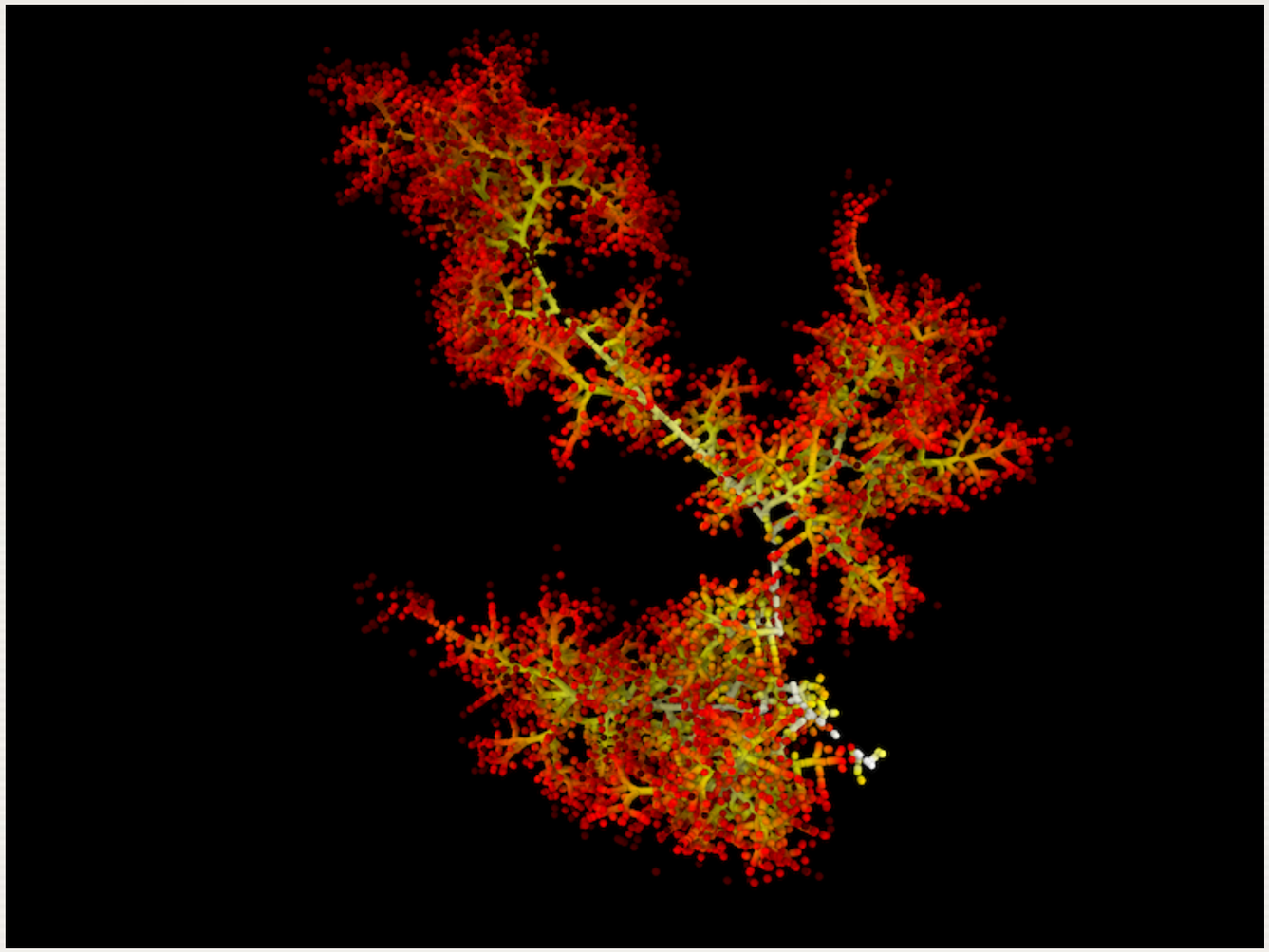
AMD Unit Database Developments

CascadesDB



https://cascadesdb.iaea.org/

IAEA

AMD Unit Database Developments

CascadesDB

Objectives

A database of molecular dynamics simulations of collision cascade simulations for the analysis and prediction of radiation damage in materials for fusion and fission applications.

Current Statistics

- 815 GB of data in 14398 simulations in 294 archives.
- Materials: W, Fe, Cu, Au, Ag, Ni, Pd, Pt
- 16 interatomic potentials represented
- 7 contributors from 5 Member States

IAEA

AMD Unit Database Developments

CascadesDB

[Online Interface: https://cascadesdb.org/cdbmeta/](https://cascadesdb.org/cdbmeta/)

CascadesDB Home Browse Search About

Search

Author name: Setyawan

Publication DOI:

Material chemical formula: W

e.g. W, Fe

500 ≤ Initial temperature /K ≤ Tmax K

50 ≤ Projectile / PKA energy /keV ≤ 100

Archive name:

Search

Results

Attribution	Material	PKA energy /keV	Initial T /K	Simulation time /ps	Number of simulations	Metadata	Data	Source
Wahyu SETYAWAN	W (bcc)	50.0	1025.0	30.0	15	html | xml | txt | json	R025 (188.1 MB)	link | bibtex
Wahyu SETYAWAN	W (bcc)	60.0	1025.0	30.0	10	html | xml | txt | json	R026 (118.6 MB)	link | bibtex
Wahyu SETYAWAN	W (bcc)	75.0	1025.0	30.0	15	html | xml | txt | json	R027 (362.2 MB)	link | bibtex

IAEA

AMD Unit Database Developments

CascadesDB

Metadata Formats

- **HTML**
- XML
- TXT
- JSON

CDB Record R027

Attribution A6

Contributor

Wahyu SETYAWAN, Pacific Northwest National Laboratory (PNNL)

Publication

Publication DOI: 10.1016/j.jnucmat.2014.12.056

Acknowledgements

This research has been partially supported by the U.S. Department of Energy, Office of Science, Office of Fusion Energy Sciences (#DE-AC06-76RL0-1830), and partially supported by the U.S. Department of Energy, Office of Science, Office of Fusion Energy Sciences and Office of Advanced Scientific Computing Research through the Scientific Discovery through Advanced Computing (SciDAC) Project on Plasma-Surface Interactions, under Award No. DE-SC0008875. Computations were performed on Olympus cluster at Pacific Northwest National Laboratory (Fusion account).

Material

Formula: **W**

Structure: **bcc**

$a = 3.183630$ Å, $b = 3.183630$ Å, $c = 3.183630$ Å.
$\alpha = 90.000000°$, $\beta = 90.000000°$, $\gamma = 90.000000°$.

Simulation includes surface? **false**

Initially perfect crystal configuration? **true**

IAEA

AMD Unit Database Developments

CascadesDB

Metadata Formats

- HTML
- **XML**
- TXT
- JSON


```
−<cdbml version="1.0">
  −<cdbrecord id="R025">
    −<attribution id="A6">
       <name>Wahyu SETYAWAN</name>
       <affiliation>Pacific Northwest National Laboratory (PNNL)</affiliation>
       <doi>10.1016/j.jnucmat.2014.12.056</doi>
      −<acknowledgements>
          This research has been partially supported by the U.S. Department of Energy, Office of Science, Office of Fusion
          Energy Sciences (#DE-AC06-76RL0-1830), and partially supported by the U.S. Department of Energy, Office of
          Science, Office of Fusion Energy Sciences and Office of Advanced Scientific Computing Research through the
          Scientific Discovery through Advanced Computing (SciDAC) Project on Plasma-Surface Interactions, under Award
          No. DE-SC0008875. Computations were performed on Olympus cluster at Pacific Northwest National Laboratory
          (Fusion account).
       </acknowledgements>
    </attribution>
   −<material>
       <formula>W</formula>
       <structure>bcc</structure>
      −<lattice_parameters>
          <a units="Å">3.183660</a>
          <b units="Å">3.183660</b>
          <c units="Å">3.183660</c>
          <alpha units="deg">90.000000</alpha>
          <beta units="deg">90.000000</beta>
          <gamma units="deg">90.000000</gamma>
       </lattice_parameters>
    </material>
    <has_surface>false</has_surface>
    <initially_perfect>true</initially_perfect>
    <PKA_atomic_number>74</PKA_atomic_number>
  −<PKA>
       <energy units="keV">50.000000</energy>
       <recoil>true</recoil>
    </PKA>
    <electronic_stopping>false</electronic_stopping>
    <thermostat>true</thermostat>
  −<thermostat_comment>
       Initial thermalization: NPT 30 ps Cascade: NVE for the first 10 ps, followed by NVT (whole system); see publication
    </thermostat_comment>
    <input_filename>therm.in cascade.in</input_filename>
    <simulation_time units="ps">30.000</simulation_time>
    <initial_temperature units="K">1025.00</initial_temperature>
  −<simulation_box>
       <box_X_length units="Å">254.6930</box_X_length>
       <box_Y_length units="Å">254.6930</box_Y_length>
```


IAEA

AMD Unit Database Developments

CascadesDB

Metadata Formats

- HTML
- XML
- **TXT**
- JSON

```
CDB Record R025
================

Attribution A6
================

Contributor: Wahyu SETYAWAN, Pacific Northwest National Laboratory (PNNL)
Publication DOI: https://doi.org/10.1016/j.jnucmat.2014.12.056

Acknowledgements
----------------
This research has been partially supported by the U.S. Department of Energy, Office of Science, Office of

Material
========
Formula: W
Structure: bcc
Lattice Parameters:
    a = 3.183660Å,
    b = 3.183660Å,
    c = 3.183660Å,
    α = 90.000000°,
    β = 90.000000°,
    γ = 90.000000°.
Simulation includes surface? false
Initially perfect crystal configuration? true

PKA
===
PKA atomic number: 74
PKA energy: 50.000000keV
PKA by recoil? true

Simulation Details
==================
Electronic stopping included? false
Electronic stopping comments:
Thermostat? true
Thermostat comments: Initial thermalization: NPT 30 ps Cascade: NVE for the first 10 ps, followed by NVT
Input filename: therm.in cascade.in
Simulation time: 30.000ps
Initial temperature: 1025.00K
Box dimensions (Å): 254.6930, 254.6930, 254.6930
Box orientation: 100, 010, 001
Interatomic potential URI: https://cascadesdb.org/potential/3
Interatomic potential filename: W_Juslin2010_AT_mod.eam.fs
Interatomic potential comment:
Interatomic potential doi: 10.1016/j.jnucmat.2012.07.023
Code: LAMMPS Version: 5Mar12

Data
====
Data archive name: 025-T1025K_50keV_data.tar.gz
```

IAEA

AMD Unit Database Developments

CascadesDB

Metadata Formats

- HTML
- XML
- TXT
- **JSON**


```
qid:                    "R025"
attribution:
  qid:                  "A6"
  contact:
    qid:                "C4"
    name:               "Wahyu SETYAWAN"
    institution:
      qid:              "I4"
      name:             "Pacific Northwest National Laboratory (PNNL)"
      country:          "United States of America"
    email:              "wahyu.setyawan@pnnl.gov"
  source_doi:           "10.1016/j.jnucmat.2014.12.056"
  source_url:           "http://dx.doi.org/10.1016/j.jnucmat.2014.12.056"
  acknowledgements:     "This research has been partially supported by the U.S. Department of Energy, Office of Science,
                        Office of Fusion Energy Sciences (#DE-AC06-76RL0-1830), and partially supported by the U.S.
                        Department of Energy, Office of Science, Office of Fusion Energy Sciences and Office of Advanced
                        Scientific Computing Research through the Scientific Discovery through Advanced Computing (SciDAC)
                        Project on Plasma-Surface Interactions, under Award No. DE-SC0008875. Computations were performed
                        on Olympus cluster at Pacific Northwest National Laboratory (Fusion account)."
material:
  chemical-formula:     "W"
  structure:            "bcc"
  lattice-parameters:
    a:                  3.18366
    b:                  3.18366
    c:                  3.18366
    alpha:              90
    beta:               90
    gamma:              90
potential:
  filename:             "W_Juslin2010_AT_mod.eam.fs"
  source-doi:           "10.1016/j.jnucmat.2012.07.023"
  uri:                  "https://cascadesdb.org/potential/3"
has-surface:            false
initially-perfect:      true
PKA-atomic-number:      74
PKA-energy:             50
recoil:                 true
electronic-stopping:    false
thermostat:             true
thermostat-comment:     "Initial thermalization: NPT 30 ps Cascade: NVE for the first 10 ps, followed by NVT (whole
                        system); see publication"
input-filename:         "therm.in cascade.in"
```


IAEA

AMD Unit Database Developments

CascadesDB

Software Developments

- Implementation of **Csaransh** (https://github.com/haptork/csaransh): a software suite developed by the Bhabha Atomic Research Centre (BARC) to post-process, explore, validate and visualize Molecular Dynamics simulations of collision cascades: Home-based Consultancy by Utkarsh Bhardwaj, BARC.
  - Defect statistics
  - Defect locations, classification, clustering
  - Comparisons between cascade simulations
  - Subcascade identification

https://cascadesdb.org/csaransh

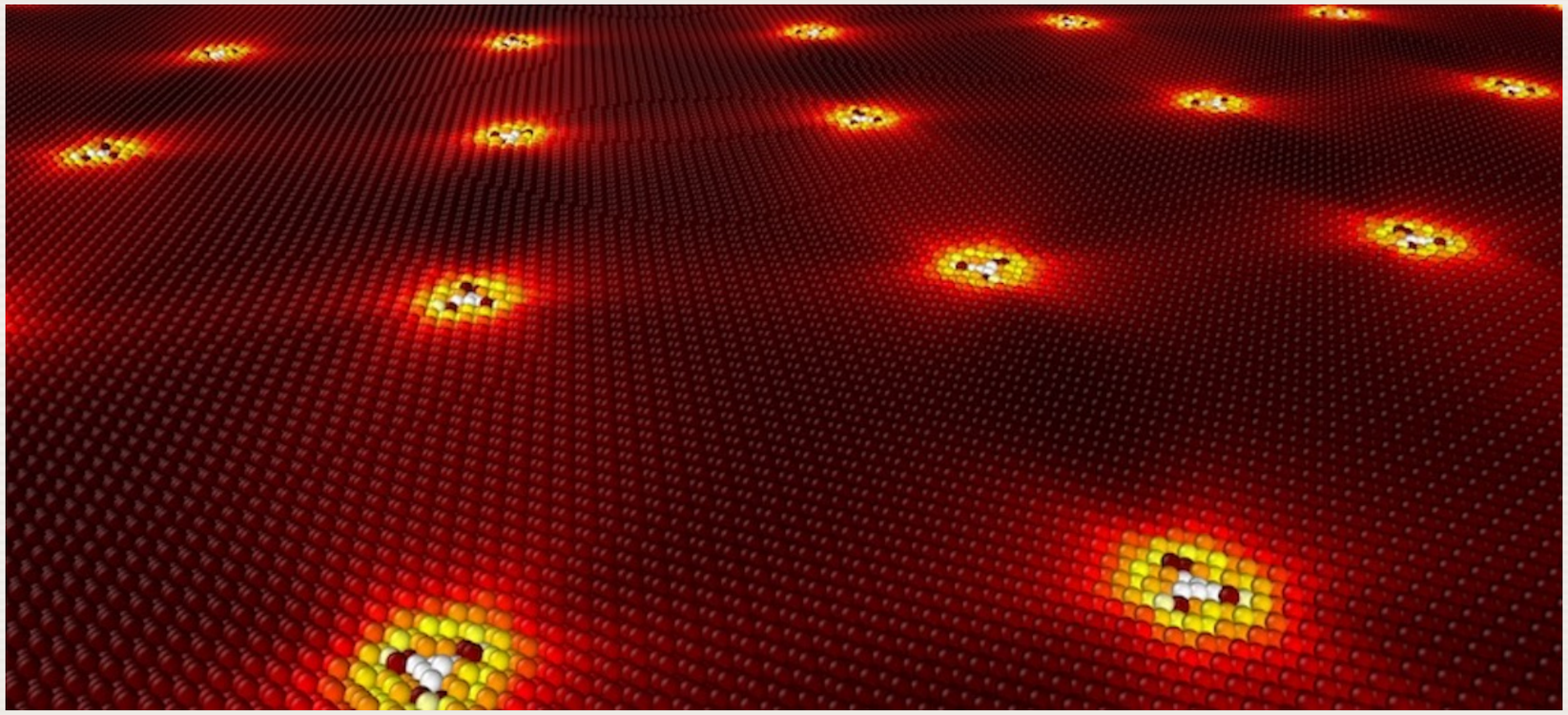
IAEA

AMD Unit Database Developments

DefectDB

Objectives

A database of DFT calculations of radiation-induced defect structures in materials of interest to nuclear fusion and fission applications. Developed in collaboration with CEA Paris-Saclay (C. Mărinică and A. Goryaeva).

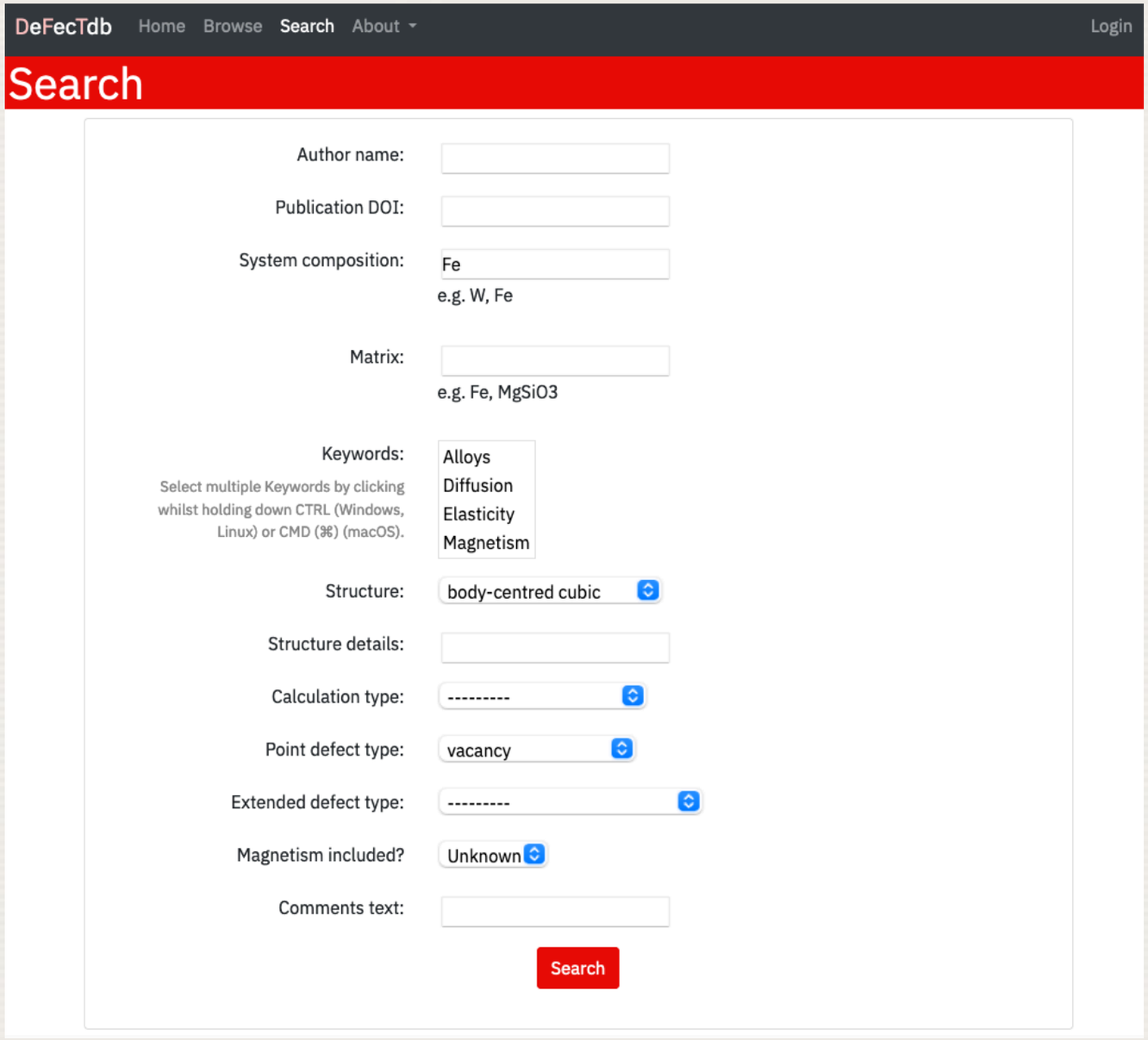


IAEA

AMD Unit Database Developments

DefectDB

[Online Interface (development): https://db-amdis.org/defectdb/](https://db-amdis.org/defectdb/)



IAEA

AMD Unit Database Developments

DefectDB

Online Interface (development): https://db-amdis.org/defectdb/

14 Results

ID	Contact	Code	Composition	Matrix	Structure	Defects
▼ | D88	Alexandra GORYAEVA	VASP	Fe_126	Fe	bcc	V(Fe),
▼ | D89	Alexandra GORYAEVA	VASP	Fe_126	Fe	bcc	V(Fe),
▼ | D115	Alexandra GORYAEVA	VASP	Fe_127	Fe	bcc	V(Fe),
▼ | D121	Alexandra GORYAEVA	VASP	Fe_127	Fe	bcc	V(Fe),
▼ | D122	Alexandra GORYAEVA	VASP	Fe_126	Fe	bcc	V(Fe),
▼ | D78	Julien DÈRES	VASP	Fe_127 C_1	Fe	bcc	V(Fe), S_S(Fe→C),
▼ | D79	Julien DÈRES	VASP	Fe_127 C_3	Fe	bcc	V(Fe), S_I(C),
▼ | D80	Julien DÈRES	VASP	Fe_127 C_4	Fe	bcc	V(Fe), S_I(C),
▼ | D81	Julien DÈRES	VASP	Fe_127	Fe	bcc	V(Fe),
▼ | D82	Julien DÈRES	VASP	Fe_127 C_1	Fe	bcc	V(Fe), S_S(Fe→C),

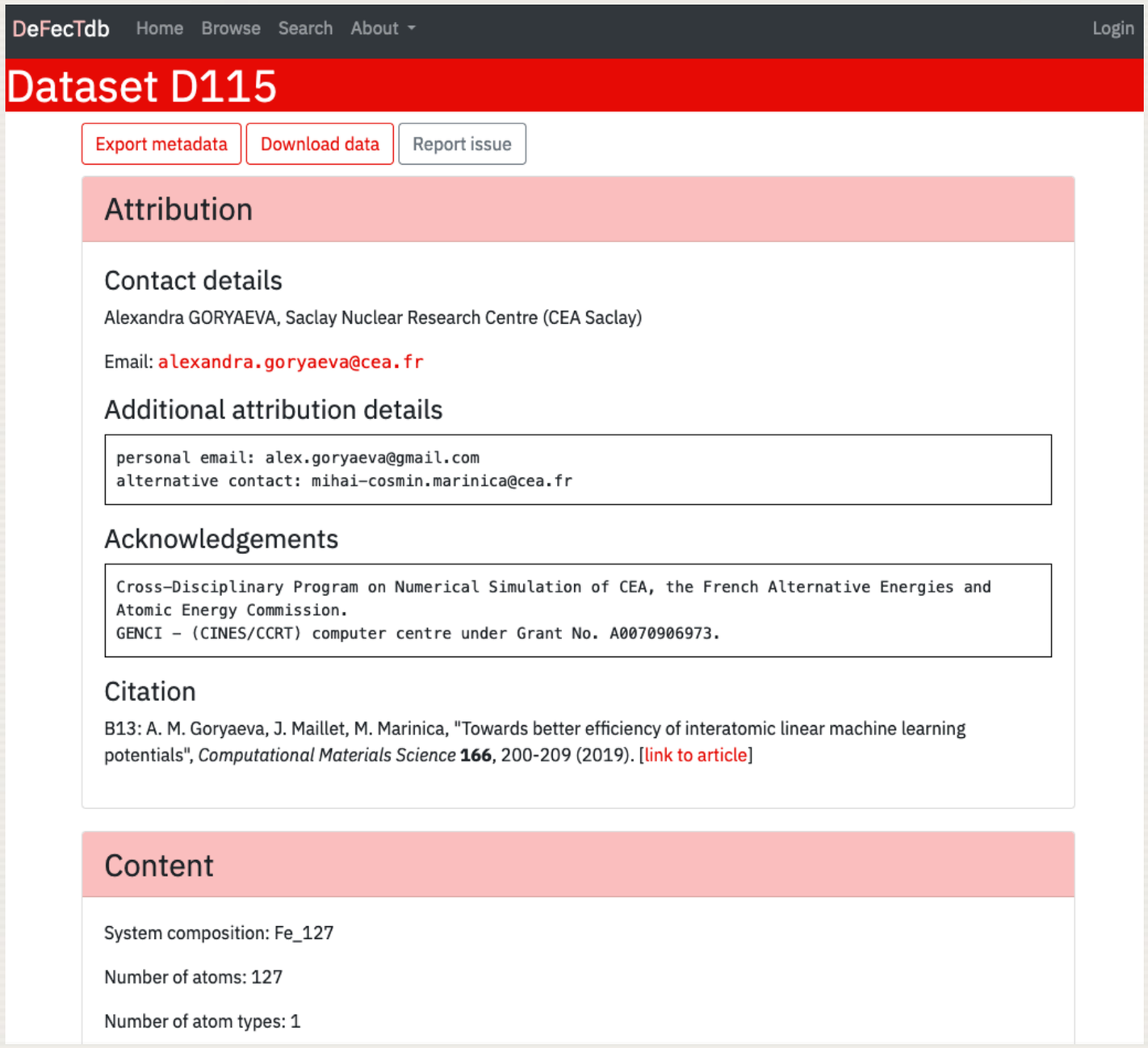
« Previous 1 2 Next »

IAEA

AMD Unit Database Developments

DefectDB

Online Interface (development): https://db-amdis.org/defectdb/



IAEA

AMD Unit Database Developments

DefectDB

[Online Interface (development): https://db-amdis.org/defectdb/](https://db-amdis.org/defectdb/)


```
qid:                                "D115"
attribution:
  qid:                              "A35"
  contact:
    qid:                            "P2"
    name:                           "Alexandra GORYAEVA"
    institution:
      qid:                          "I1"
      name:                         "Saclay Nuclear Research Centre (CEA Saclay)"
      country:                      "France"
    email:                          "alexandra.goryaeva@cea.fr"
  source_doi:                       "10.1016/j.commatsci.2019.04.043"
  source_url:                       "https://dx.doi.org/10.1016/j.commatsci.2019.04.043"
  general-comments:                 "personal email: alex.goryaeva@gmail.com\r\nalternative contact: mihai-cosmin.marinica@cea.fr"
  acknowledgements:                 "Cross-Disciplinary Program on Numerical Simulation of CEA, the French Alternative Energies and Atomic Energy Commission.
                                     \r\nGENCI - (CINES/CCRT) computer centre under Grant No. A0070906973."
content:
  system-composition:               "Fe_127"
  matrix:                           "Fe"
  structure:                        "bcc"
  content-comment:                  "The uploaded configuration is accompanied by INCAR and OUTCAR"
  point-defects:
    0:
      defect-type:                  "vacancy"
      number:                       1
      matrix-atom:                  "Fe"
calculation:
  calculation-type:                 "relax"
  code:
    name:                           "VASP"
    version:                        "5.4.1"
  exchange-correlation:             "GGA"
  exchange-correlation-comment:     "PBE"
  kpoints:                          "5 5 5 0.5 0.5 0.5"
  Ecut:                             400
  smearing-type:                    "Methfessel-Paxton"
  smearing-energy:                  0.25
  pseudopotential:
    name:                           "PAW_PBE Fe_pv"
    class:                          "paw"
    semicore:                       true
  convergence-criterion:            1e-7
  magnetism-included:               true
  calculation-comment:              "The uploaded configuration is accompanied by INCAR and OUTCAR"
url:                                "https://db-amdis.org/defectdb/data/agoryaeva/Fe_monovacancy_a0_2.833068.tar.gz"
```


JSON metadata

DeFecTdb Home Browse Search About Login

Dataset D115

Export metadata | Download data | Report issue

Attribution

Contact details

Alexandra GORYAEVA, Saclay Nuclear Research Centre (CEA Saclay)

Email: alexandra.goryaeva@cea.fr

Additional attribution details

```
personal email: alex.goryaeva@gmail.com
alternative contact: mihai-cosmin.marinica@cea.fr
```

Acknowledgements

```
Cross-Disciplinary Program on Numerical Simulation of CEA, the French Alternative Energies and
Atomic Energy Commission.
GENCI - (CINES/CCRT) computer centre under Grant No. A0070906973.
```

Citation

B13: A. M. Goryaeva, J. Maillet, M. Marinica, "Towards better efficiency of interatomic linear machine learning potentials", *Computational Materials Science* **166**, 200-209 (2019). [link to article]

Content

System composition: Fe_127

Number of atoms: 127

Number of atom types: 1

AMD Unit Database Developments

DefectDB

Future Developments

- Data **upload** functionality: JSON metadata -> Database records, as for CascadesDB
- More data: from CEA and (esp.) EDF – Home-based consultancy pending
- Migration to official IAEA domain (defectdb.iaea.org?)

AMD Unit Database Developments

AMBDAS

Atomic and Molecular Bibliographic Data System

- Old interface: https://www-amdis.iaea.org/AMBDAS/
- New interface: https://amdis.iaea.org/db/ambdas
- 51106 classified and described records
- Adoption of new plasma process classifications: https://amdis.iaea.org/databases/processes: v2.1, December 2020, following Technical Meeting in November 2019 (https://amdis.iaea.org/meetings/software-tools/)
- Development of new admin tools to improve reference management (DOI → database record):
  - F. M. Skinner, I. E. Gordon, C. Hill, R. J. Hargreaves, K. E. Lockhart, L. S. Rothman, “Referencing Sources of Molecular Spectroscopic Data in the Era of Data Science: Application to the HITRAN and AMBDAS Databases”, *Atoms* **8**(2), 16 (2020)
- Population of database in cooperation with Korea Institute of Fusion Energy (KFE) through Practical Arrangements, and NIST (Alexander Kramida).

IAEA

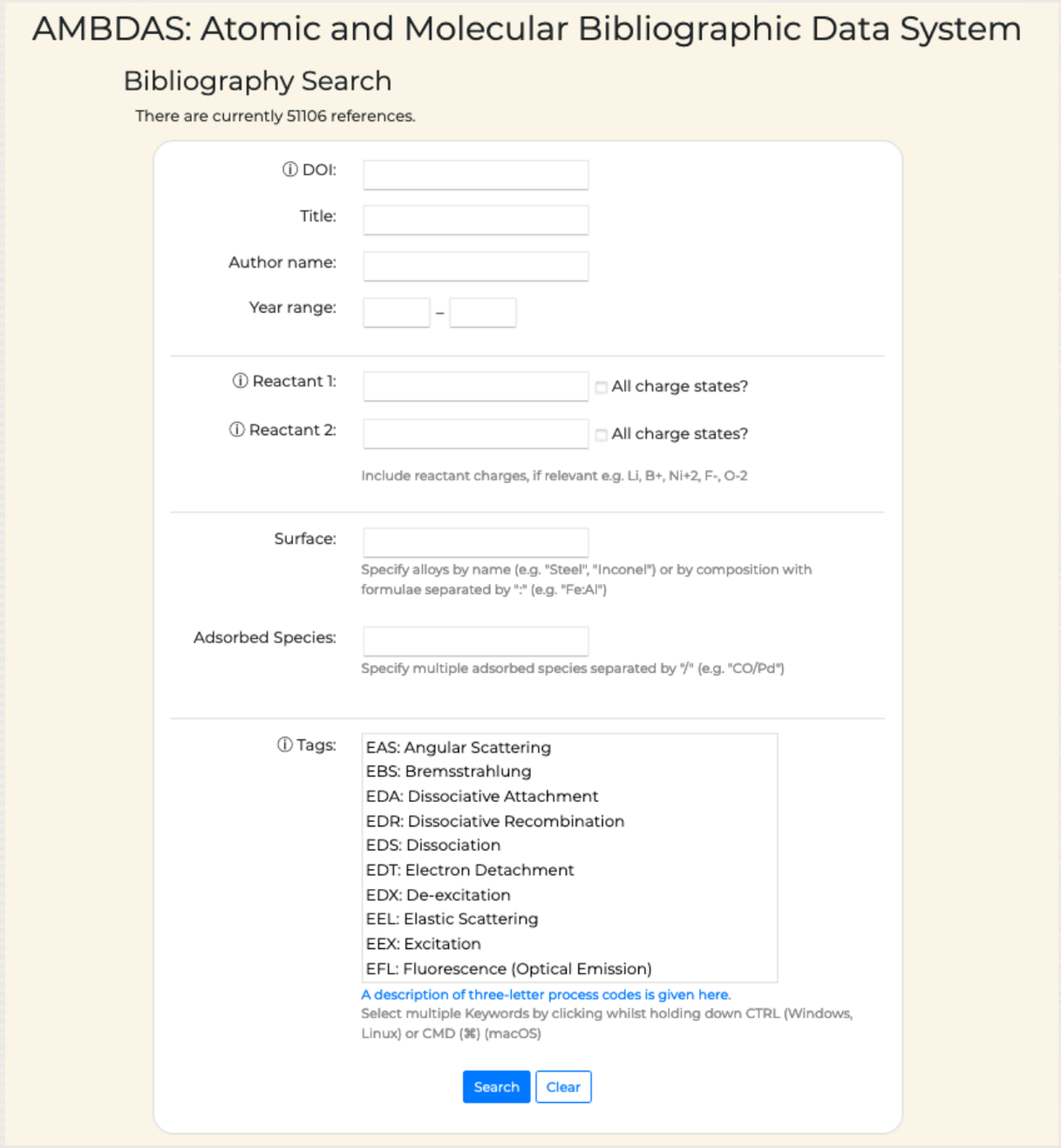
AMD Unit Database Developments

AMBDAS

[Atomic and Molecular Bibliographic Data System]

Search by:

- DOI
- Title
- Author name
- Year range
- Reactants, surfaces, adsorbed species
- Tags (process classification)



IAEA

AMD Unit Database Developments

AMBDAS

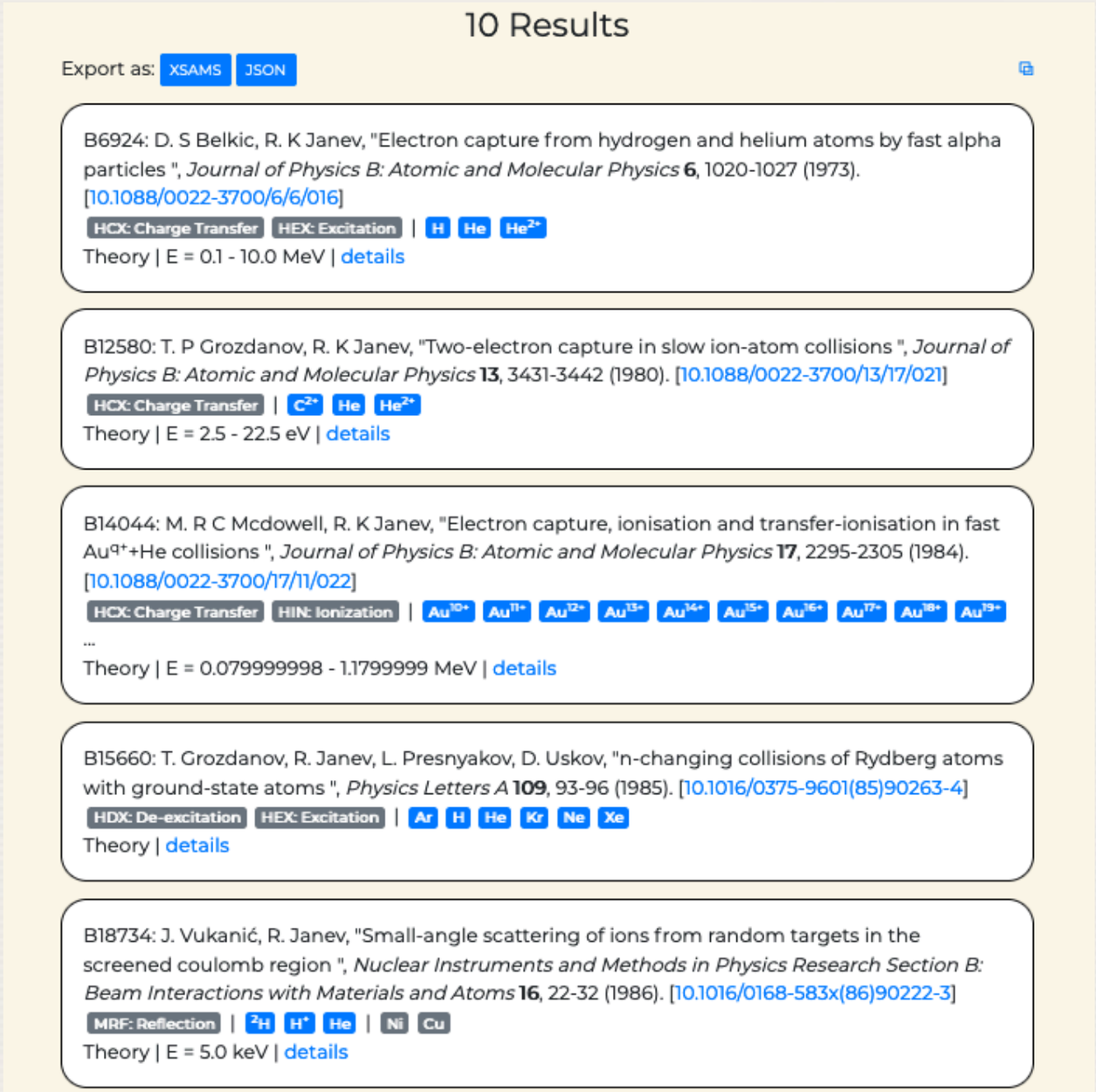
Atomic and Molecular Bibliographic Data System

Records

- Citation
- DOI
- Tags (process classification)
- Species
- Theory / Experiment
- Energy range

Export formats

- XSAMS
- JSON



IAEA

AMD Unit Database Developments

ALADDIN

A Labelled Atomic Data Interface

- Old interface: https://www-amdis.iaea.org/ALADDIN/
- New interface:
  - Vienna-based Consultant (Dipti) from August 2021
  - Home-based Consultant (Martin) for software tools / migration (to Jan 2022)
  - Better search functionality
  - Updated process classification
  - Easier data upload functionality
  - Improved download functionality (archives, by publication)
  - API

IAEA

AMD Unit Database Developments

ALADDIN2

ALADDIN → ALADDIN2

- Old interface: 21607 entries
- New interface: 7646 entries
- Issues
  - Inconsistent or incorrect representation of atomic and molecular states (1500+ datasets)
    - Charge error cases - 382 datasets (fixed)
    - Stoichiometry error cases – 1,426 datasets
  - Missing product cases – 2,567 datasets
  - ~ 3,000 out of 21,607 datasets need to be checked on a case-by-case basis.
  - 371 references updated with doi which also corrected incorrect bibliographic data.
  - Removed some of the bad datasets
- Fit function library:
  - Fortran functions as provided in the old version of ALADDIN
  - Plan to provide the python versions of fit functions.

IAEA

AMD Unit Database Developments

CollisionDB

- Development interface: https://db-amdis.org/collisiondb/
- 100,000+ plasma collisional datasets
  - Based around standards for describing species, states and processes
  - Standard data exchange format (JSON metadata)
  - API (under development)

IAEA

AMD Unit Database Developments

CollisionDB

Newest datasets relating to Be and related species in edge plasmas

Status of collisional data involving Be and its molecular species uploaded to collisionDB

Reactants	# Datasets	Data type	Process type	Reference
e-, Be	193	Cross sections	EEX, EIN	IAEA + NIST evaluation
e-, Be^+	105	Cross sections	EEX, EIN	IAEA + NIST
e-, BeH	400	Cross sections	EXE, EXV	*JPB* **53**, 135202 (2020)
e-, BeD	400	Cross sections	EXE, EXV	*JPB* **53**, 135202 (2020)
e-, BeT	400	Cross sections	EXE, EXV	*JPB* **53**, 135202 (2020)
e-, BeH^+	324	Rate-coefficients	EXV, EDR	*ADNDT* **115-116**, 287-308 (2017)
e-, BeD^+	576	Rate-coefficients	EXV, EDR	*PSST* **27**, 025015 (2018)
e-, BeT^+	783	Rate-coefficients	EXV, EDR	*ADNDT* **139**, 101414 (2021)
H^+, Be^+	52	Cross sections	HCX, HEX, HIN, HDX	Vapour shielding CRP
Li, Be^{3+}	30	Cross sections	HCX	Vapour shielding CRP
H, Be^{4+}	9	Cross sections	HCX, HEX, HIN	Neutral beams CRP

IAEA

AMD Unit Database Developments

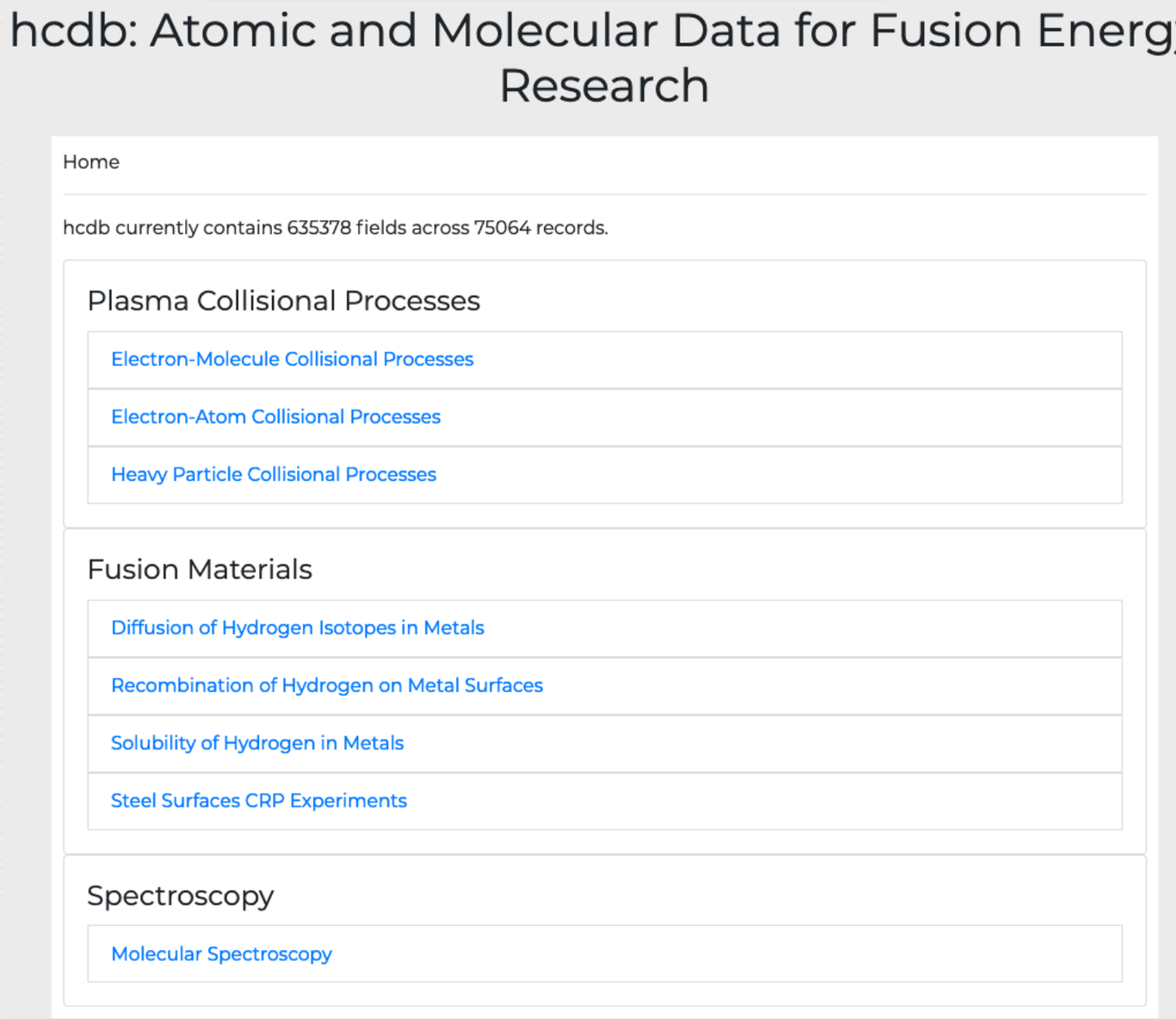
hcdb

Hierarchical Database for generic, labelled data

Development interface: https://db-amdis.org/hcdb/

Uses:

- Heterogeneous data
  - Arbitrary physical quantities
  - Ranged values
  - Descriptive text
  - Experimental data
  - Images
  - Described tabular data
- Unvalidated data
- Links to external data resources
- Integration with visualization tools



IAEA

AMD Unit Database Developments

hcdb

Hierarchical Database for generic, labelled data

Click through to records

Home > Steel Surfaces CRP Experiments

Steel Surfaces CRP Experiments

48 / 48 records shown.

pk	doi	Contact name	Steel type	T /K	ϕ /$m^{-2}.s^{-1}$	Γ /m^{-2}	Ion energy	D_{tot} /m^{-2}
R6091	-	Golubeva	Eurofer	443	3e+21	3e+24 – 7.3e+25	-	-
R6092	-	Golubeva	Rusfer	443	3e+21	3e+24 – 7e+25	-	-
R6093	-	Golubeva	Rusfer	below melting	1e+23 – 1e+24 [D pulsed high heat plasma loading, 0.3 MJ/m2, 1 ms]	in 1 pulse big uncertainity; 1 and 5 pulses (see "ion flux" column)	-	1e+20 – 3.7e+20
R6094	-	Golubeva	Eurofer	below melting	1e+23 – 1e+24 [D pulsed high heat plasma loading, 0.3 MJ/m2, 1 ms]	in 1 pulse big uncertainity; 1 and 5 pulses (see "ion flux" column)	-	1.3e+20 – 1.5e+20
R6095	-	Golubeva	F82H	below melting	1e+23 – 1e+24 [D pulsed high heat plasma loading, 0.3 MJ/m2, 1 ms]	in 1 pulse big uncertainity; 1 and 5 pulses (see "ion flux" column)	-	4.8e+19 – 1.1e+20
R6096	-	Golubeva	CLAM	below melting	1e+23 – 1e+24 [D pulsed high heat plasma loading, 0.3 MJ/m2, 1 ms]	in 1 pulse big uncertainity; 1 and 5 pulses (see "ion flux" column)	-	1.8e+20 – 2.3e+20

IAEA

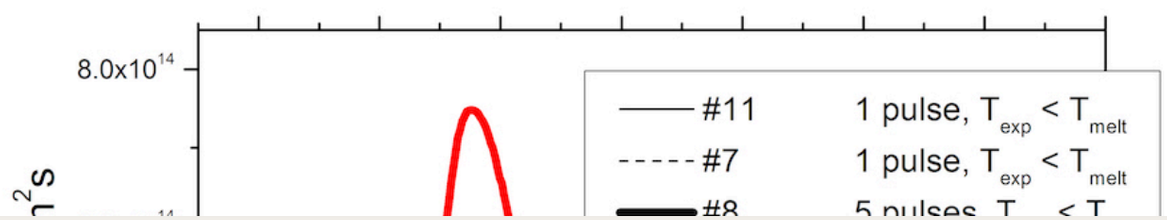
AMD Unit Database Developments

hcdb

Hierarchical Database for generic, labelled data

Home > Steel Surfaces CRP Experiments > R6094

Contact name		Golubeva
Steel type		Eurofer
Ion flux	ϕ /$m^{-2}.s^{-1}$	1e+23 – 1e+24 [D pulsed high heat plasma loading, 0.3 MJ/m2, 1 ms]
Ion fluence	Γ /m^{-2}	in 1 pulse big uncertainity; 1 and 5 pulses (see "ion flux" column)
Ion energy per D	E /eV	20 – 30
Sample thickness	t /mm	2
Sample temperature	T /K	below melting
Sample temperature measurement location		backside; heat transfer to cooling system
Analysis method		TDS
Retained deuterium	D_{tot} /m^{-2}	1.3e+20 – 1.5e+20
Image files		Fig_3_AG.jpg, Fig_Total_Ret_AG.jpg

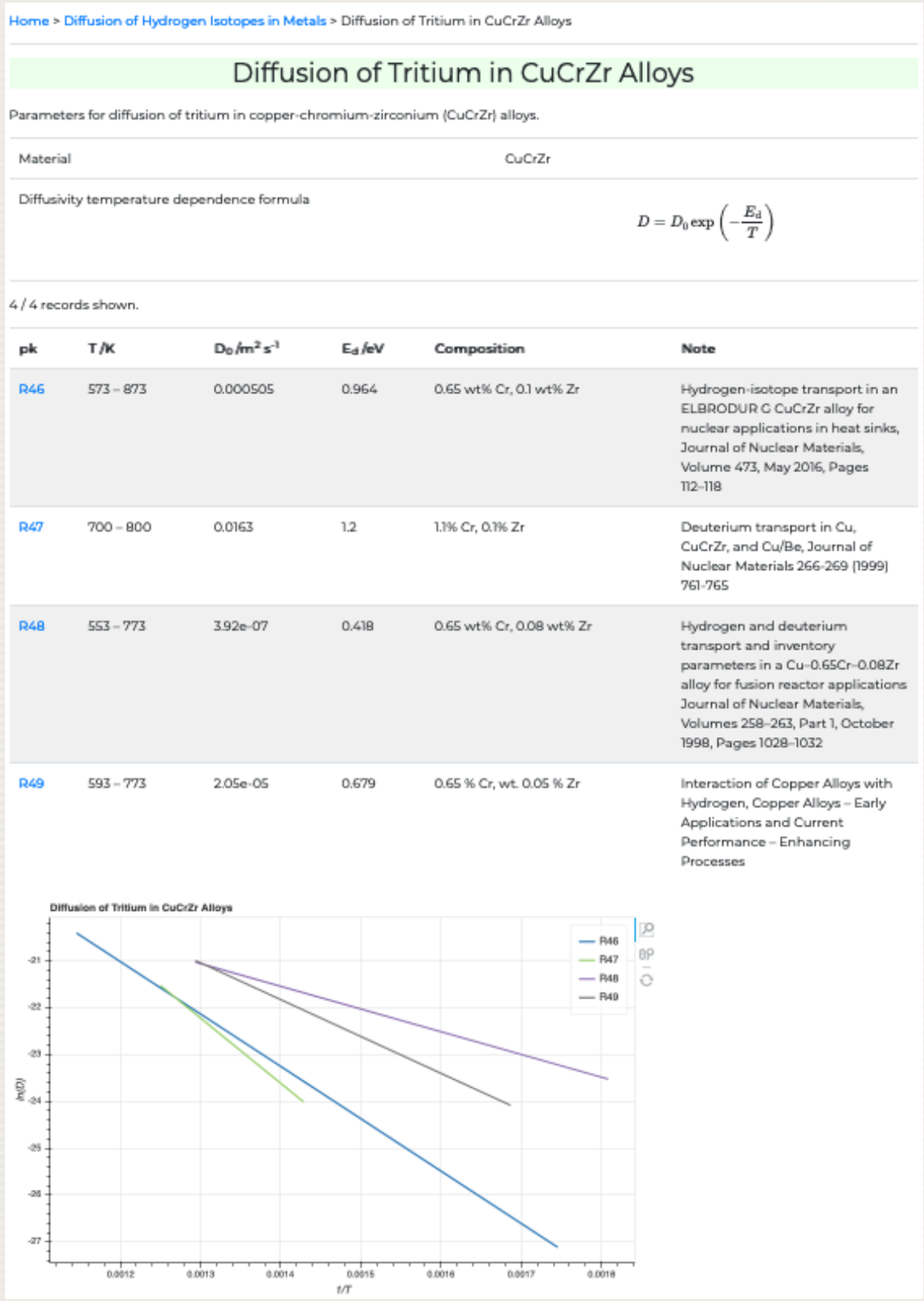


IAEA

AMD Unit Database Developments

hcdb

- Data Comparisons through Interactive charts
- References
- Contact Details
- Contextual Information (units, formulas)



Home > Diffusion of Hydrogen Isotopes in Metals > Diffusion of Tritium in CuCrZr Alloys

Diffusion of Tritium in CuCrZr Alloys

Parameters for diffusion of tritium in copper-chromium-zirconium (CuCrZr) alloys.

Material	CuCrZr
Diffusivity temperature dependence formula	$D = D_0 \exp\left(-\frac{E_d}{T}\right)$

4 / 4 records shown.

pk	T /K	D_0 /m^2 s^{-1}	E_d /eV	Composition	Note
R46	573 – 873	0.000505	0.964	0.65 wt% Cr, 0.1 wt% Zr	Hydrogen-isotope transport in an ELBRODUR C CuCrZr alloy for nuclear applications in heat sinks, Journal of Nuclear Materials, Volume 473, May 2016, Pages 112-118
R47	700 – 800	0.0163	1.2	1.1% Cr, 0.1% Zr	Deuterium transport in Cu, CuCrZr, and Cu/Be, Journal of Nuclear Materials 266-269 (1999) 761-765
R48	553 – 773	3.92e-07	0.418	0.65 wt% Cr, 0.08 wt% Zr	Hydrogen and deuterium transport and inventory parameters in a Cu-0.65Cr-0.08Zr alloy for fusion reactor applications Journal of Nuclear Materials, Volumes 258–263, Part 1, October 1998, Pages 1028–1032
R49	593 – 773	2.05e-05	0.679	0.65 % Cr, wt. 0.05 % Zr	Interaction of Copper Alloys with Hydrogen, Copper Alloys – Early Applications and Current Performance – Enhancing Processes

AMD Unit Database Developments

Clerval

A database of institutions and events of relevance to the use, calculation and measurement of atomic, molecular and plasma-material interaction data in nuclear fusion research.

- https://amdis.iaea.org/clerval/
- Institutions (339)
- People (770; local version only)
- Events (Conferences, Workshops, Meetings)
- Databases and other resources

- Linked by Keywords

IAEA