

# Databases and Knowledge Base for Plasma-Matter Interaction for Fusion

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Atomic and Molecular Data Unit, Nuclear Data Section

26-28 September 2012



# International Coordination of A+M/PSI Data Research for Fusion

Consultants  
Meetings  
(CM)

Fusion Plasma  
Modelling

Measurements

Theories

Publications  
(INDC, APID,  
Bulletin)

Coordinated Research  
Projects (CRP)

Technical  
Meetings  
(TM)

Data  
Production

Data  
Compilation

Data  
Evaluation

Databases  
(AMBDAS,  
GENIE,  
ALADDIN,  
Wiki...)



IAEA

# Online AM/PSI Data Services:

## <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](#)

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### Databases

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ALADDIN  
OPEN-ADAS  
GENIE  
KNOWLEDGE BASE

### On-Line Computing

Overview  
HEAVY  
AAEXCITE  
RATES  
LANL Codes  
FLYCHK

### Activities

IFRC Subcommittee  
CRP  
Publications  
Meetings  
Workshops  
Data Centre Network  
Code Centre Network  
XSAMS

### Contacts

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## 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 D<sub>2</sub>

FC Factors &  
A-values of  
H<sub>2</sub> & Isotopes

- Online Computing Capabilities

Code  
Centres  
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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 Documents  
INDC Reports  
Publications



Computer  
Codes

### IAEA Meetings

Jun 20-22, 2012  
Consultant Meeting  
on Data Evaluation  
and the  
Establishment of a  
Standard Library of  
A+M/PMI Data for  
Fusion

Aug 29-31, 2012  
2nd RCM of CRP on  
Spectroscopic and  
Collisional Data for  
W from 1 eV to 20  
keV

Sep 4-7, 2012  
Joint IAEA-NFRI  
Technical Meeting on  
Data Evaluation for  
Atomic, Molecular  
and Plasma-Material  
Interaction  
Processes in Fusion  
NFR, Daejon, Korea

Sep 26-28, 2012  
1st RCM of CRP on  
Data for Erosion and  
Tritium Retention in  
Beryllium Plasma

### AM/PSI Meetings

May 21-25, 2012  
20th Plasma-Surface  
Interaction  
Conference Aachen,  
Germany

May 29-31, 2012  
11th International  
Workshop on  
Hydrogen Isotopes  
in Fusion Reactor  
Materials, Schloss  
Ringberg, Germany

September 2-7,  
2012: 16th in a  
series of  
International  
Conferences on  
Plasma Physics

# Databases for PMI Research

- Plasma-Surface Interaction Data
  - ALADDIN: Numerical Database
  - AMBDAS: Bibliographic database
  - Dust Particle Database
- Plasma Spectroscopic Analysis for PSI Data
  - ALADDIN: Atomic and Molecular Collisional Data
  - AMBDAS: Bibliographic database
  - GENIE: Atomic Structure, Transition Probabilities & Collisional Data
  - OPEN-ADAS: Publically Available Fundamental Data Used by ADAS
  - FLYCHK: Charge State Distributions

# Databases : ALADDIN

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

- Data list: <http://www-amdis.iaea.org/ALADDIN/datalist.php>
  - Data from 1980-2006 for evaluated / compiled data
  - Data from CRPs recently
  - ~17600 sets for A&M data (~ 8500 rad. rec. APID 16)
  - ~ 6200 data for Surface data
- Data Development
  - Consultancy by Eckstein on reflection and penetration data
  - TM on “Improving the Database for Physical and Chemical Sputtering”
- Be Surface Data
  - Mostly Eckstein’s work
  - Björkas recent work
  - UCSD’s work

# ALADDIN PSI Database

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

ALADDIN

Go to data selection Filter from selection Reset request

### Process

- Reflection
- Chemical Sputtering
- Physical Sputtering
- Radiation Enhanced Sublimation
- Penetration

Projectile	Surface	Chemical Component
H D T [3]He	Be Graphite α-Carbon CFC	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
Behrash 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

# Databases: AMBDAS

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

- Bibliographic data for spectroscopy from NIST
- No data for collisions and plasma-surface interaction data available since 2010
- No publication of international bulletin on atomic and molecular data for fusion
- Need a provider of collisional data and PSI data
- ~ 100 Data for Plasma-Be(Surface) Interaction

# Search on Be Surface: 111 Results

## AMBDAS: Query Output

111 references found. Processing the output...

1. D. Nishijima, R. P. Doerner, M. J. Baldwin, G. De Temmerman  
*Erosion yields of deposited beryllium layers.*  
J. Nucl. Mater. **390-391**, 132 (2009). doi:[10.1016/j.jnucmat.2009.01.144](https://doi.org/10.1016/j.jnucmat.2009.01.144)

Experiment | 5-140 eV | [Reactant Data](#)

2. M. Reinelt, Ch. Linsmeier  
*Ion implanted deuterium retention and release from clean and oxidized beryllium.*  
J. Nucl. Mater. **390-391**, 568 (2009). doi:[10.1016/j.jnucmat.2009.01.103](https://doi.org/10.1016/j.jnucmat.2009.01.103)

Experiment | 1 keV | [Reactant Data](#)

3. M. Ait El Fqih, P.-G. Fournier  
*Optical emission from Be, Cu and CuBe targets during ion beam sputtering.*  
Nucl. Instrum. Methods Phys. Res. B **267**, 1206 (2009). doi:[10.1016/j.nimb.2009.01.159](https://doi.org/10.1016/j.nimb.2009.01.159)

Experiment | 5 keV | [Reactant Data](#)

4. J. Sun, H. Watanabe, M. Tona, T. Watanabe, N. Nakamura, C. Yamada, S. Ohtani  
*K and L x-ray emission from hollow atoms produced in the interaction of slow H-like ( $l^{52+}$ ) and bare ( $l^{53+}$ ) ions with different target materials.*  
Phys. Rev. A **77**, 032901 (2007). doi:[10.1103/PhysRevA.77.032901](https://doi.org/10.1103/PhysRevA.77.032901)

Experiment | 182-186 eV | [Reactant Data](#)

5. Y. Zhao, G. Xiao, X. Zhang, Z. Yang, Y. Zhang, W. Zhan, X. Chen, F. Li  
*X-ray emission of hollow atoms formed by highly charged argon and xenon ions below a beryllium surface.*  
Nucl. Instrum. Methods Phys. Res. B **258**, 121 (2007). doi:[10.1016/j.nimb.2006.12.178](https://doi.org/10.1016/j.nimb.2006.12.178)

Experiment | 204-450 keV | [Reactant Data](#)

6. M. Reinelt, Ch. Linsmeier  
*Temperature programmed desorption of 1 keV deuterium implanted into clean beryllium.*  
Phys. Scr. **T128**, 111 (2007). doi:[10.1088/0031-8949/2007/T128/022](https://doi.org/10.1088/0031-8949/2007/T128/022)

Experiment | 1 keV | [Reactant Data](#)

7. H. Paul  
*On the gas-solid difference in stopping power for low energy ions.*  
Nucl. Instrum. Methods Phys. Res. B **262**, 13 (2007). doi:[10.1016/j.nimb.2007.04.283](https://doi.org/10.1016/j.nimb.2007.04.283)

Experiment and Theory | 0.025-0.05 MeV/amu | [Reactant Data](#)

8. Y. Zhao, G. Xiao, X. Zhang, Z. Yang, W. Zhan, X. Chen, F. Li  
*X-ray spectroscopy of hollow argon atoms formed on a beryllium surface.*  
Nucl. Instrum. Methods Phys. Res. B **245**, 72 (2006). doi:[10.1016/j.nimb.2005.11.081](https://doi.org/10.1016/j.nimb.2005.11.081)

Experiment | Undef. | [Reactant Data](#)

## AMBDAS: Reactant Data for Ref. 1

List of available reactant/surface codes

Reactant(s):  $H^+$   
Surface(s): **Be**  
Sputtering

Reactant(s):  $H_2^+$   
Surface(s): **Be**  
Sputtering

Reactant(s):  $D^+$   
Surface(s): **Be**  
Sputtering

Reactant(s):  $D_2^+$   
Surface(s): **Be**  
Sputtering

Query time: 0 sec

- A. I. Belyayeva
- O. Benka
- H. Bergsaker
- J. Bohdansky
- A. Bonanno
- V. N. Bondarenko
- M. Boustimli
- D. K. Brice
- R. A. Causey
- R. S. Chauhan
- X. Chen
- Y. P. Cherdantsev
- V. N. Chernikov
- I. P. Chernov
- R. W. Conn
- S. Datz
- J. W. Davis
- W. Degel
- Z. J. Ding
- R. P. Doerner



Key

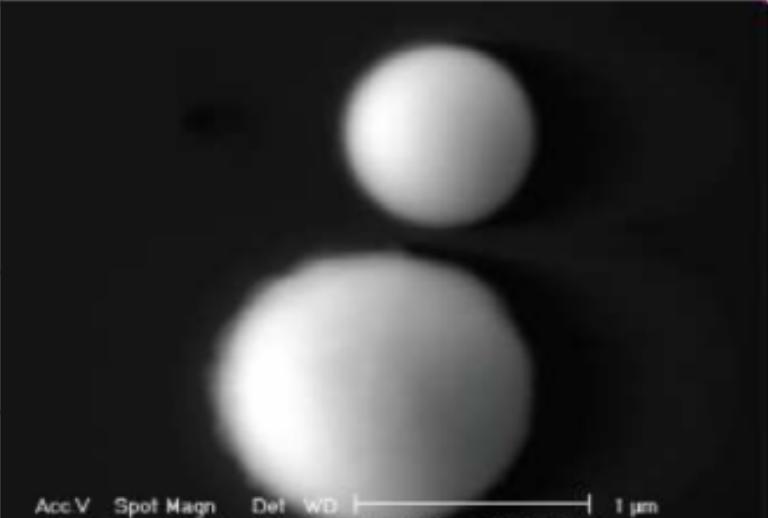
# Planned Databases : Dust particles

in collaboration with IPP-Garching

IPP

## Classification system selection

Classification scheme: IAEA CRP 2011-v.1.0

Class no.: 1/10	Name: Tungsten droplet	
Description	Typical SEM image	
Shape e.g. Elongation: > 0.72 Circularity: > 0.92 Convexity: > 0.90	 A scanning electron micrograph showing two distinct, spherical tungsten droplets against a dark background. The droplets have a smooth surface texture.	
Surface morphology e.g. smooth		
Element composition e.g. Dominant Element(s): W	Acc.V 20.0 KV Spot Mag. 3.0 35000x Det. WD GSE 10.4 5.0 mBar V5_29_03.TIF 1 μm	
Identified Sources Arcs Melting	Impact on Safety $\text{WO}_3$ formation	Impact on Operation disruption

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  - OPEN-ADAS: Publically Available Fundamental Data Used by ADAS
  - FLYCHK: Charge State Distributions

# Databases Search Engine: GENIE

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

- Radiative properties : 9 Databases
- Collisional data : 6 Databases

**GENIE**  
A General Internet Search Engine for Atomic Data

Transition Probabilities  
Wavelengths  
Energy Levels

Ion: Be I

Enter wavelength in Å:

From 1 to 10000

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

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



Electron Impact Cross Sections  
and/or Rate Coefficients

Ion: Be I+

Excitation      [?](#)

Ionization      [?](#)

Dielectronic recombination      [?](#)

Cross sections      [?](#)

Rate coefficients      [?](#)

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

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

# FLYCHK: Charge state distributions

## 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 non-LTE (Non-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, see 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 code can calculate steady-state plasmas with electron temperatures from 0.5 eV to 100 keV and electron densities from  $10^{12} \text{ cm}^{-3}$  to  $10^{24} \text{ cm}^{-3}$ . Click the element in the periodic table for more 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 are provided 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 rates. These are provided for the same range of plasma conditions as the Charge state distributions. The details of the methods are found at the [FLYCHK Rates information page](#).

1 H	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: 1E12 - 1E24 cm-3 <a href="#">click here for limitations of FLYCHK results</a>												2 He				
3 Li	4 Be	5 B	6 C	7 N	8 O	9 F	10 Ne	11 Na	12 Mg	13 Al	14 Si	15 P	16 S	17 Cl	18 Ar		
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
55 Cs	56 Ba	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn	
87 Fr	88 Ra	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Uut	114 Uuq	115 Uup	116 Uuh	117 Uus	118 Uuo	



# Knowledge base (wiki style)

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

- Introduction
- Data Needs
  - Magnetic Confinement Fusion
  - Inertial Confinement Fusion
  - Atomic Data
  - Molecular Data
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  - Code Centers Network
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  - Data Producers Directory
  - Data Exchange Forum
- Special Topics
  - IAEA Coordinated Research Projects (CRP)
  - IAEA Workshops
  - NLTE Kinetics Code Comparison Workshops
  - ITPA (International Tokamak Physics Activity)
  - European Fusion Development Agreement (EFDA)
- Fusion Research
  - Magnetic Confinement Fusion Research
  - Inertial Confinement Fusion Research

# Data Development Project

- Data Users
  - Modellers, Spectroscopists, Experimentalists, ... etc
- Data sets of interest
  - Sputtering yields, Reflection coefficients, Retention ... etc
  - Interaction potential surfaces, Surface binding energies ... etc
- Data formats
  - Numbers, Images, Movies(?) ... etc
- Independent Variables
  - Surface temperatures, Ion energies, Angles, Surface morphologies, Fluences, Compositions, Exposure times, Plasma properties ... etc
- Input Variables for this research
  - Plasma spectroscopic analysis, Molecular reaction data... etc