Cross Sections and/or Rate Coefficients</p> <p>Ion: <input type="text" value="C 3+"/></p> <table border="1"><tr><td><input checked="" type="radio"/> Excitation</td><td rowspan="3"><input type="button" value="?"/> Cross sections <input checked="" type="checkbox"/> Rate coefficients <input checked="" type="checkbox"/></td></tr><tr><td><input type="radio"/> Ionization</td></tr><tr><td><input type="radio"/> Dielectronic recombination</td></tr></table> <table border="1"><tr><td>IAEA ALADDIN Database</td><td><input checked="" type="checkbox"/></td><td><input type="button" value="?"/></td></tr><tr><td>NIFS AMDIS Database</td><td><input checked="" type="checkbox"/></td><td><input type="button" value="?"/></td></tr><tr><td>CAMBD Collisional Processes</td><td><input checked="" type="checkbox"/></td><td><input type="button" value="?"/></td></tr><tr><td>NIST Atomic Cross Sections</td><td><input checked="" type="checkbox"/></td><td><input type="button" value="?"/></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="button" value="?"/> Cross sections <input checked="" type="checkbox"/> Rate coefficients <input checked="" type="checkbox"/>	<input type="radio"/> Ionization	<input type="radio"/> Dielectronic recombination	IAEA ALADDIN Database	<input checked="" type="checkbox"/>	<input type="button" value="?"/>	NIFS AMDIS Database	<input checked="" type="checkbox"/>	<input type="button" value="?"/>	CAMBD Collisional Processes	<input checked="" type="checkbox"/>	<input type="button" value="?"/>	NIST Atomic Cross Sections	<input checked="" type="checkbox"/>	<input type="button" value="?"/>
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Code Centre Network (CCN) Activities

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

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

- Online computing
 - Downloadable codes
 - Direct contacts with the CCN for any expertise
-
- Online codes on Heavy Particles collisions
 - Online codes on Average Approximation
 - Online codes on Rate coefficients
 - Results and Link to Los Alamos atomic physics codes
 - Results and Link to FLYCHK code

IAEA Online Calculation Capabilities

- **Average Approximation** <http://www-amdis.iaea.org/AAEXCITE/>
 - J. Peek provided code for electron impact excitation cross sections of ions
 - For any ion and configuration in real time
- **Heavy particle collisions** <http://www-amdis.iaea.org/HEAVY/>
 - A. Dubois, JP Hansen and P. Vainstein provided code for calculation of cross sections for excitation, ionization and charge exchange for bare nucleus on hydrogenic target
 - Registration required
- **Effective Ionization/Recombination Rates** <http://www-amdis.iaea.org/RATES/>
 - Results from collisional radiative calculations of plasmas are available, as carried out with the Los Alamos modeling codes
 - Level population distributions and Radiative Power rates are obtained.

Interface to Remote Online Capabilities

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

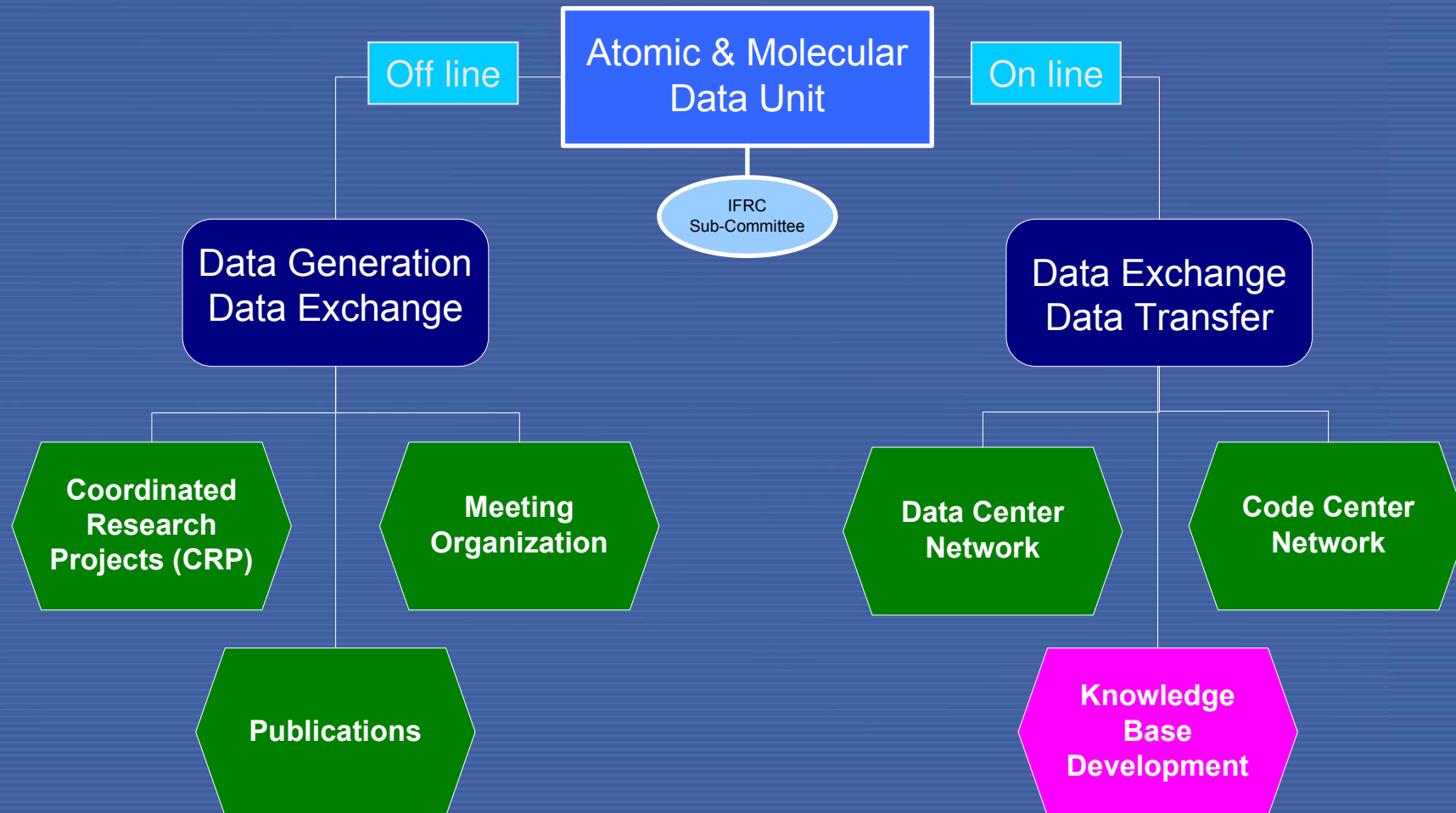
- An interface to run Los Alamos atomic physics codes to calculate atomic structure and electron impact excitation and ionization cross sections
- Complete data sets of for Argon, Chlorine and Silicon atoms (~ 2GB)
 - CRP for "Atomic Data For Heavy Element Impurities in Fusion Reactors"
 - Level energies and statistical weights of the ground and excited levels
 - Oscillator strengths and electron-impact excitation cross-sections, photo-ionization and electron-impact ionization cross-sections

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

- An interface to run a Collisional-Radiative code FLYCHK at NIST to calculate ionization distributions and spectral properties of elements from Hydrogen to Gold.
- Average Charge State of elements from Hydrogen to Gold in a wide range of plasma conditions of $0.5 \text{ eV} \leq T_e \leq 100 \text{ keV}$ and $10^{12} \text{ cm}^{-3} \leq N_e \leq 10^{24} \text{ cm}^{-3}$.



New Knowledge Base Development

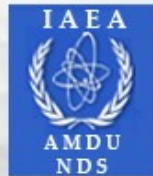


Knowledge Base Motivation

- Background: Limitations of Databases in Data Collection & Dissemination
 - Modeling requires an Extensive Set of Data (LANL data ~ 2GB)
 - Limited Description on Data Sources, Quality and Validity
 - “Lost In Translation” of Comprehensive Knowledge by Numerical Representation (Particularly CRP Results on Plasma-Matter Interaction)
 - Web 2.0 Technology – facilitate interactive information sharing, interoperability, user-centered design and collaboration on the web. A Web 2.0 site allows its users to interact with each other as contributors to the website's content in contrast to websites where users are limited to the passive viewing of information that is provided to them .
- Organization
 - Use of Wiki pages --- A+M Data Unit in a Coordinator role
 - Community Ownership: Voluntary Content Contribution and Peer Review
 - Central location – Direct Data Storage or Link to Data Sources
 - More information on Data and their Applications in a Context
 - Closer Community Network → Foster Collaboration on a Focused Topic

Knowledge Base Overview

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



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

Introduction [\[edit\]](#)

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 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 [\[edit\]](#)

Magnetic Confinement Fusion [\[edit\]](#)

- 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 [\[edit\]](#)

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- 2 Data Needs
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 - 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 Requests
 - 4.3 Data Exchange Forum
- 5 Special Topics
 - 5.1 IAEA Coordinated Research Projects (CRP)
 - 5.2 IAEA Workshops
 - 5.3 NLTE Kinetics Code Comparison Workshops
- 6 Fusion Research
 - 6.1 Magnetic Confinement Fusion Research
 - 6.2 Inertial Confinement Fusion Research

knowledge base

- Main Page
- Data Needs
- Data Sources
- Data Exchange
- Special Topics
- Fusion Research

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search

Go

Search

toolbox

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

Knowledge Base Status

- Plasma-Matter Interaction Data Needs
 - APID Volumes <http://www-amdis.iaea.org/publications/APID/>
 - INDC Reports and Consultant's Reports
<http://www-amdis.iaea.org/publications/INDC/>
- CRP Activities
 - Participants Presentation <http://www-amdis.iaea.org/CRP/>
 - APID Volume and INDC Reports
 - Contributed Papers from CRP Participant
- CRP on Characterization of Size, Composition and Origins of Dust in Fusion Devices
 - Summary of Participants Presentations at the 1st RCM
 - Reviews on the Wiki pages are highly appreciated

Knowledge Base Future Work

- Improvement Needed:
 - Place Holders for Wiki Pages
 - Citations and References
 - More Linking of Contents for Comprehensive Overview
 - Search Option on Words
 - <http://nds121.iaea.org/alberto/mediawiki-1.6.10/index.php>
 - Migration to MySQL
- Contributing to the Knowledge Base
 - Help available at the Knowledge Base
 - Registration Provided for CRP Participants and Consultants

Conclusions

IAEA AMD Unit Activities

Coordinated Research Projects (CRP)

Meetings and Workshops

Publications

Data Centre Network (DCN) Activities

Code Centre Network (CCN) Activities

Knowledge Base for A+M/PSI data for fusion

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