Databases and Knowledge Base for Plasma-Matter Interaction for Fusion

H.-K. Chung and B. Braams

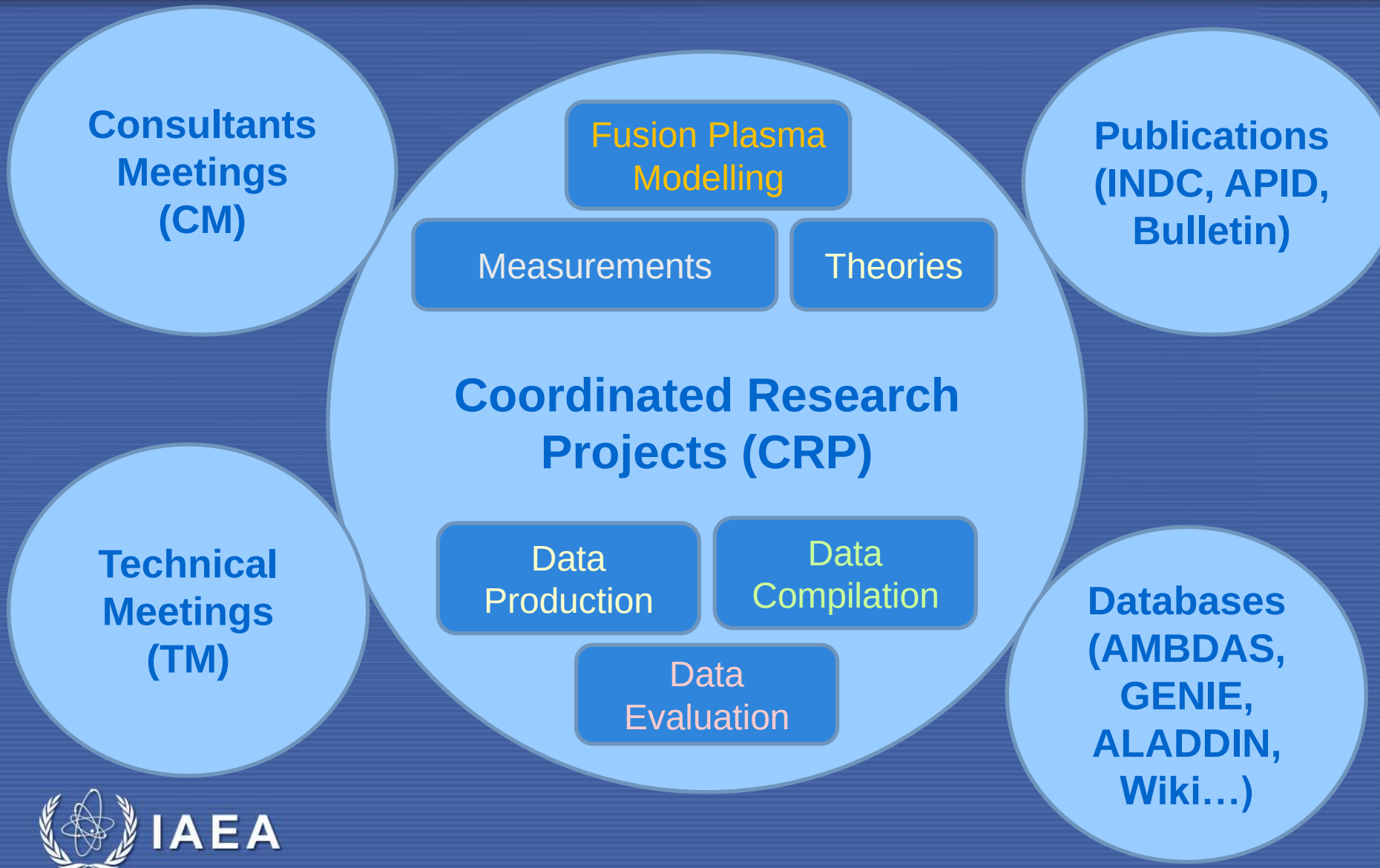
Atomic and Molecular Data Unit, Nuclear Data Section

26-28 September 2012

IAEA

International Atomic Energy Agency

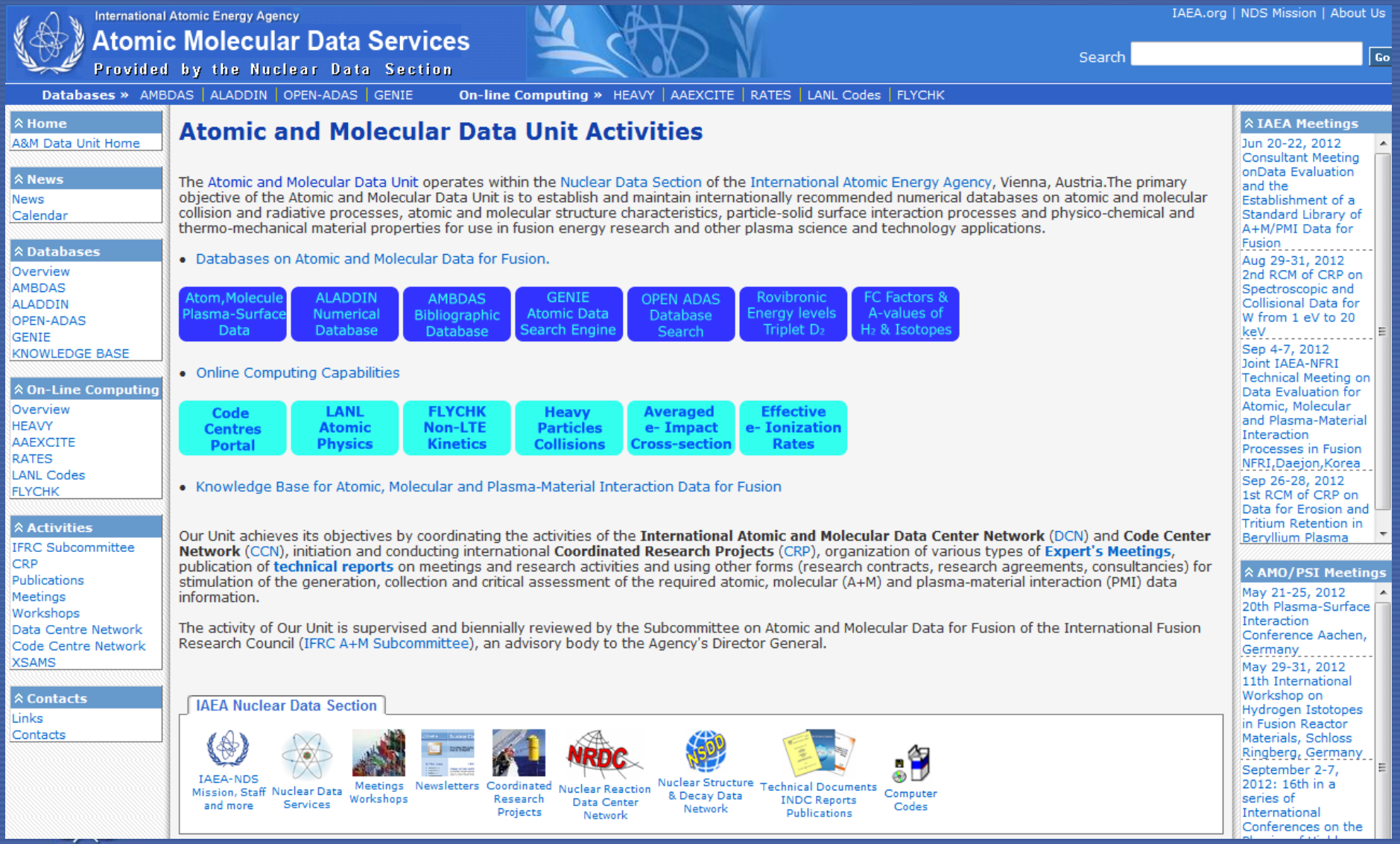
International Coordination of A+M/PSI Data Research for Fusion



IAEA

Online AM/PSI Data Services:

http://www-amdis.iaea.org



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

IAEA

Databases : ALADDIN

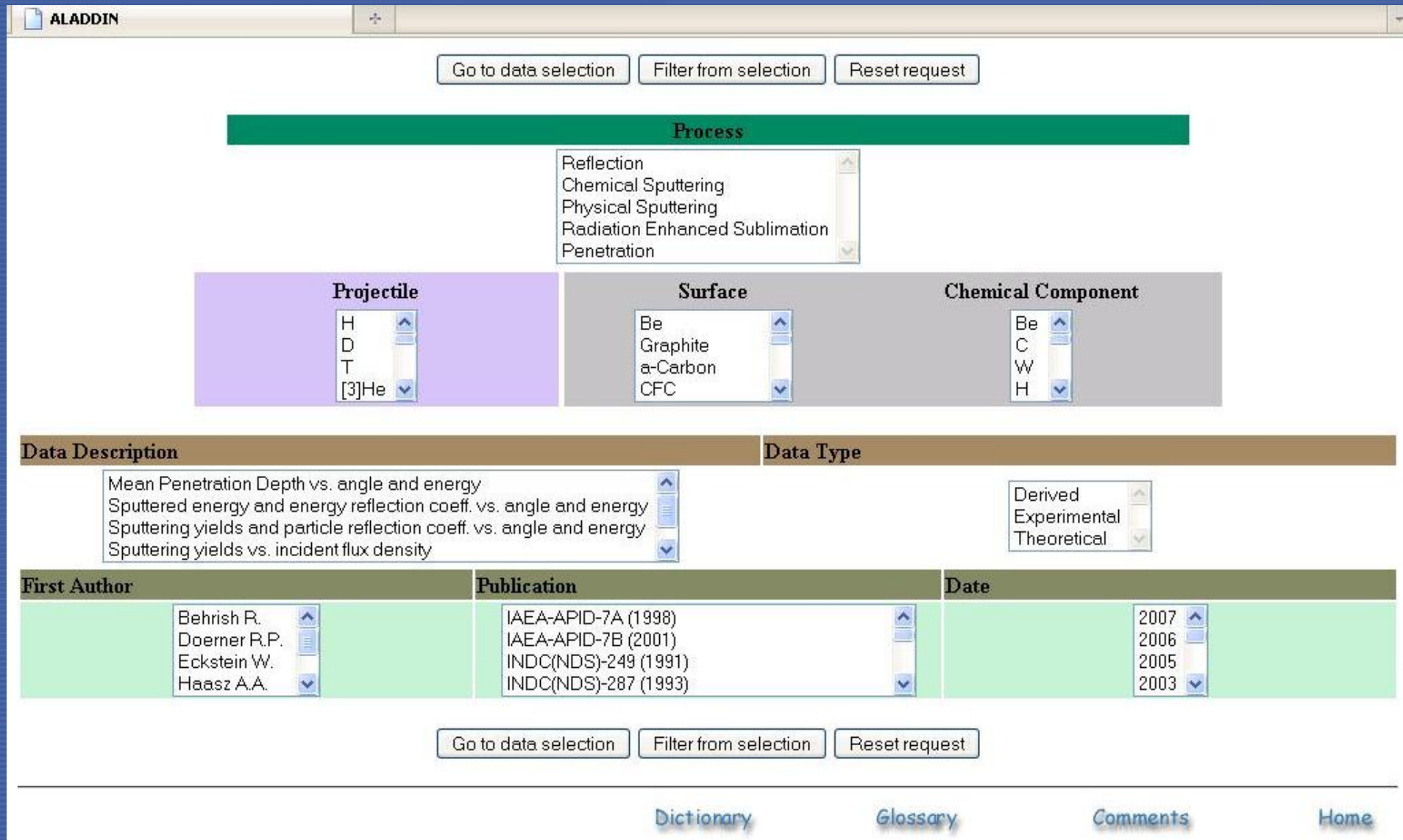
http://www-amdis.iaea.org/ALADDIN

- 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

IAEA

ALADDIN PSI Database

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



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

IAEA

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

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

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

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 (I^{52+}) and bare (I^{53+}) ions with different target materials.
   Phys. Rev. A **77**, 032901 (2007). doi: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

Experiment | 204-450 keV | Reactant Data

6. M. Reinelt, Ch. Linsmeier
   Temperature programmed desorption of 1 keV deuterium implanted into clean beryllium.
   Phys. Scr. T**128**, 111 (2007). doi: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

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

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

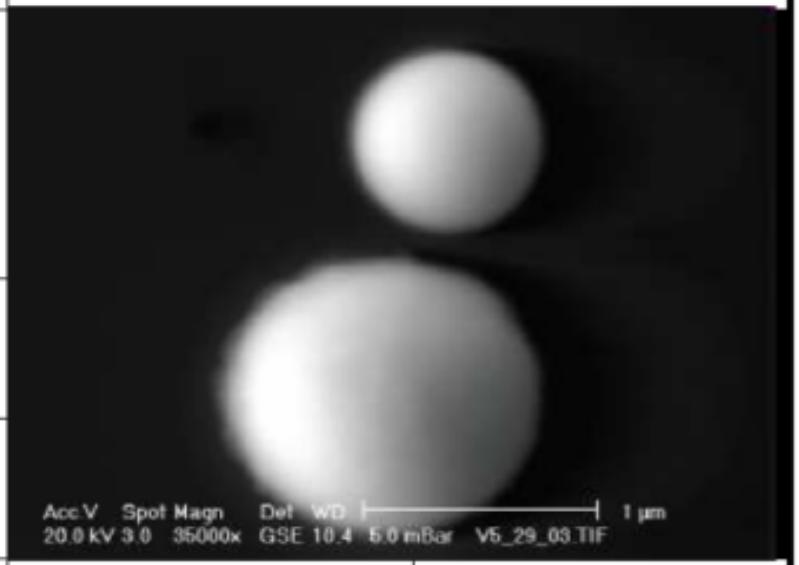
Query time: 0 sec

- A. I. Belyayeva
- O. Benka
- H. Bergsaker
- J. Bohdansky
- A. Bonanno
- V. N. Bondarenko
- M. Boustimi
- 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

Planned Databases : Dust particles

in collaboration with IPP-Garching

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		
Surface morphology e.g. smooth		
Element composition e.g. Dominant Element(s): W		
Identified Sources Arcs Melting	Impact on Safety WO_3 formation	Impact on Operation disruption

Databases for PMI Research

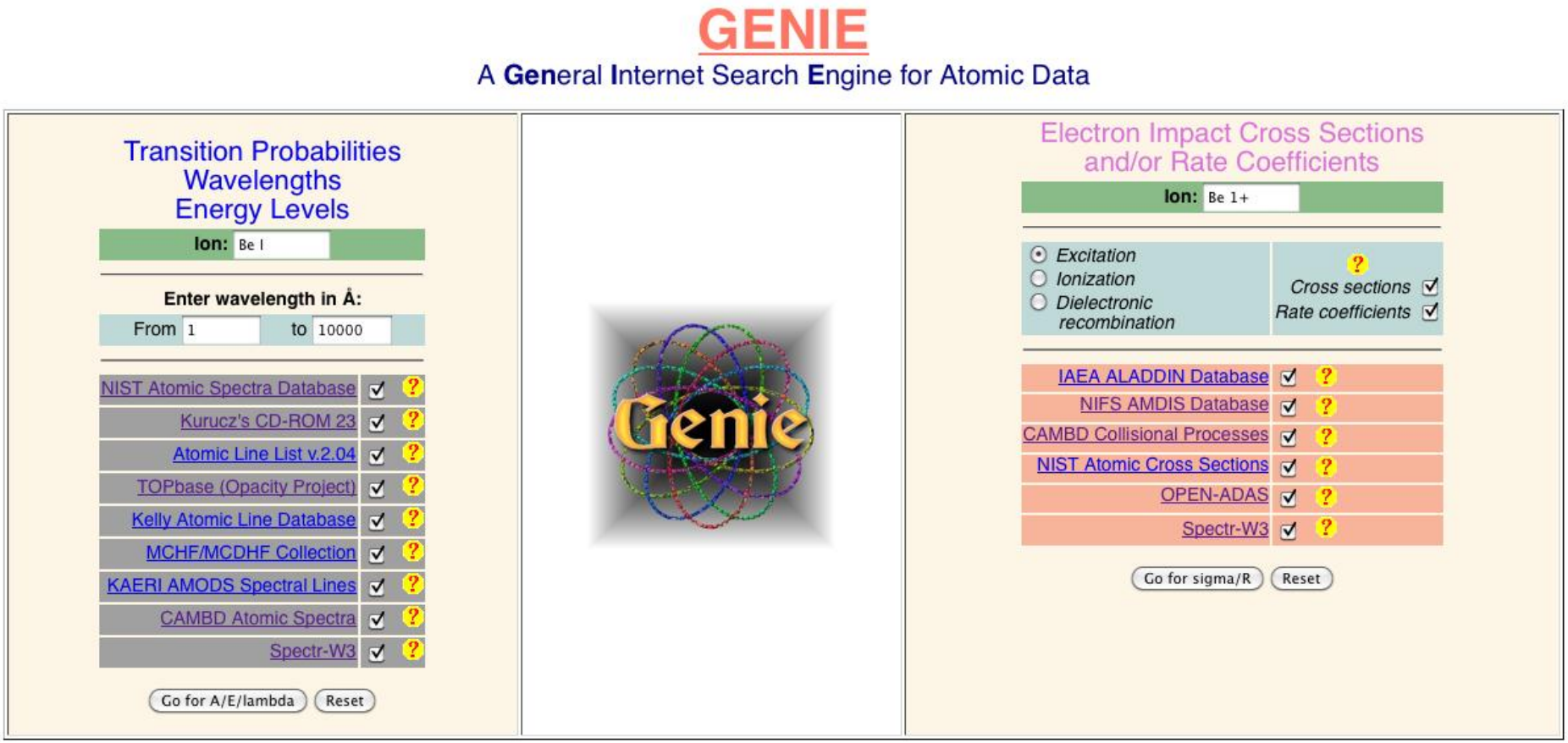
- Plasma-Surface Interaction Data
  - ALADDIN: Numerical Database
  - AMBDAS: Bibliographic database
  - Dust Particle Database
- Plasma Spectroscopic Analysis for PSI Data
  - ALADDIN: Atomic and Molecular Collisional Data
  - AMBDAS: Bibliographic database
  - GENIE: Atomic Structure, Transition Probabilities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

IAEA

Databases Search Engine: GENIE

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

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



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 eleme
Thermodynamic Equilibrium) conditions. The code is currently available at the **password-protected NIST website.** For more information on details, validity and li
FLYCHK information page .

Steady-State Charge State Distributions

Average charge states <Z> of atoms from Z=1 (Hydrogen) to Z=79 (Gold) are calculated by FLYCHK code and plotted over a wide range of plasma conditions. Th
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
information on <Z>, Charge State Distribution and Total Radiative Power Loss Rates of the element.

Rate Coefficients at Coronal Equilibirum for Plasma Modeling Applications

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

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
click here for limitations of FLYCHK results

1 H																	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
  - Plasma-Material Interaction Data
- Data Sources
  - Online Databases
  - Data Centers
  - Code Centers Network
- Data Exchange
  - 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

IAEA

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

IAEA