Forschungszentrum Jülich
Germany
25 – 27 November 2024

Atomic, Molecular and Plasma-Material Interaction Data Activities at the IAEA

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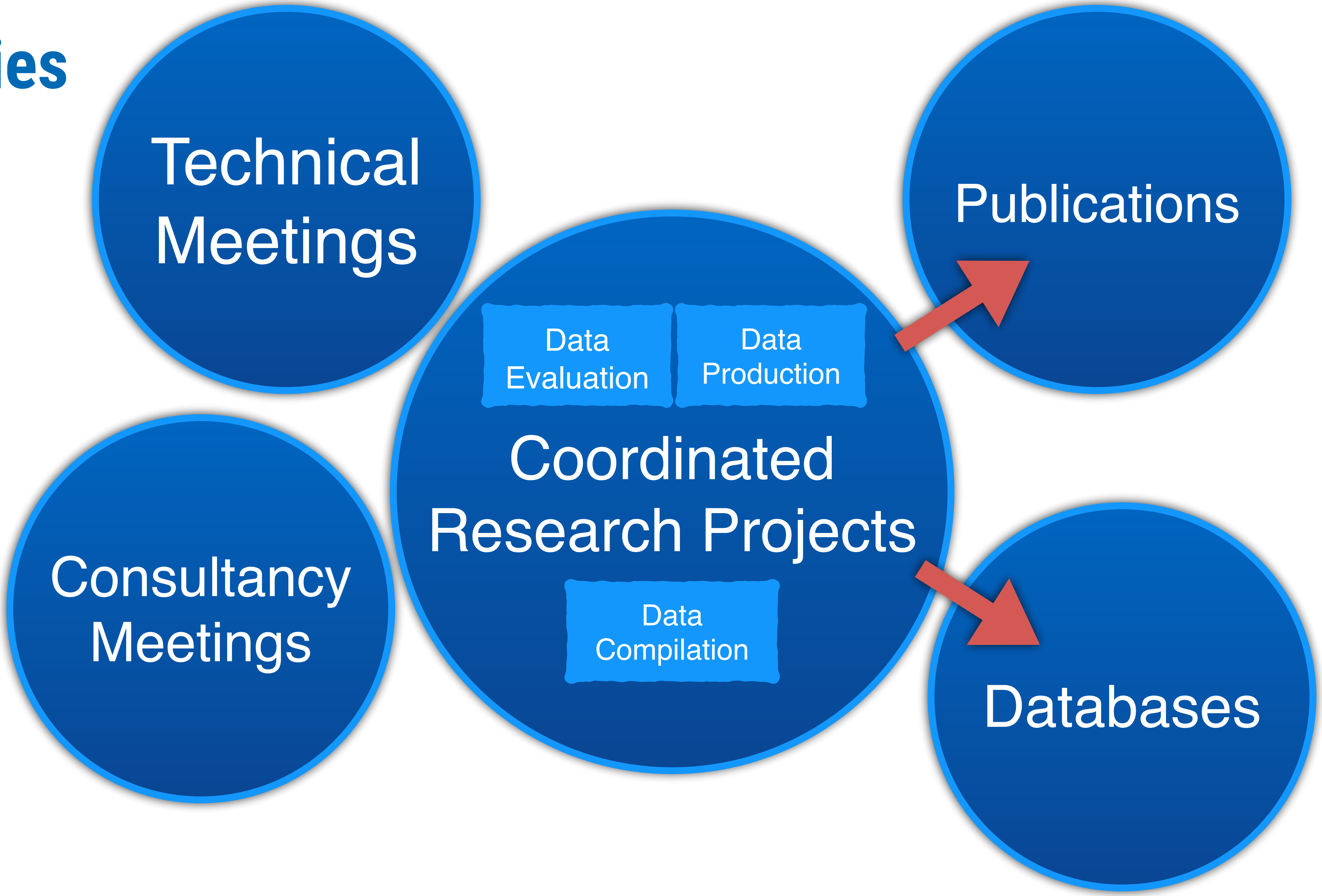
Atomic and Molecular Data Unit
International Atomic Energy Agency

Activities


Technical Meetings
Publications
Data Evaluation
Data Production
Coordinated Research Projects
Consultancy Meetings
Data Compilation
Databases

Coordinated Research Projects (CRPs)

Collaborative Research and Development: https://amdis.iaea.org/CRP/

- Focussed research programme to address a specific topic in fundamental data for fusion energy
- Usually 5 years in duration
- 10 – 20 participating institutions
- Research Agreements and Research Contracts
- Output data and report

Coordinated Research Projects (CRPs)

✓ Completed since 2014; ◉ ongoing and; ✦ planned

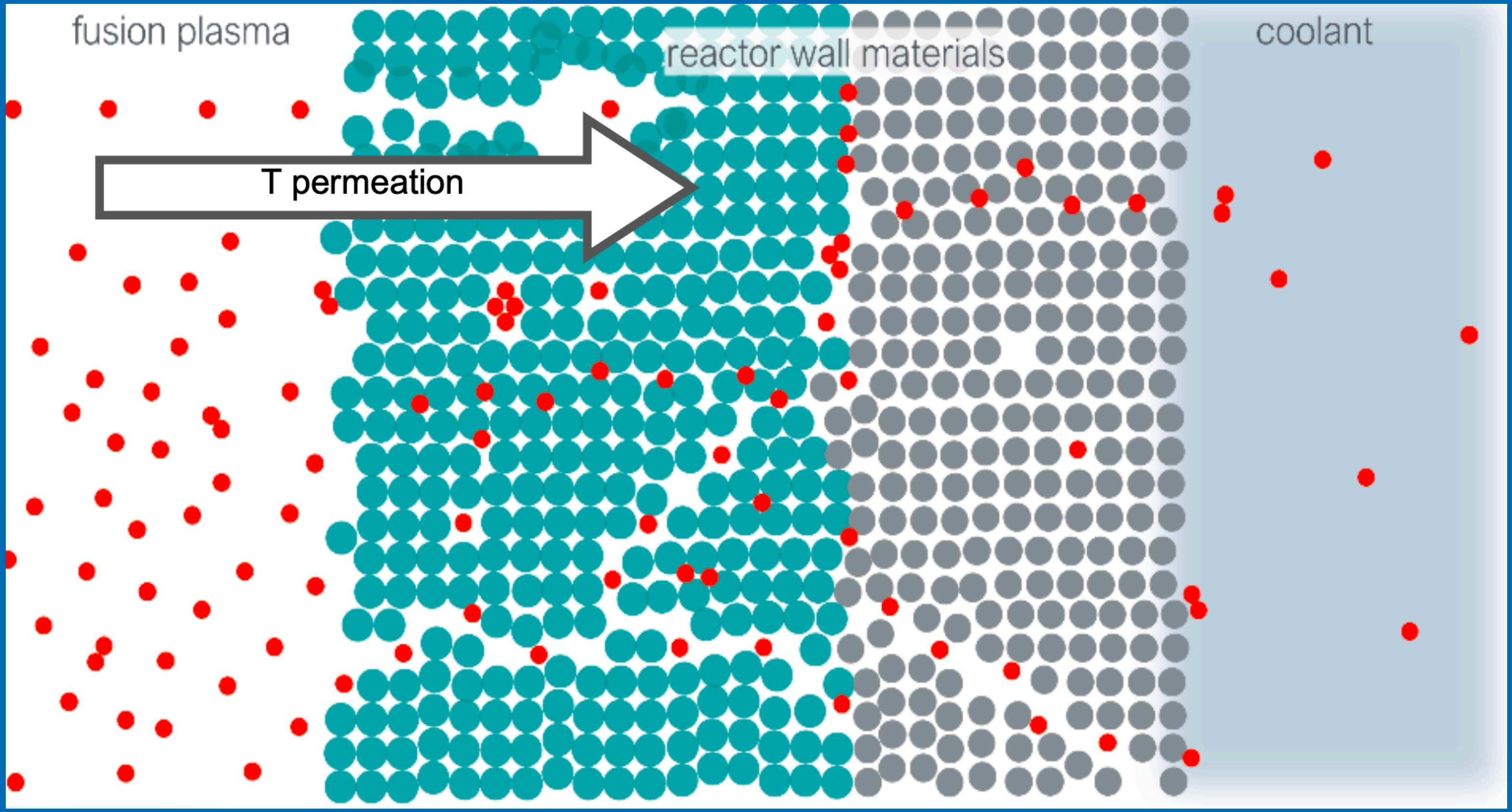
- ✓ Data for Erosion and Tritium Retention in Beryllium Plasma-Facing Materials (2011 – 2016)
- ✓ Atomic and Molecular Data for State-Resolved Modelling of Hydrogen and Helium and Their Isotopes in Fusion Plasma (2012 – 2016)
- ✓ Plasma-wall Interaction with Irradiated Tungsten and Tungsten Alloys in Fusion Devices (2013 – 2019)
- ✓ Plasma-wall Interaction with Reduced-activation Steel Surfaces in Fusion Devices (2015 – 2020)
- ✓ Data for Atomic Processes of Neutral Beams in Fusion Plasma (2017 – 2022)
- ✓ Atomic Data for Vapour Shielding in Fusion Devices (2019 – 2023)
- ◉ Hydrogen Permeation in Nuclear Materials (2020 –)
- ◉ Atomic Data for Injected Impurities in Fusion Plasmas (2023 –)
- ◉ The Formation and Properties of Molecules in Edge Plasmas (2023 –)
- ✦ Properties of Tungsten Ions in Fusion Plasmas (2025 –)

Hydrogen Permeation in Nuclear Materials

CRP, 2020 – present

To enhance the knowledge base and reduce uncertainties in data concerning the migration of hydrogen in materials in fusion reactors

- Divertor and main chamber: W, RAFM; joining materials: Cu, CuCrZr0.1
- Parameters affecting hydrogen permeation, trapping, retention and release
- Effect of neutron-induced damage
- Effect of surface chemistry



Hydrogen Permeation in Nuclear Materials

CRP, 2020 – present

- 20 Participants, 15 Member States
- 1st Research Coordination Meeting: Nov 2020
- Technical Meeting on *Nuclear Fusion Fuel Permeation in Reactor First Wall Components*: October 2021
- Technical Meeting on *Effects of Hydrogen Supersaturation and Defect Stabilization in Nuclear Fusion Materials*: April 2022
- 2nd Research Coordination Meeting: February 2023
- 3rd Research Coordination Meeting: December 2024

- Center for Energy Research, UCSD, United States of America
- Bhabha Atomic Research Centre, India
- National Research Nuclear University MEPhI, Russia
- SCK CEN, Belgium
- Shizuoka University, Japan
- Forschungszentrum Jülich (FZJ), Germany
- Department of Nuclear Engineering, University of Tennessee, United States of America
- Lanzhou Institute of Chemical Physics, Chinese Academy of Sciences, China
- Kyung Hee University, South Korea
- Institute of Plasma Physics, Chinese Academy of Sciences (ASIPP), China
- National Atomic Energy Commission, Argentina
- Centre d'Etudes Nucleaires de Cadarache, Association EURATOM-CEA, France
- Institute of Applied Physics, The National Academy of Sciences, Ukraine
- Jožef Stefan Institute, Slovenia
- Uppsala University, Sweden
- Physique des Interactions Ioniques et Moléculaires (PIIM), Aix-Marseille Université (AMU), France
- Beihang University, China
- Culham Centre for Fusion Energy, United Kingdom
- Department of Physics, University of Helsinki, Finland
- Max Planck Institute for Plasma Physics, Garching, Germany

Hydrogen Permeation in Nuclear Materials

CRP, 2020 – present

Round-Robin Subtasks

- Gas-Driven Permeation (GDP) for Fusion Materials
  - EUROFER97, 30 – 550 °C, 10 – 1000 mbar
  - CEA, FZJ, Kurchatov, ASIPP, CNEA, IPP Garching
- Thermal Desorption Spectroscopy (TDS)
  - 0.1 dpa self-damaged W
  - D-plasma exposure / D high-energy implantation / D_2 thermal exposure

Hydrogen Permeation in Nuclear Materials

CRP, 2020 – present

Round-Robin Subtasks

- Hydrogen in Neutron-irradiated Materials
  - Irradiation of W by SCK-CEN (Belgium) up to 1 dpa
  - Studies on permeation and defect-evolution
  - Analysis by GDP, PDP, TDS, PAS, NRA
  - Participants: INL, MEPhI, UKAEA, U. Helsinki
  - First campaign (2017 – 2019)
  - Second campaign (2022 –) to include W, CuCrZr, Mo, Fe, steels

Atomic Data for Injected Impurities in Fusion Plasmas

CRP, 2023 – present

Scope

- Species, in order of priority:
  - Ar, N, Ne (all ionization states)
  - Kr, Xe (ionization states present for $T_i > 500$ eV)
  - Li, B

Processes

- Charge Exchange (HCX) with H^0
- Electron Impact Excitation (EEX)
- Dielectronic Recombination (ERD) for Ar and Ne (state resolved)
- Spectra (line strengths and wavelengths)
- Collisions with He^{2+} for energies > 100 keV.

Atomic Data for Injected Impurities in Fusion Plasmas

CRP, 2023 – present

9 Participants, 8 Member States

- Institute of Plasma Physics, Chinese Academy of Sciences (ASIPP), China
- Faculty of Science and Engineering, Curtin University, Australia
- Vilnius University, Lithuania
- Indian Institute of Technology, Roorkee, India
- National Center of Nuclear Sciences and Technologies (CNSTN), Tunisia
- Laboratoire de Chimie Physique – Matière et Rayonnement (LCPMR), Sorbonne Université, France
- Instituto de Física del Sur (IFISUR), Universidad Nacional del Sur (UNS), Argentina
- Institute for Nuclear Research (ATOMKI), Hungary
- Institute of Modern Physics, Chinese Academy of Sciences (IMPCAS), China

Atomic Data for Injected Impurities in Fusion Plasmas

CRP, 2023 – present

- Theory (data production)
  - Interactions of C, N, O, Ne, Ar, W with H, D, T, He and H_2 (and isotopologues) [Curtin]
  - Ar^{q+}, N^{q+} and Ne^{q+} spectra (quasi-relativistic HF) [Vilnius]
- Experiment (data production)
  - State-resolved single electron capture cross sections between He and H_2 (~H) and Ar^{q+}, N^{q+} and Ne^{q+} ; Dielectronic recombination rates for Ar^{q+} [IMPCAS]
- Evaluation of data
  - Comparison with LHD and EBIT spectra [NIFS]
  - Radiative Divertor experiments with Ar/D_2 and Ne/D_2 seeding at EAST [ASIPP]

The Formation and Properties of Molecules in Edge Plasmas

CRP, 2023 – present

Scope

- Species, in order of priority:
  - H_2, BH, BeH, BeH^+ (and isotopologues)
  - LiH
  - OH and water-derived species
  - WH

Processes

- Molecular Assisted Recombination / Ionization / Dissociation (H_2)
- Spectra (esp. OH, BH)
- Dissociative attachment, mutual neutralization, ion conversion, dissociative recombination (for H_2)
- Electron impact excitation, ionization and dissociation

The Formation and Properties of Molecules in Edge Plasmas

CRP, 2023 – present

10 Participants, 8 Member States

- Scottish Church College, India
- University College London, United Kingdom
- Stockholm University, Sweden
- Faculty of Science and Engineering, Curtin University, Australia
- American University of Beirut, Lebanon
- Politehnica University of Timișoara, Romania
- National Institute for Fusion Science, Japan
- Culham Centre for Fusion Energy, United Kingdom
- Université le Havre Normandie, France
- Forschungszentrum Jülich (FZJ), Germany

The Formation and Properties of Molecules in Edge Plasmas

CRP, 2023 – present

Processes relating to Molecular Hydrogen in the detached divertor plasma

- Molecular Assisted Recombination: contribution to plasma volume recombination and hence reduced ion particle flux:
    1. $H_2(v) + e^- \rightarrow H^- + H$ (dissociative attachment)

       $H^- + H^+ \rightarrow H + H$ (mutual neutralization)
    2. $H_2(v) + H^+ \rightarrow H_2^+ + H$ (ion conversion)

       $H_2^+ + e^- \rightarrow H + H$ and $H_2^+ + H_2 \rightarrow H_3^+ + H$ (dissociative recombination)
- Molecular Assisted Ionization

  $H_2^+ + e^- \rightarrow H^+ + H^+ + 2\,e^-$
- Molecular Assisted Dissociation

  $H_2^+ + e^- \rightarrow H + H^+ + e^-$ and $H_2^+ + e^- \rightarrow H + H$

The Formation and Properties of Molecules in Edge Plasmas

CRP, 2023 – present

Boron Hydrides

- Boronization to harden the first wall and act as an oxygen getter is necessary for non-Beryllium metal surfaces
- Expect BHn from desorbed B–H bonds on the surface to enter the edge plasma and dissociate.
- BH spectroscopy can be a good diagnostic for real time monitoring of the deposition and desorption processes near the wall surface, as CH molecular spectroscopy is in carbon machines

Properties of Tungsten Ions in Fusion Plasmas

CRP, 2025 – present

To address data needs in the area of the ionization balance and spectroscopic and collisional properties of tungsten at temperatures between 1 keV and 10 keV

- Ionisation from metastable states of low ionisation stages of W
- Neutral and proton collisions with low ionisation stages of W
- Spectroscopic analysis of low and medium ionisation stages of W

https://amdis.iaea.org/CRP/tungsten-ions

First Research Coordination Meeting expected March 2025.

Networks

Collaborative Research and Development

- Data Centres Network (DCN): https://amdis.iaea.org/DCN/
  - Data standards, priorities, database infrastructure, data dissemination
- Global Network for the Atomic and Molecular Physics of Plasmas (GNAMPP): https://amdis.iaea.org/GNAMPP/
  - Data evaluation and comparison, experimental validation of calculated data, research collaboration and knowledge-exchange
- Code Centres Network (CCN): https://amdis.iaea.org/CCN/
  - Modelling and calculation of data for fusion energy applications; simulations of radiation damage in nuclear materials

Databases

https://amdis.iaea.org/databases/

- Bibliographic Data
- Plasma Collisional Processes
- Radiation Damage in Materials
- Institutions, Events, External Databases

AMBDAS: Atomic and Molecular Bibliographic Data System

AMBDAS: Legacy interface

ALADDIN: Numerical database of evaluated collisional cross sections and plasma-material interaction data

CollisionDB: Numerical database of collisional data

CascadesDB: Database of Molecular Dynamics simulations of collision cascades in materials of relevant to fusion research

DefectDB: Database of DFT calculations of radiation-induced defects in nuclear-relevant materials

Clerval: Database of institutions, people and events related to atomic and molecular data

Databases

https://amdis.iaea.org/databases/

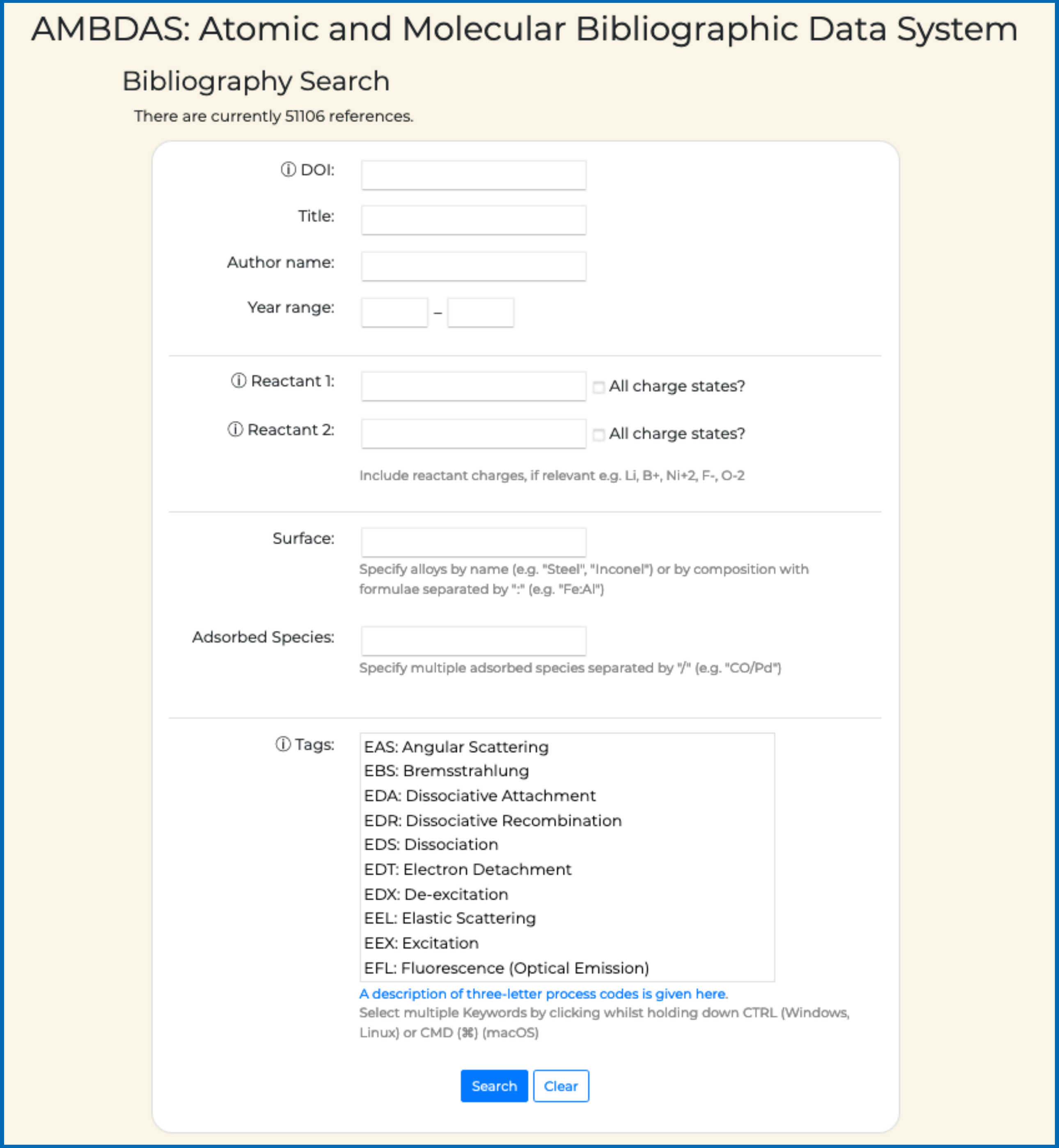
Data Standards and Tools

- Plasma collisional processes classification
  https://amdis.iaea.org/databases/processes/
- Molecular state quantum numbers:
  https://amdis.iaea.org/cbc/
- Atomic and Molecular species and states standards and parser
  PyValem: https://github.com/xnx/pyvalem
- Bibliographic management and integration tools
  PyRef: https://github.com/xnx/django-pyref
- Atomic and molecular process database framework
  Django-Valem: Bibliographic management and integration tools
  https://github.com/xnx/django-valem

AMBDAS

https://amdis.iaea.org/db/ambdas

- 52397 classified and described records
- Populated by cooperation with:
  - Korea Institute of Fusion Energy
  - NIST (Alexander Kramida)
  - Consultancies
- Search by:
  - DOI
  - Title
  - Author name
  - Year range
  - Reactants, surfaces, adsorbed species
  - Tags (process classification)



AMBDAS

https://amdis.iaea.org/db/ambdas

- Records:
  - Citation
  - DOI
  - Tags (process classification)
  - Species
  - Theory / Experiment
  - Energy range
- Records:
  - XSAMS (XML)
  - JSON

10 Results

Export as: XSAMS JSON

B6924: D. S Belkic, R. K Janev, "Electron capture from hydrogen and helium atoms by fast alpha particles ", *Journal of Physics B: Atomic and Molecular Physics* **6**, 1020-1027 (1973). [10.1088/0022-3700/6/6/016]
HCX: Charge Transfer HEX: Excitation | H He He^{2+}
Theory | E = 0.1 - 10.0 MeV | details

B12580: T. P Grozdanov, R. K Janev, "Two-electron capture in slow ion-atom collisions ", *Journal of Physics B: Atomic and Molecular Physics* **13**, 3431-3442 (1980). [10.1088/0022-3700/13/17/021]
HCX: Charge Transfer | C^{2+} He He^{2+}
Theory | E = 2.5 - 22.5 eV | details

B14044: M. R C Mcdowell, R. K Janev, "Electron capture, ionisation and transfer-ionisation in fast Au^{q+}+He collisions ", *Journal of Physics B: Atomic and Molecular Physics* **17**, 2295-2305 (1984). [10.1088/0022-3700/17/11/022]
HCX: Charge Transfer HIN: Ionization | Au^{10+} Au^{11+} Au^{12+} Au^{13+} Au^{14+} Au^{15+} Au^{16+} Au^{17+} Au^{18+} Au^{19+} ...
Theory | E = 0.079999998 - 1.1799999 MeV | details

B15660: T. Grozdanov, R. Janev, L. Presnyakov, D. Uskov, "n-changing collisions of Rydberg atoms with ground-state atoms ", *Physics Letters A* **109**, 93-96 (1985). [10.1016/0375-9601(85)90263-4]
HDX: De-excitation HEX: Excitation | Ar H He Kr Ne Xe
Theory | details

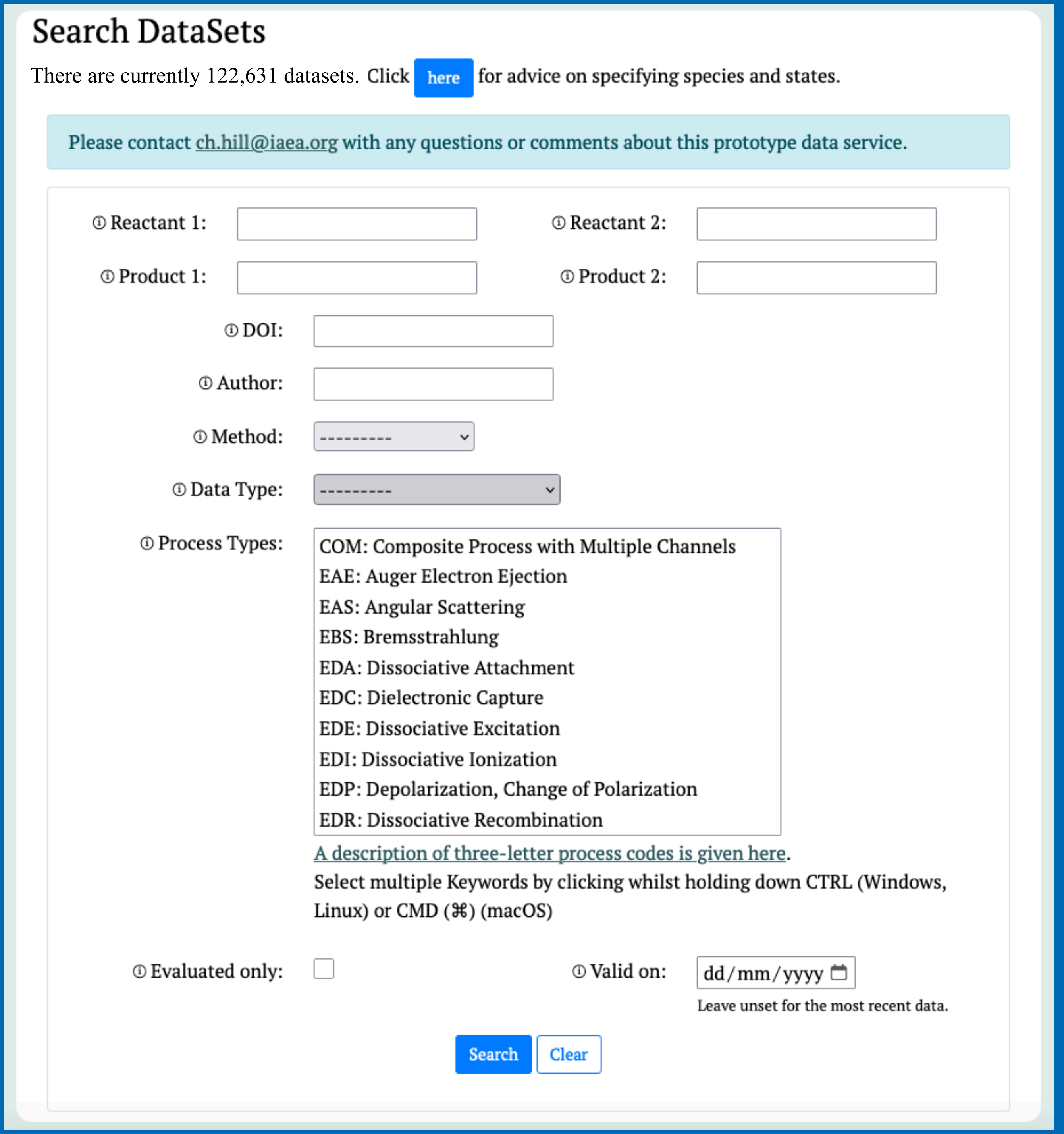
B18734: J. Vukanić, R. Janev, "Small-angle scattering of ions from random targets in the screened coulomb region ", *Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms* **16**, 22-32 (1986). [10.1016/0168-583x(86)90222-3]
MRF: Reflection | ^{2}H H^{+} He | Ni Cu
Theory | E = 5.0 keV | details

CollisionDB

https://amdis.iaea.org/db/collisiondb

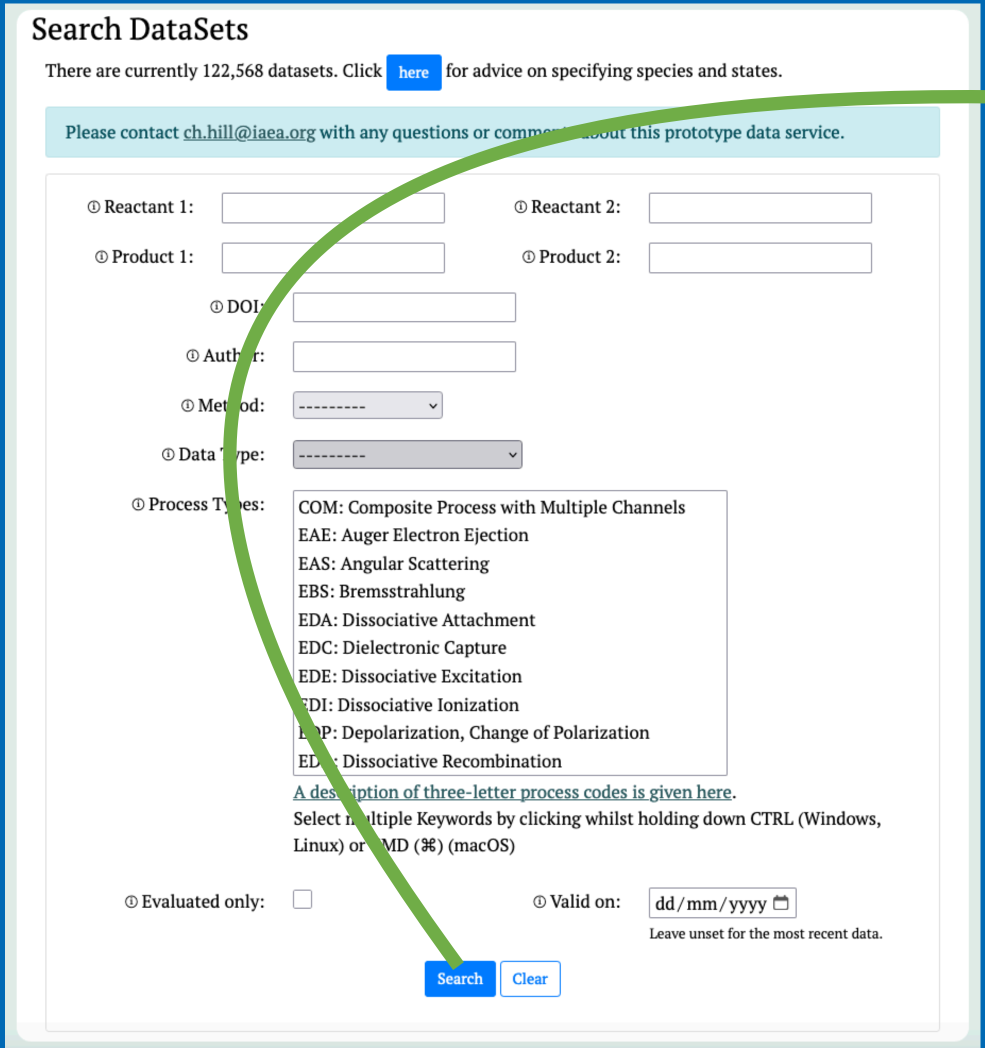
Plasma collisional processes: cross sections and rate coefficients

- 122631 datasets
- Validation
- Unit standardization
- Canonicalize reaction
- DOI resolution
- Numerical checks
- Physics checks
- Provenance preservation
- API and Python library, PyCollisionDB



CollisionDB

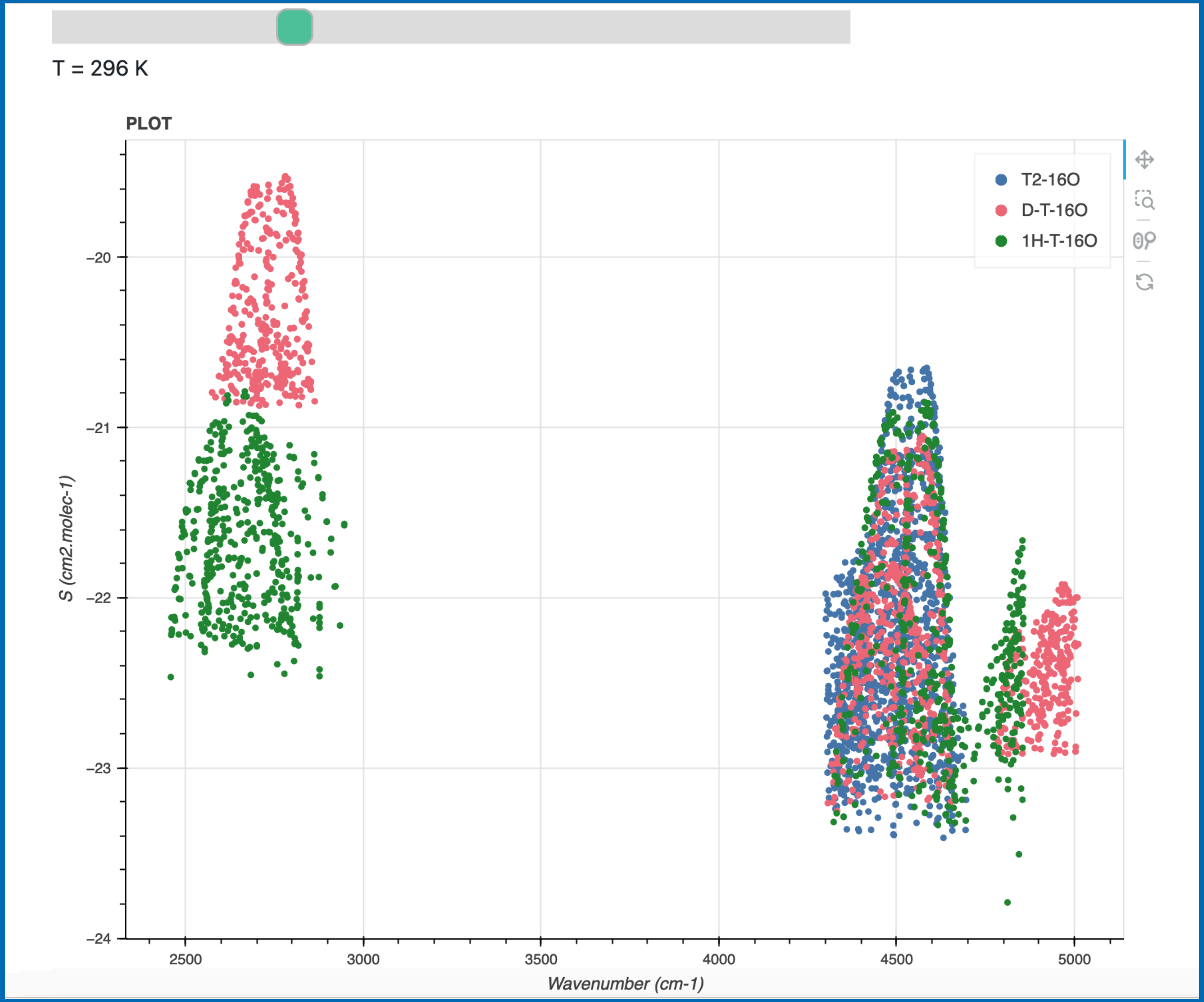
https://amdis.iaea.org/db/collisiondb



C. Hill, Dipti, K. Heinola, M. Haničinec, "CollisionDB: A new database of atomic and molecular collisional processes with an interactive API", *Atoms* **12**(4), 20 (2024).

stmDB: Spectra of Tritiated Molecules

https://db-amdis.org/stmdb

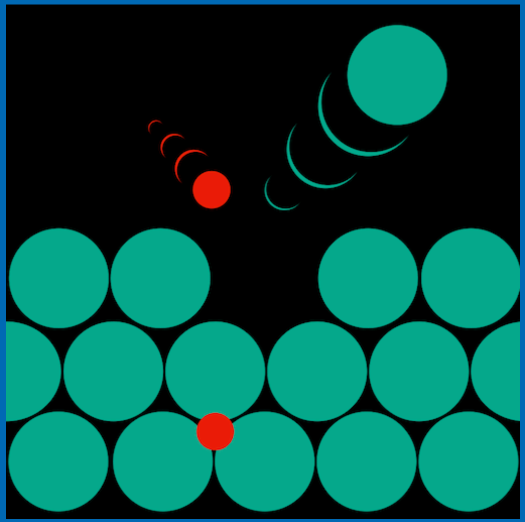


pwiDB: Plasma-wall interaction database

https://db-amdis.org/pwidb

A database of plasma-surface and plasma-(bulk) material interaction data for fusion energy research applications.Hydrogen in Neutron-irradiated Materials

- Sputtering
- Retention
- Reflection



- Diffusivity
- Solubility (Sieverts constants)
- Permeation

pwiDB: Plasma-wall interaction database

https://db-amdis.org/pwidb

Search Plasma-Surface Interaction Data

We have 25 PSI datasets available.

Process: ---------

Particle-surface interaction process

Species / Particle: D, D2, H, T

Surface: Li, LiOD, LiOH, Li2O

DOI:

DOI with or without https://doi.org/ prefix

Author:

Filter Reset

Search Plasma-Material Interaction Data

We have 365 PMI datasets available.

Process: ---------

Particle-material interaction process

Species / Particle: D, H, T

Material: Ag, Al, Al2O3, Al2O3-Er2O3

Alloy: 1.4914SS, 14YWT-SM13, 316L, 316L(N)-IG

DOI:

DOI with or without https://doi.org/ prefix

Author:

Method: ---------

Scaled? Unknown

Filter Reset

pwiDB: Plasma-wall interaction database

https://db-amdis.org/pwidb

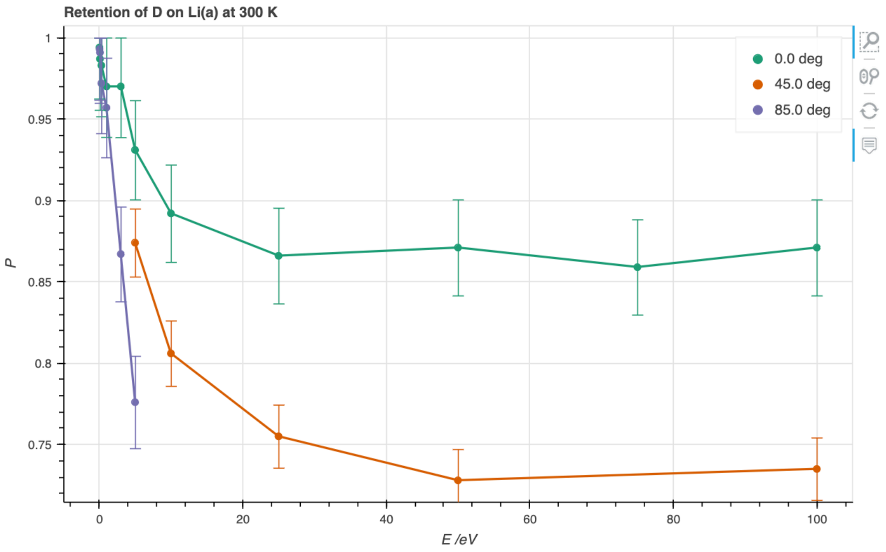
e.g. “Retention of D on amorphous Lithium”

Plasma-Surface Interaction Data Set 85

Retention of D on Li(a) at 300 K

1. B1: P. Krstic, E. Ostrowski, F. Domínguez-Gutierrez, S. Abe, B. Koel, "Sputtering and reflection processes from amorphous lithium surfaces by low-energy impacts of H and D atoms and D_2 molecules ", *Journal of Nuclear Materials* **568**, 153848 (2022). [10.1016/j.jnucmat.2022.153848]
2. B2: P. S. Krstic, S. Abe, E. Schiltz-Rouse, E. T. Ostrowski, B. E. Koel, "Energy, angle, and temperature dependencies of the sticking of D atoms on Li surfaces ", *Journal of Applied Physics* **131** (2022). [10.1063/5.0096816]

$P(E)$ $P(\theta)$



$P(E)$ $P(\theta)$

Retention of D on Li(a) at 300 K

angle = 0.0 deg	**E /eV**	**P**	**unc**
	0.025	0.994	0.0315
	0.1	0.987	0.0314
	0.3	0.983	0.0314
	1.0	0.97	0.0311
	3.0	0.97	0.0312
	5.0	0.931	0.0305
	10.0	0.892	0.0299
	25.0	0.866	0.0294
	50.0	0.871	0.0295
	75.0	0.859	0.0293
	100.0	0.871	0.0295

pwiDB: Plasma-wall interaction database

https://db-amdis.org/pwidb

e.g. "Diffusion of H in Steel (all alloys)"

Plasma-Material Interaction Data Set 176

Diffusivity of H in Steel

Download JSON

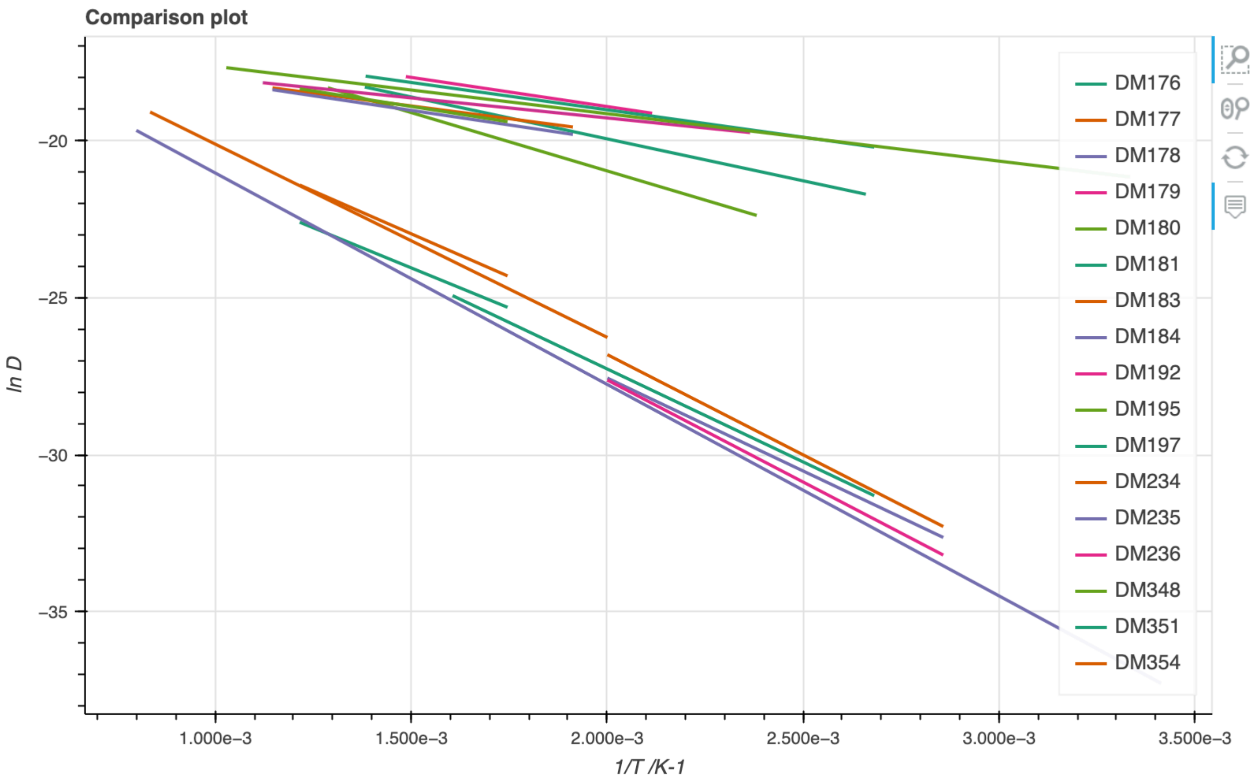
$$D = D_0 \exp\left(-\frac{E_\mathrm{d}}{k_\mathrm{B}T}\right)$$

[In the above formula, the Boltzmann constant is expressed in $\mathrm{eV\,K^{-1}}$.]

- Material: Steel
- Alloy: SS316L
- Method: Experiment
- Data scaled for isotope mass? No

- D_0 = 7.66e-08 $\mathrm{m^2\,s^{-1}}$
- E_d = 0.44 eV
- T = 573 – 823 K

1. B73: K. Forcey, D. Ross, J. Simpson, D. Evans, "Hydrogen transport and solubility in 316L and 1.4914 steels for fusion reactor applications ", *Journal of Nuclear Materials* **160**, 117-124 (1988). [10.1016/0022-3115(88)90038-4]



17 Matching Data Sets

ID	Process	Species	Material / Alloy
DM176	Diffusivity	H	Steel / SS316L
DM177	Diffusivity	H	Steel / 316SS
DM178	Diffusivity	H	Steel / SS316L

pwiDB: Plasma-wall interaction database

https://db-amdis.org/pwidb

e.g. "Diffusion of H in Steel (all alloys)"

Plasma-Material Interaction Data Set 176

Diffusivity of H in Steel

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```
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qualified_id: "DM176"
process: "Diffusivity"
process_types:
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    description: "Diffusion"
method: "Experiment"
scaled: false
material: "Steel"
species:
  qualified_id: "F3"
  text: "H"
  charge: 0
comment: "Heat treated 316L SS, Pressure dependence of permeability: ~P^0.5 for 316L. Data provided by M. Lavrentiev (UKAEA, 2024) with permission from STEP."
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  0:
    qualified_id: "B73"
    authors: "K. Forcey, D. Ross, J. Simpson, D. Evans"
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    journal: "Journal of Nuclear Materials"
    volume: "160"
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    page_end: "124"
    year: 1988
    doi: "10.1016/0022-3115(88)90038-4"
    bibcode: "1988JNuM..160..117F"
    url: "https://dx.doi.org/10.1016/0022-3115(88)90038-4"
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  Ed:
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    units: "eV"
  Trange:
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    1: 823
```

Workshops at the Abdus Salam International Centre for Theoretical Physics (ICTP)

Residential Courses of 1 – 2 weeks at the ICTP in Trieste, Italy:
https://amdis.iaea.org/workshops/

- 2025: Joint IAEA-ICTP-MAMBA School on Materials Irradiation: from Basics to Applications
- 2024: Data for Modelling Atomic and Molecular Processes in Plasmas
- 2021: Atomistic Modelling of Radiation Damage in Nuclear Systems
- 2021: Atomic Processes in Plasmas: Data-Driven Research
- 2019: Atomic and Molecular Spectroscopy in Plasmas

Questions

- How can data needs be communicated, discussed and prioritised?
- What format are data required?
- How are the data incorporated in codes?
- Is there a need for API access to major databases?
- What about tools for converting between formats?
- What can be done to encourage standardisation in the description of AM & PMI species, states and processes?
- How important is our bibliographic database, AMBDAS?
- How widely-used is ALADDIN in comparison with CollisionDB

IAEA