LXCat discussion session, Wednesday evening (Oct 30), at GEC 2019

Organized by Klaus Bartschat and approximately 50 participants

Klaus Bartschat opened the discussion session with a short introduction so as to define the scope of the LXCat project. This was followed by an on-line walk through the LXCat website presented by Jacob Stephens. These two introductory talks were followed by short talks from participants. Klaus made a special effort to encourage participation from the A&M community who generates data needed for modeling plasmas, and several of the talks were contributions from A&M community. We hope to see their data soon on LXCat. Other short talks were intended to highlight data needs in the plasma modeling community.

The session lasted about 90 minutes and was quite lively. We are looking forward to GEC 2020 where there will again be a LXCat discussion session one evening. Please send a message with your suggestions for what you would like to see included to the LXCat team at info@lxcat.net.

The LXCat project (initiated at LAPLACE in 2010)

LXCat is a web-based, community-wide project for the curation of

data needed in modeling low-temperature plasmas

Electron + neutral
cross sections / oscillator strengths/ swarm parameters

Ion + neutral
cross sections / interaction potentials / swarm parameters

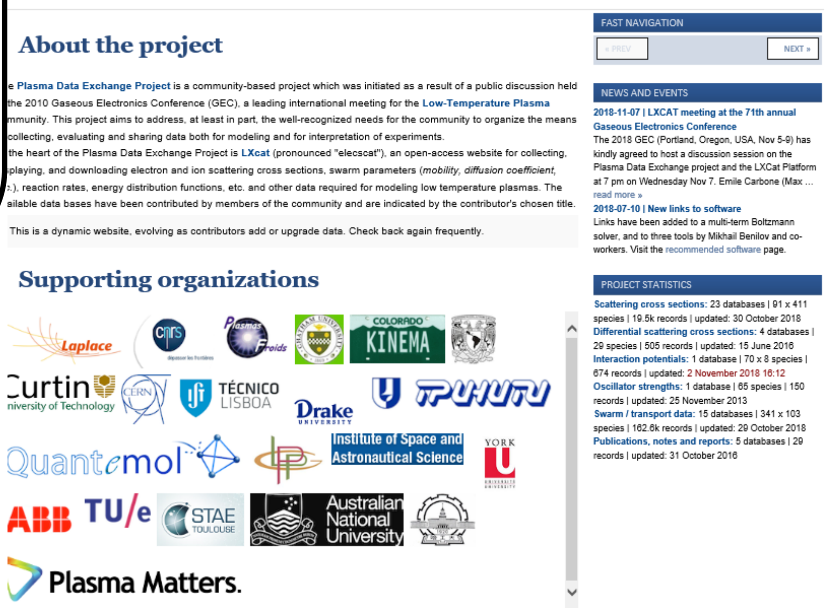
Plasma-surface interactions

Plasma chemistry

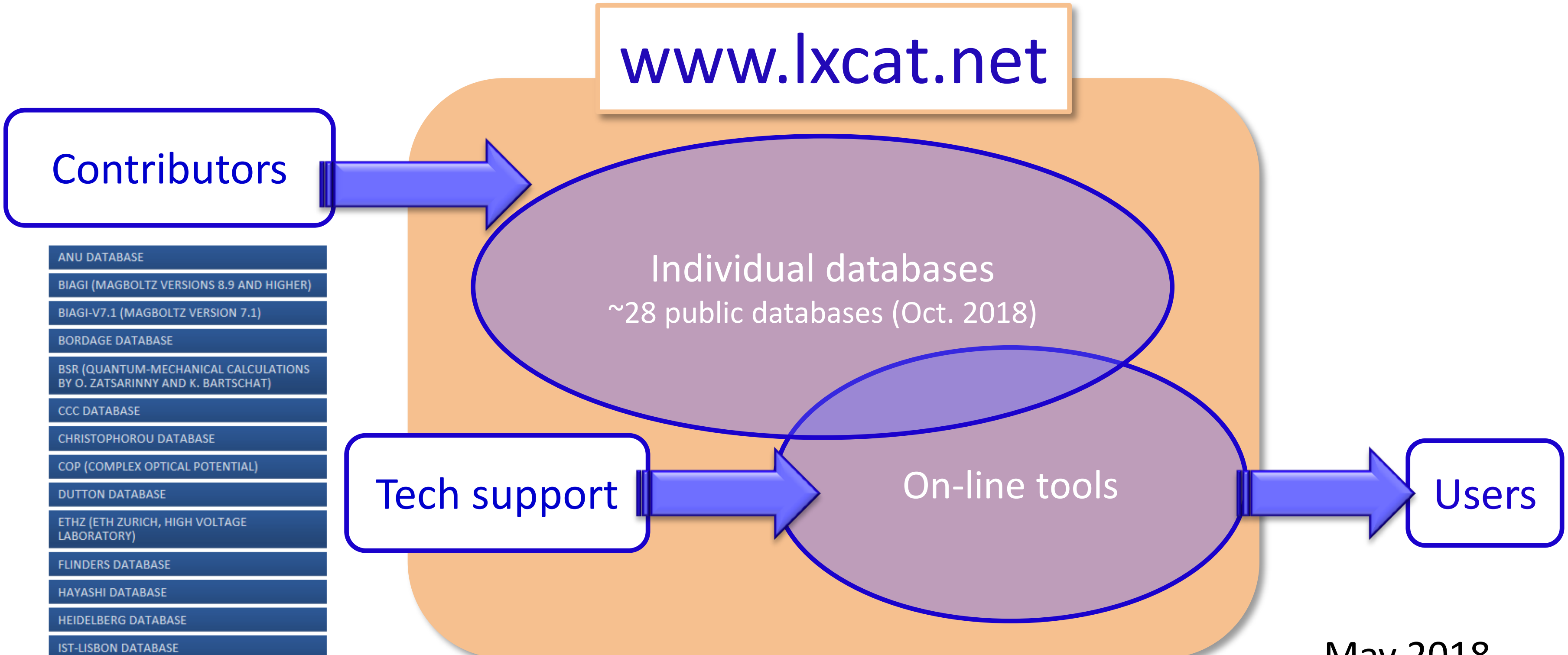
Radiation

LXCat

ELECtron (and ion) SCATtering



LXCat structure – on-line tools & users



- ANU DATABASE
- BIAGI (MAGBOLTZ VERSIONS 8.9 AND HIGHER)
- BIAGI-V7.1 (MAGBOLTZ VERSION 7.1)
- BORDAGE DATABASE
- BSR (QUANTUM-MECHANICAL CALCULATIONS BY O. ZATSARINNY AND K. BARTSCHAT)
- CCC DATABASE
- CHRISTOPHOROU DATABASE
- COP (COMPLEX OPTICAL POTENTIAL)
- DUTTON DATABASE
- ETHZ (ETH ZURICH, HIGH VOLTAGE LABORATORY)
- FLINDERS DATABASE
- HAYASHI DATABASE
- HEIDELBERG DATABASE
- IST-LISBON DATABASE
- ITIKAWA DATABASE
- LAPLACE (MEASUREMENTS AFTER 1975)
- MORGAN (KINEMA RESEARCH & SOFTWARE)
- NGFSRDW DATABASE
- PHELPS DATABASE
- PUECH DATABASE
- QUANTEMOL DATABASE
- SIGLO DATABASE
- TRINITI DATABASE
- UBC DATABASE
- UNAM DATABASE
- VIEHLAND DATABASE
- BOLSIG+ SOLVER

May 2018

A recent statistic: There are over 70 visitors per day on the average.

S Pancheshnyi *et al.*, *Chem. Phys.* **398**, 148 (2012)
LC Pitchford *et al*, *Plasma Process. Polym*. **14,** 1600098 (2017)

Contributors to the LXCat project (2010 to Sept 2018)

Website conception: S Pancheshnyi, (France /Switzerland)

Contributors:

Scattering cross sections (compilations, quantum calculations, measurements) : MC Bordage, V. Puech, LC Pitchford (France); SF Biagi, D Brown, J Tennyson (UK); K Bartschat, WL Morgan, AV Phelps, J. Stephens, L Viehland, MC Zammit, O Zatsarinny (USA); LL Alves, C Ferreira, V Guerra (Portugal); NA Dyatko, IV Kochetov, AP Napartovich (Russia); Y Itikawa (Japan); I Bray, S Buckman, M Brunger, L Campbell, D Fursa, McEachran (Australia); A Stauffer (Canada); RK Gangwar, L Sharma, R Srivastava (India)

Oscillator strengths: C Brion (Canada)

Transport/rate coefficients (compilations, measurements) : L Viehland, AV Phelps (USA); S Chowdhury (France), J de Urquijo (Mexico); LL Alves, V Guerra (Portugal); Christophorou (Greece); A Chachereau, CM Franck, P Haefliger, A Hoesl, M M Hildebrandt (Germany); L Rabie (Switzerland); X-M Zhu (China); I Jogi (Estonia)

Ion-neutral interaction potentials: L Viehland (USA)

Initial website development: S Pancheshnyi, (France /Switzerland); B Chaudhury (India),

Tech support: W Graef, D Mihailova, J van Dijk (The Netherlands); M Hopkins, B Yee (USA), Pancheshnyi

Outreach: K Bartschat (USA), E Carbone (Germany), LC Pitchford (France), Y-K Pu (China)

On-line Bolsig+ : GJM Hagelaar (France); S Pancheshnyi (Switzerland)

Servers: Eindhoven Technical Univ. & Univ Toulouse

LXCat demonstration

Jacob Stephens

Short Introduction

From the website:

...an open-access website for **collecting**, **displaying**, and **downloading** electron and ion **scattering cross sections**, **swarm parameters** (*mobility, diffusion coefficient, etc.*), **reaction rates**, energy distribution functions, etc. and other data required for modeling **low temperature plasmas**...

https://www.lxcat.net/home

Goal

- Only be a gateway to data, provide platform:
  - for contributors
  - for users
  - be community driven

- LXCat does **not own** the data (proper references)
- LXCat does **not recommend** data

Technical Support Team

- Wouter Graef (Plasma Matters)
- Sergey Pancheshnyi (ABB)
- **Matt Hopkins**, Benjamin Yee (Sandia)
- Diana Mihailova (Plasma Matters)
- Jan van Dijk (Eindhoven University of Technology)

Plasma-MDS and INPTDAT for publication and re-use of digital research data

Markus M. Becker

SPONSORED BY THE

Federal Ministry of Education and Research

The 72nd Annual Gaseous Electronics Conference
October 30, 2019

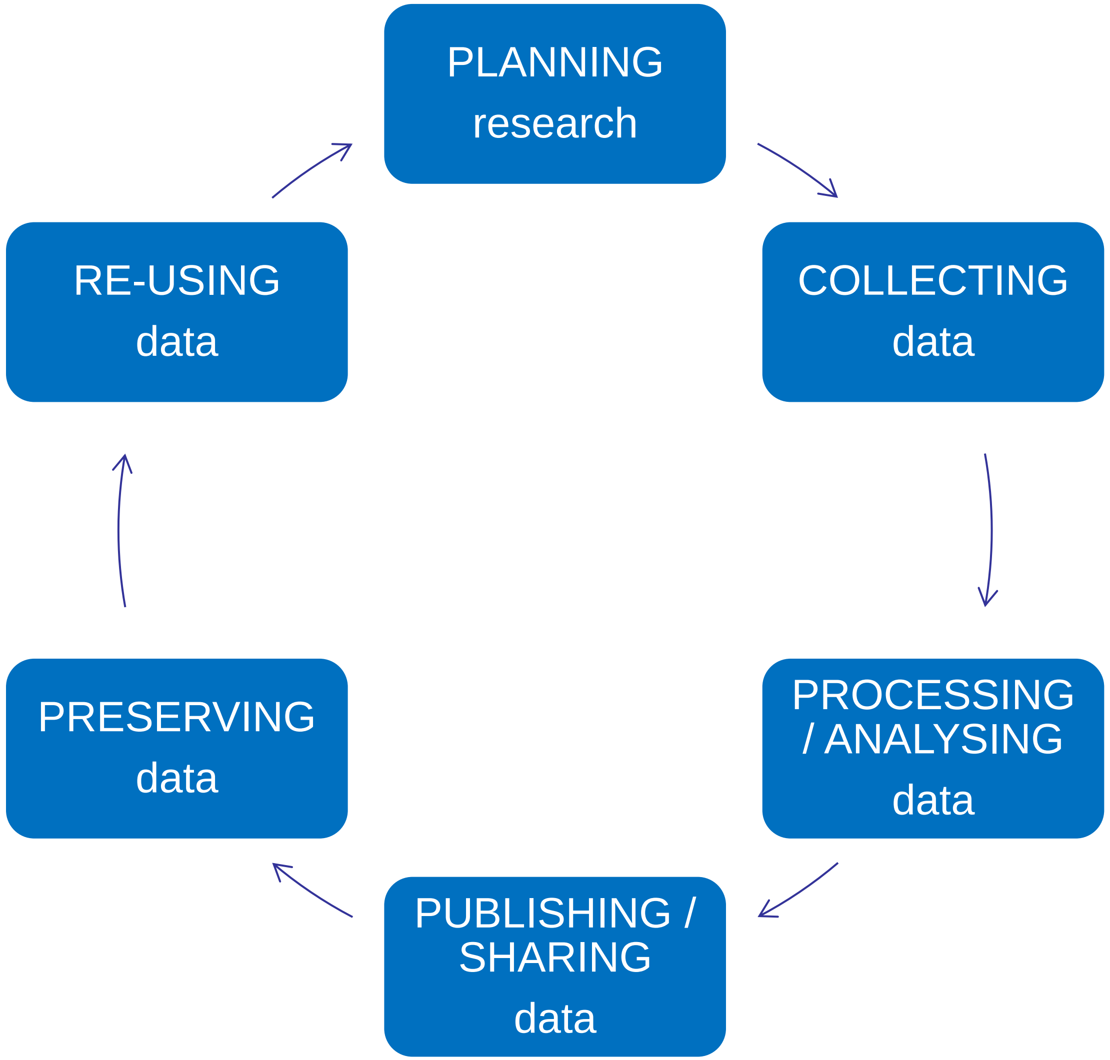
Leibniz Gemeinschaft

FROM IDEA TO PROTOTYPE

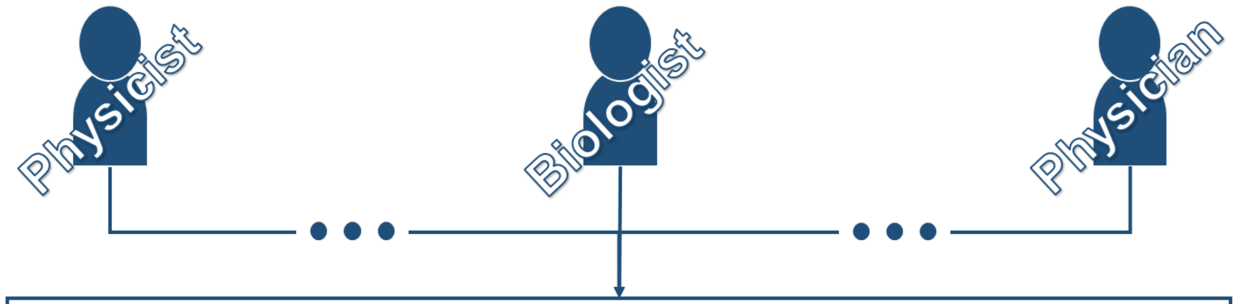
Reasons for sharing digital research data

- Transparency and reproducibility of research
- Validation of research results
- Visibility, scientific recognition and reputation
- External requirements (e.g. publishers, funders)

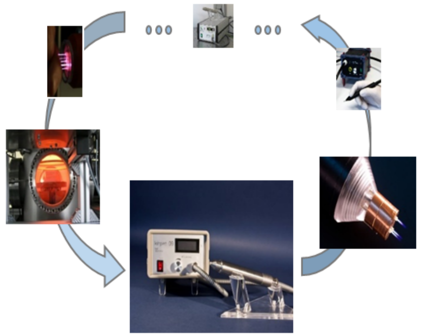
➢ Enable full research data life-cycle



Concept



INPTDAT data platform



- Storage and sharing of research data
- Reference to corresponding publications
- Content indexing and full-text search
- Direct linking and visualisation of data records
- Directory of plasma sources and applications

Benefit

- Version-safe long-term archiving of research data according to the guidelines of good scientific practice.
- Simplified reuse of interdisciplinary research data, especially for researchers from other fields.
- Merging of heterogeneous research data from different fields of science → generation of new scientific findings.

Realized by

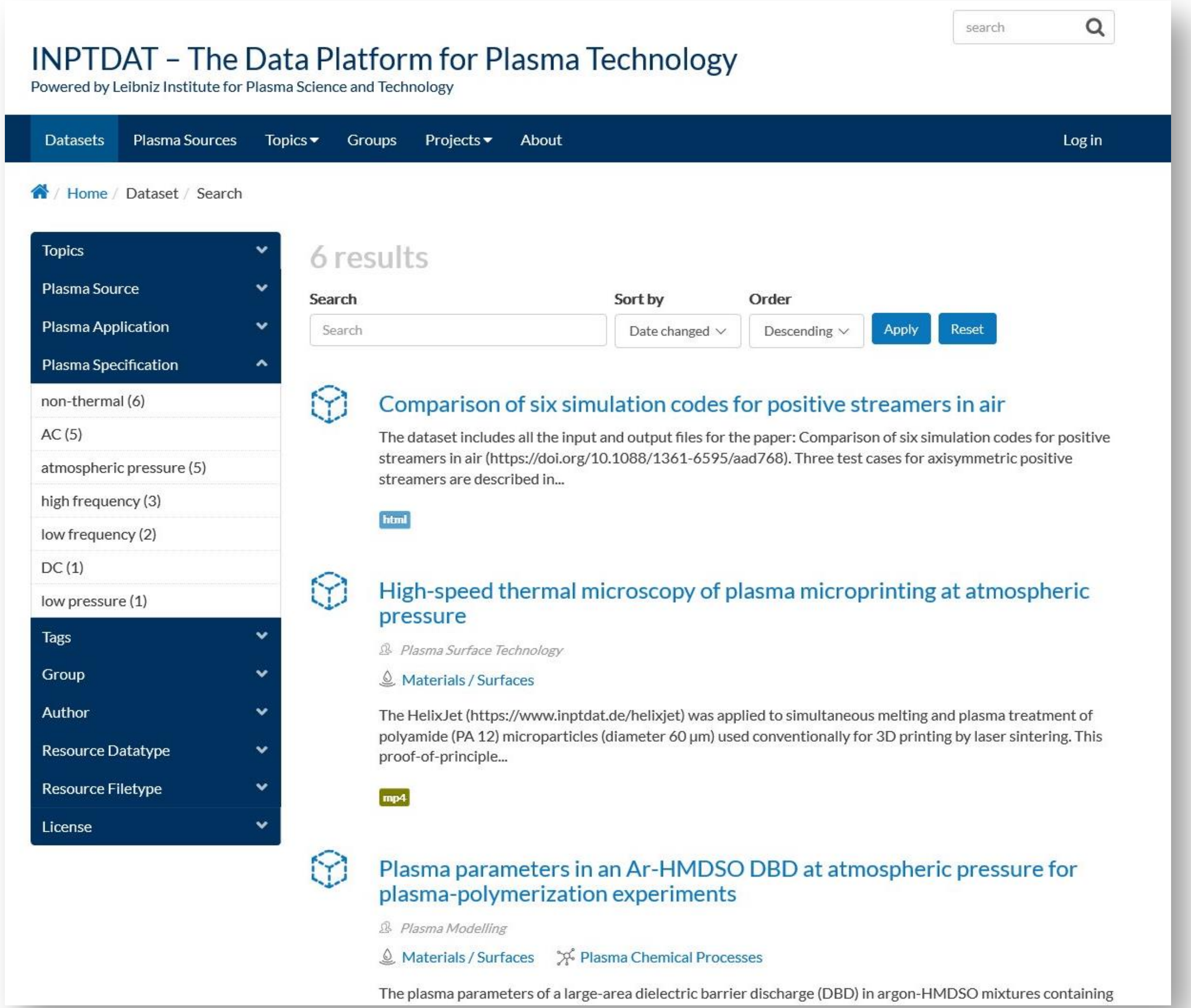
1. subject-specific **metadata schema**
2. institutional **data platform**

Metadata schema Plasma-MDS

- Subject-specific metadata schema for annotation of research data in low-temperature plasma physics
- Extension to basic schemas (Dublin Core, DataCite)
- Metadata fields for description of
    - plasma source
    - plasma medium
    - plasma target
    - diagnostics / modelling / simulations
    - resources (data)

- To be reviewed after initial phase of growing usage
- Development of a community standard as a long-term perspective

INPTDAT (https://www.inptdat.de)



Data platform for low-temperature plasma physics featuring

- data publications with DOI
- Plasma-MDS for data annotations
- faceted search
- online visualization
- plasma source catalog
- API based access to (meta)data
- links to external data resources (e.g. in university repositories)

➢ prototype for community platform

Summary

- **Plasma-MDS:** first attempts to develop a schema for annotation of data in low-temperature plasma physics
- **INPTDAT:** data platform using Plasma-MDS for publication and re-use of research data
- Activities will be continued to support data-driven plasma science
- Linking with LXCat and joint activities on data management for plasma physics could be very fruitful
    - assurance of data quality
    - development of standards for labeling of data
    - …

Contact

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Markus Becker

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Phone: +49 - 3834 - 554 3821

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FAIR data principles (https://www.go-fair.org/fair-principles/)

Findable

F1. (Meta)data are assigned a globally unique and persistent identifier

F2. Data are described with rich metadata (defined by R1)

F3. Metadata clearly and explicitly include the identifier of the data they describe

F4. (Meta)data are registered or indexed in a searchable resource

Accessible

A1. (Meta)data are retrievable by their identifier using a standardized communications protocol

A2. Metadata are accessible, even when the data are no longer available

Interoperable

I1. (Meta)data use a formal, accessible, shared, and broadly applicable language for knowledge representation

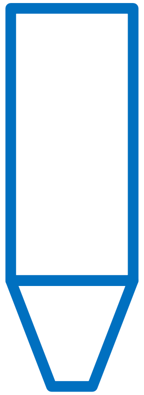
I2. (Meta)data use vocabularies that follow FAIR principles

I3. (Meta)data include qualified references to other (meta)data

Reusable

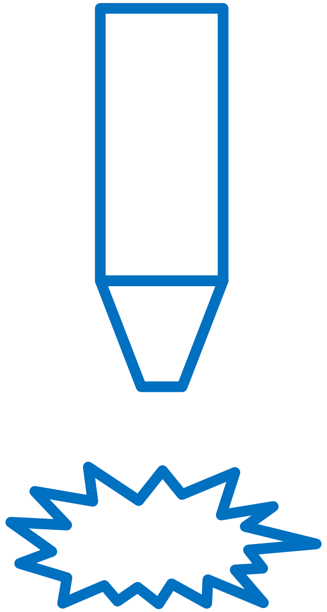
R1. Meta(data) are richly described with a plurality of accurate and relevant attributes

Plasma source (CCP, APPJ, COST-Jet…)



Metadata field
plasma.source.name
plasma.source.application
plasma.source.specification
plasma.source.properties
plasma.source.procedure

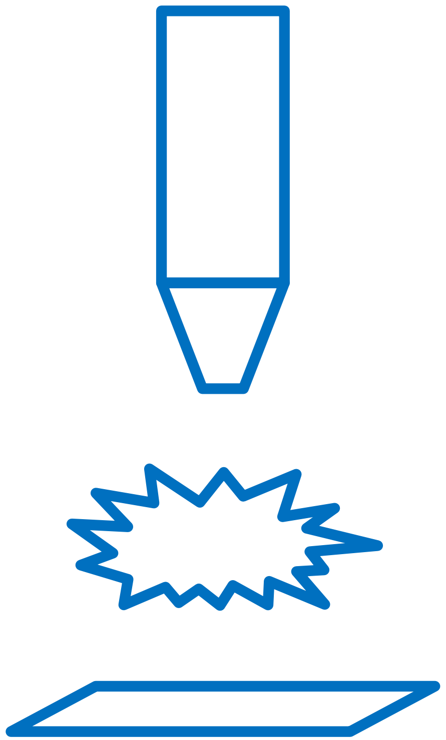
Plasma medium (air, Ar, O2…)



Metadata field
plasma.source.name
plasma.source.application
plasma.source.specification

Metadata field
plasma.medium.name
plasma.medium.properties
plasma.medium.procedure

Plasma target (distilled water, silicon wafer, E. coli…)

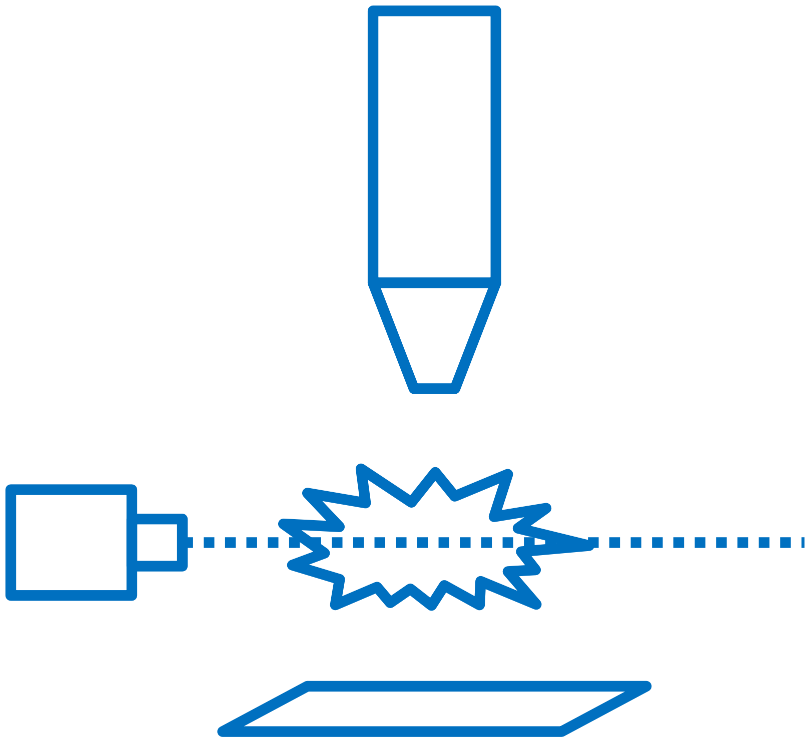


Metadata field
plasma.source.name
plasma.source.application
plasma.source.specification

Metadata field
plasma.source.name

Metadata field
plasma.target.name
plasma.target.properties
plasma.target.procedure

Diagnostics / modelling / simulations (OES, XPS, PIC-MCC…)



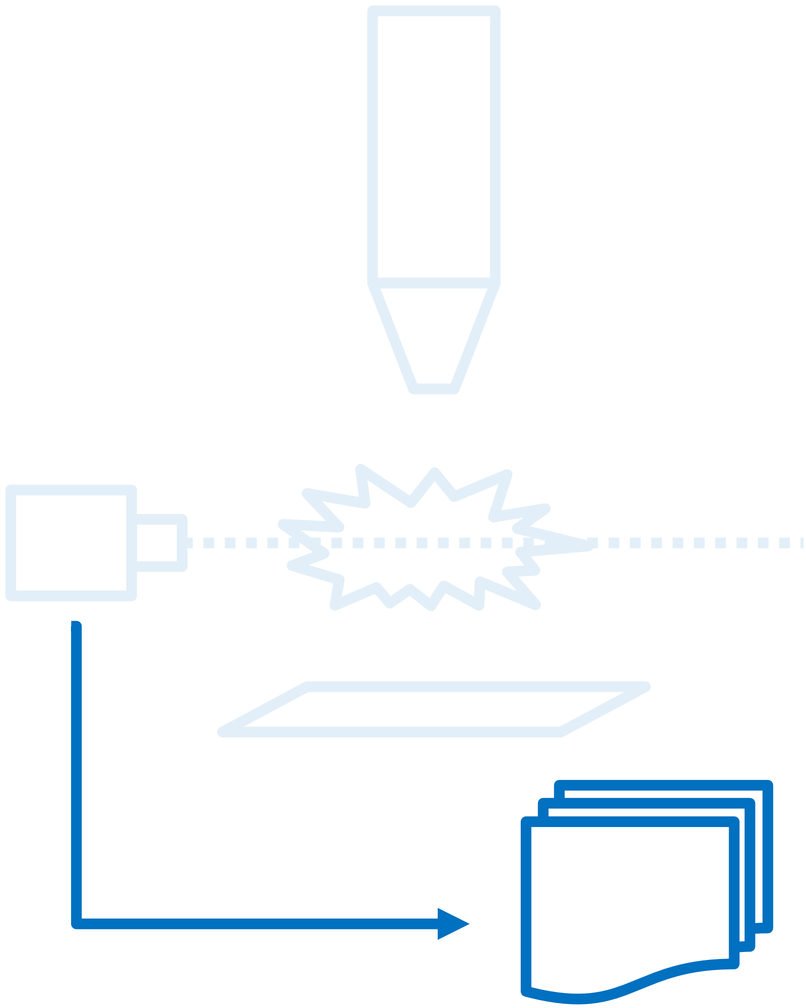
Metadata field
plasma.source.name
plasma.source.application
plasma.source.specification

Metadata field
plasma.s

Metadata field
plasma.diagnostics.name
plasma.diagnostics.properties

Metadata
plasma.t
plasma.target.properties
plasma.target.procedure

Resources (data shared with the dataset)



Metadata field
plasma.source.name
plasma.source.application
plasma.source.specification

Metadata field
plasma.resource.filetype
plasma.resource.datatype
plasma.resource.range
plasma.resource.quality

Search view

Datasets | Innovations | Plasma Sources | Topics | Groups | About | Log in

Home / Dataset / Search

Topic

Plasma Source

- CCP (1)
- HF plasma jet (1)
- ntAPPJ (1)

Plasma Application

Plasma Specification

- AC (2)
- high frequency (2)
- non-thermal (2)
- atmospheric pressure (1)

2 results

Search | Sort by | Order

Search | Date changed | Descending | Apply | Reset

Correlation of helicality and rotation frequency of filaments in the ntAPPJ

Plasma Surface Technology

Surfaces/Materials

The self-organized behaviour (locked mode) of filaments in the non-thermal atmospheric pressure plasma jet (ntAPPJ) couples a spatial patterning of the discharge (helical symmetry) and a regular motion (steady rotation). The dataset represents...

3x csv png

Dataset view

Datasets | Innovations | Plasma Sources | Topics | Groups | About | Log in

Plasma Surface Technology

The Department for Plasma Surface Technology bundles years of experience in development of plasma-assisted processes for modification of surfaces for applications, as well as in the high-tech sector, e.g.

Correlation of helicality and rotation frequency of filaments in the ntAPPJ

Surfaces/Materials

The self-organized behaviour (locked mode) of filaments in the non-thermal atmospheric pressure plasma jet (ntAPPJ) couples a spatial patterning of the discharge (helical symmetry) and a regular motion (steady rotation). The dataset represents the mean rotation frequency of filaments in the capillary with a diameter of 4 mm and the corresponding geometric characteristics: helicality and/or filament inclination angles were measured along with the gas temperature under varying discharge conditions (electric power and argon flow rate).

plasma jet · self-organisation

Field	Value
Group	Plasma Surface Technology
Authors	

Resource view

Correlation of helicality and rotation frequency at 8 W

The data table shows the correlation of helicality and rotation frequency of plasma filamants at a power of 8 W. From the images of filaments, the angle of inclination alpha has been obtained. The helicality k has been calculated according to the equation k=tan(alpha)/r. Here, r is the radial position of filaments in the capillary, and alpha is measured from the line parallel to the jet axis. The corresponding rotation frequency of filaments has been measured by means of laser schlieren deflectometry (LSD).

CSV node807_data-table_8w.csv

Data Preview: Note that by default the preview only displays up to 100 records. Use the pager to flip through more records or adjust the start and end fields to display the number of records you wish to see.

Grid | Graph | 5 records | « 1 – 5 » | Search data ... | Go » | Filters | Fields

Rotation frequency [Hz]	Helicality [rad/mm]	Gas flow rate [slm]

Interactive online visualization

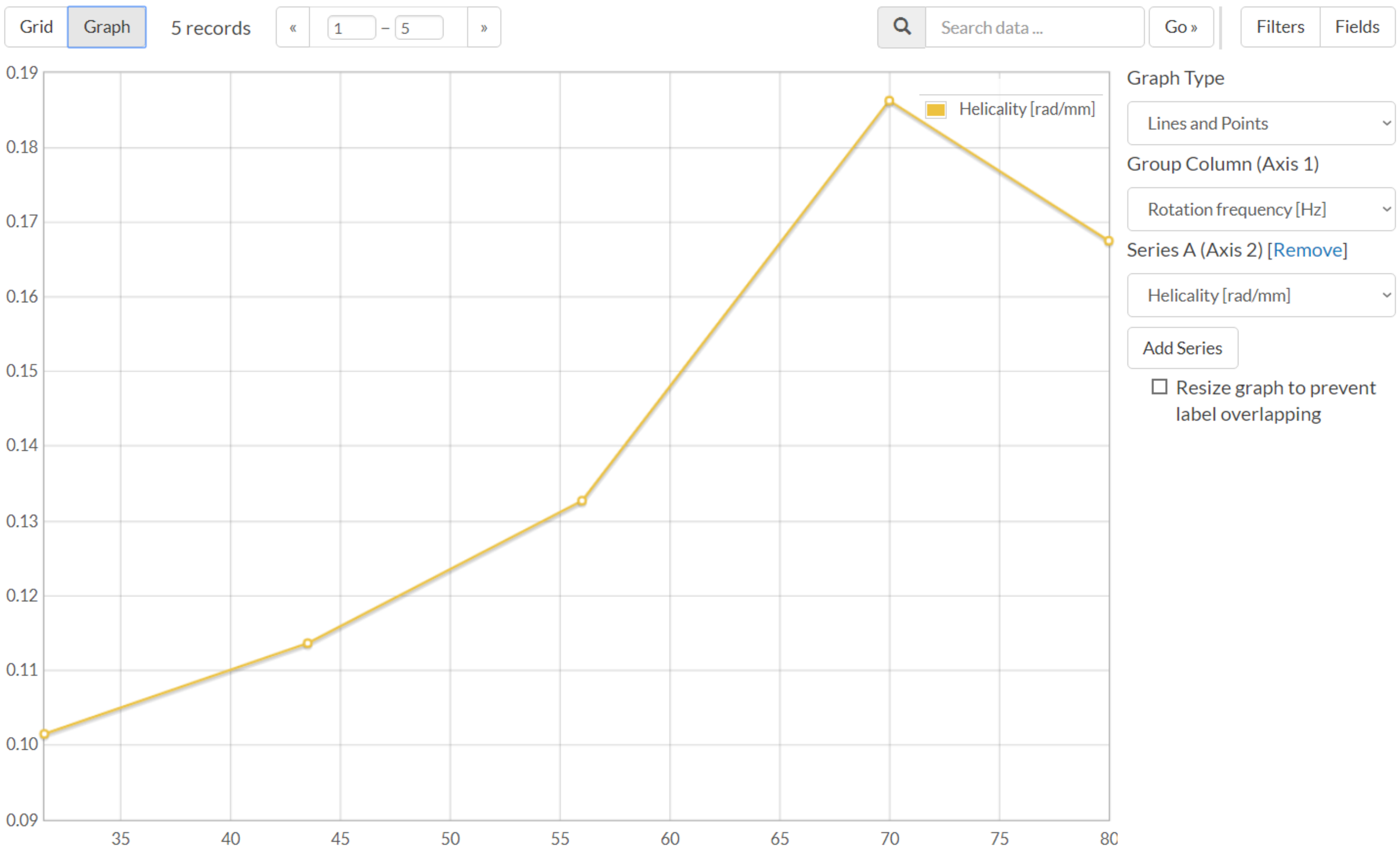
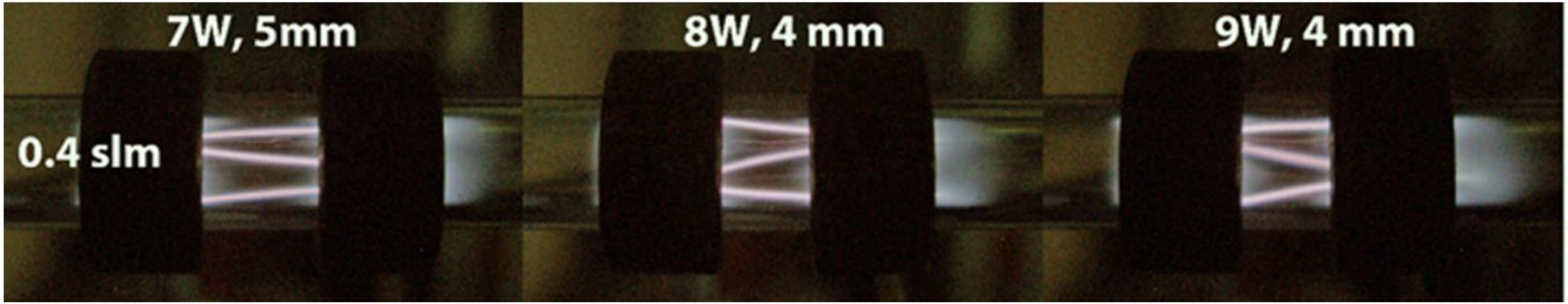


Image preview

Images of filaments

Images of filaments for different power and gas flow rate. From these images, the angle of inclination has been obtained.

node807_image_inclination.png



Find data by standardized metadata (DataCite)

Other Access

The information on this page (the dataset metadata) is also available in these formats.

DataCite | Plasma-MDS

via the DKAN API

<siteurl>/api/3/action/package_show_**datacite**

→ For DOI retrieval

id: "a170d151-9a19-422a-b9ee-b1ed76d8b1ad"
@context: "http://schema.org"
@type: "Dataset"
url: "https://vpc-inptdat.intranet.inp-greifswald.de/node/807"
name: "Correlation of helicality and rotation frequency of filaments in the ntAPPJ"
author:
  0:
    @type: "Person"
    name: "Schäfer, Jan"
publisher:
  @type: "Organisation"
  name: "INPTDAT"
datePublished: "2019-03-25"
description: "The self-organized behaviour (locked mode) of filaments in the non-thermal atmospheric pressure plasma jet (ntAPPJ) couples a spatial

Find data by standardized metadata (Plasma-MDS)

Other Access

The information on this page (the dataset metadata) is also available in these formats.

DataCite | Plasma-MDS

via the DKAN API

<siteurl>/api/3/action/package_show_**plasma**

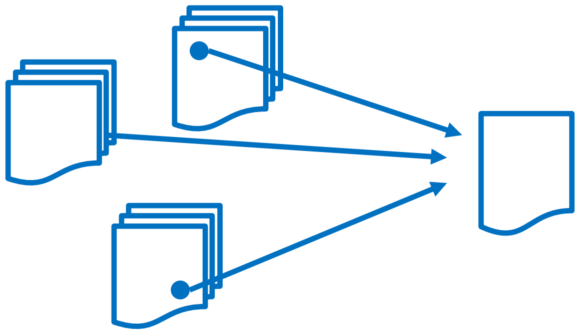

```
▼ plasma.source:
    name:              "ntAPPJ, HF plasma jet"
    application:       "PECVD"
  ▼ specifications:    "AC, atmospheric pressure, non-thermal, high
                        frequency"
  ▼ properties:        "Non-thermal atmospheric pressure plasma jet
                        (capacitively coupled) operated in a self-
                        organized regime (locked mode). Power: 7 - 9
                        W; Frequency: 27.12 MHz; Flow rate: 400 - 800
                        sccm argon; Electrodes: ring configuration,
                        distance 5 mm, width 5 mm; Capillary: inner
                        diameter 4 mm, outer diameter 6 mm"
▼ plasma.medium:
    name:              "Ar"
  ▼ properties:        "Flowrate: 0.4 to 0.8 slm; Pressure: 1 bar;
                        Temperature: 300 to 1000 K; Purity: argon 6.0"
    procedures:        "Standard conditions of the argon gas are
                        assured."
  plasma.target:       []
```

Retrieve data in standardized format

- Data uploaded to the internal Datastore are directly accessible for automated data processing and reuse

<site url>/api/action/datastore/search.json?resource_id=<id>&<**parameters**>

- API parameters provide broad functionality
  - data filters
  - access specific fields
  - joining multiple tables
  - statistical operations (min/max, avg, variance…)



{"help":"Search a datastore table. :param resource_id: id or alias of the data that is going to be selected.","success":true,"result":{"fields":[{"id":"Rotation frequency [Hz]","type":"float"},{"id":" Helicality [rad/mm]","type":"float"},{"id":" Gas flow rate [slm]","type":"float"}],"resource_id":["abb84522-084f-4ca6-b8a8-9efe02bf6ef5"],"limit":5,"total":5,"records":[{"Rotation frequency [Hz]":"31.5"," Helicality [rad/mm]":"0.101514"," Gas flow rate [slm]":"0.4"},{"Rotation frequency [Hz]":"43.5"," Helicality [rad/mm]":"0.113656"," Gas flow rate [slm]":"0.5"},{"Rotation frequency [Hz]":"56"," Helicality [rad/mm]":"0.132726"," Gas flow rate [slm]":"0.6"},{"Rotation frequency [Hz]":"70"," Helicality [rad/mm]":"0.186263"," Gas flow rate [slm]":"0.7"},{"Rotation frequency [Hz]":"80"," Helicality [rad/mm]":"0.167507"," Gas flow rate [slm]":"0.8"}]}}

Current status of efforts towards a full CO_2 chemistry coupling electron/vibrational kinetics
(a step-by-step work program)

V Guerra, T Silva, M Grofulovic, P Ogloblina, L Terraz, T Dias, LL Alves – IPFN, Portugal
O Guaitella, AS Morillo-Candas, C Drag, A Chatterjee, JP Booth – LPP, France
B Klarenaar, A Silva, R Engeln – TU/e, The Netherlands

Swarm-derived electron-scattering cross sections
✓ CO_2 (published paper; data @ IST-Lisbon database)
✓ O_2 (published paper; data @ IST-Lisbon database)
✓ CO (published paper; data to be released @ IST-Lisbon database)

✓ Electron dissociation cross section for CO_2
- L. Polak and D. Slovetsky, Int. J. Radiat. Phys. Chem., 8, 257-282, 1976

✓ Electron dissociation rate coefficient for CO_2 (paper accepted)
- Calculation integrating the CS over the eedf (obtained using a complete cross section dataset)
- Good agreement with FTIR time-dependent measurements (direct validation)
- Good agreement with time-evolution of CO density in a “building-up” experiment (indirect validation)

Current status of efforts towards a full CO_2 chemistry coupling electron/vibrational kinetics
(a step-by-step work program)

VV and VT rate coefficients for reactions involving the first 72 vibrational levels
based on first-order SSH and SB perturbation theories
(corresponding to $\nu_1^{max}=2$, $\nu_2^{max}=5$ and $\nu_3^{max}=5$)
✓ validated against time-resolved in situ FTIR measurements of the vibrational populations in the afterglow of pulsed DC discharges (published paper)
✓ validated against time-resolved measurements of T_g in the afterglow of pulsed DC discharges (paper in preparation)

e-impact excitation / deexcitation rate coefficients for reactions involving the first 72 vibrational levels
(corresponding to $\nu_1^{max}=2$, $\nu_2^{max}=5$ and $\nu_3^{max}=5$)
✓ validated against time-resolved in situ FTIR measurements of the vibrational populations, in pulsed DC glow discharges (published paper)

e-impact, VV and VT rate coefficients for CO_2-N2
✓ validated against time-resolved in situ FTIR measurements, in pulsed DC glow discharges (accepted paper)

Electron and chemical kinetics in vibrationally "cold" CO_2 plasmas
✓ validated against O and CO measurements in continuous DC glow discharges (paper in preparation)

Current status of efforts towards a full CO_2 chemistry coupling electron/vibrational kinetics

(a step-by-step work program)

What we don't know

- ✗ e-impact, VV and VT rate coefficients for reactions involving higher vibrational levels
- ✗ general revision of gas temperature dependence for VV and VT rate coefficients
- ▪ Rate coefficients for reactions involving CO_2-CO, CO_2-O, CO-CO, etc (work in progress)

e-impact / h-impact rate coefficients and mechanisms involving O_2 / O / O_3

- Validation work in progress involving IPFN / LPP / MSU
  (DC glow discharge)

Current needs for data and validation are substantially focused on mechanisms involving heavy species

- Is LXCat evolving towards the inclusion of data for plasma chemistry ?

Molecular CCC data and LXCat

Liam H. Scarlett*, Dmitry V. Fursa#, Igor Bray, Mark C. Zammit
*liam.scarlett@postgrad.curtin.edu.au
#d.fursa@curtin.edu.au

Curtin University
Los Alamos NATIONAL LABORATORY EST. 1943

Current work: *vibrationally-resolved* electron-scattering on H_2.

Scattering on ground electronic ($X\,{}^1\Sigma_g^+$) state to 18 singlet and triplet excited electronic states:

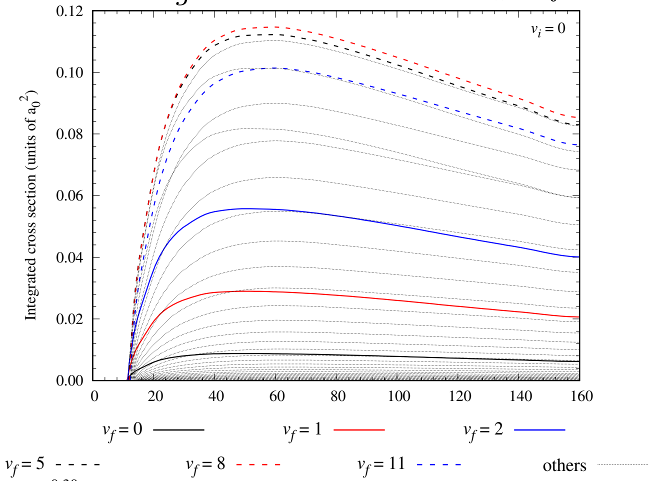
- 15 initial vibrational levels in $X\,{}^1\Sigma_g^+$ state
- 330 total bound vibrational levels in excited electronic states + dissociative excitation
- = more than 5000 cross sections

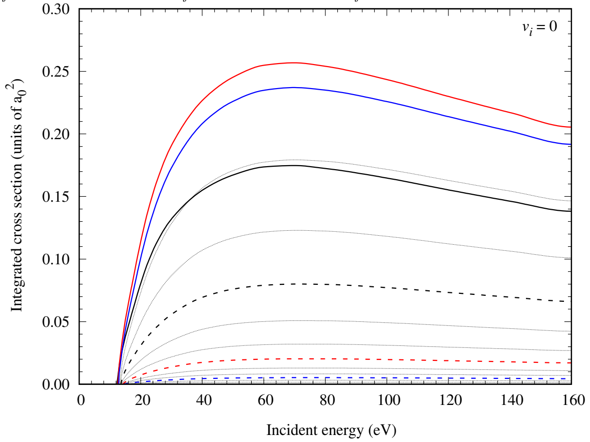
Calculations for D_2 will more than double the number of cross sections (more vibrational levels in heavier molecules)

Bound levels in H_2

state	N_{bound}	state	N_{bound}
$X\ {}^1\Sigma_g^+$	15	$b\ {}^3\Sigma_u^+$	0 (dissociative)
$B\ {}^1\Sigma_u^+$	40	$a\ {}^3\Sigma_g^+$	22
$EF\ {}^1\Sigma_g^+$	33	$c\ {}^3\Pi_u$	22
$C\ {}^1\Pi_u$	14	$e\ {}^3\Sigma_u^+$	8
$B'\ {}^1\Sigma_u^+$	10	$h\ {}^3\Sigma_g^+$	4
$GK\ {}^1\Sigma_g^+$	8	$d\ {}^3\Pi_u$	21
$I\ {}^1\Pi_g$	4	$g\ {}^3\Sigma_g^+$	20
$J\ {}^1\Delta_g$	18	$i\ {}^3\Pi_g$	4
$H\ {}^1\Sigma_g^+$	66	$j\ {}^3\Delta_g$	18
$D\ {}^1\Pi_u$	18		

$X\ {}^1\Sigma_g^+(v_i = 0) \to B\ {}^1\Sigma_u^+(v_f)$





$X\ {}^1\Sigma_g^+(v_i = 0) \to C\ {}^1\Pi_u(v_f)$

Future directions for the molecular CCC project:

Rotational excitations

Scattering on excited electronic states

More complex molecules: HeH^+ and beyond

$\Longrightarrow$ many more large datasets on the way

Molecular CCC data and LXCat

Liam H. Scarlett*, Dmitry V. Fursa#, Igor Bray, Mark C. Zammit
*liam.scarlett@postgrad.curtin.edu.au
#d.fursa@curtin.edu.au

Uploading large datasets to LXCat:

- Impossible to upload thousands of files manually.
  - Need a *user friendly* process for uploading data in an automated way.
- Large number of additional species will make the LXCat interface unusable:
  - Current CCC H_2 data will add an additional 15 target species and 15+ for each new molecule.
  - Several hundred additional excited-state species for each molecule.

Browsing data

- LXCat interface should allow definition of substates
  - e.g. users select electronic state first and on subsequent pages select vibrational/rotational levels.

Downloading data

- Option of downloading an entire dataset as an archived directory with files organized in an easy-to-navigate structure?
  - At present entire sets of data can only be downloaded as a single file.

GEC 2019 LXCat Community Discussion" Wednesday, Oct. 30, 6:30 p.m

M. A. Khakoo, California State U. Fullerton, USA

Experimental differential scattering of low energy electrons from gaseous targets- funded by NSF.

Motivated to provide differential cross section data to test current electron scattering models. Differential (angle) **energy loss spectroscopy**

- H_2 elastic electron scattering and inelastic electronic excitation of the B, c, a, C and E/F electronic states at $E_0 < 20$eV – tests of the Curtin U. CCC model (Zammit, Fursa, Scarlett, Tapley and Bray).
- CO electron excitation of the a, a', A valence states- tests of the UCL R-Matrix model (Masin, Dora and Tennyson)
- Bio-relevant molecules- tests of the multi-channel Schwinger method (Bettega, Homem, Lima, Mu-Tao, Machado)
- Rare Gases excitation lowest valence states, (Bartschat, Zatsarinny)

Elastic Electron Scattering.

#	Gas	E_0 (eV)	θ (°)	Reference
	Elastic Scattering			
1	H_2	1 - 30	10 - 130	Muse et al. J. Phys. B, **41** 095203 (2008)
2	N_2	1 - 30	10 - 130	Muse et al. J. Phys. B, **41** 095203 (2008)
3	Ethylene C_2H_4	2, 5, 10, 20, 30	10 - 130	Khakoo et al. J. Phys. B, **40** 3601 (2007)
3	Ethylene C_2H_4	0.5 - 100	5 - 130	Khakoo et al. Physical Review A, **93** 012710 (2016)
5	Acetaldehyde CH_3CHO	1 - 50	5 - 130	Gauf et al. Phys. Rev. A, **89** 022708 (2014)
6	Pentane C_5H_{12}	1 - 100	5 - 130	Fedus et al. Phys. Rev. A, **91** 42701 (2015)
7	Hexafluoropropene C_3F_6	0.5 - 20	10 - 130	Sakaamini et al. J. Phys. B, 52 25206 (2019)
8	Methanol CH_3OH	1 - 100	"	Khakoo et al. Phys. Rev. A, **77** 042705 (2008)
9	Ethanol C_2H_5OH	1 - 100	"	Khakoo et al. Phys. Rev. A, **77** 042705 (2008)
10	n-Propanol C_3H_7OH	1 - 100	5 - 130	Khakoo et al. Phys. Rev. A, 78 062714 (2008)
11	n-Butanol C_4H_9OH	1 - 100	5 - 130	Khakoo et al. Phys. Rev. A, 78 062714 (2008)
12	isoPropanol C_3H_7OH	1 - 30	10 - 130	Bettega et al. Phys. Rev. A, **84** 042702 (2011)
13	isoButanol C_4H_9OH	1 - 100	5 - 130	Fedus et al. Phys. Rev. A, **90** 032708 (2014)
14	Water H_2O	1 - 100	5 - 130	Silva et al. Phys. Rev. Letts. **101**, 033201 (2008)
14	Water H_2O	1 - 100	"	Khakoo et al. Phys. Rev. A, **78** 052710 (2008)
14	Water H_2O Errata	"	"	Khakoo et al. Phys. Rev. A. **87** 049902(E) (2013)
15	EthylVinylEther $CH_3CH_2OCH{=}CH_2$	0.738 - 50	10 - 130	Khakoo et al. Phys. Rev. A, **81** 022720 (2010)
16	Methyl Chloride CH_3Cl	0.5 - 100	5 - 125	Navarro et al. J. Phys. B, **48** 195202 (2015)
17	Ethyl Chloride C_2H_5Cl	1 - 30	10 - 125	Sakaamini et al. J. Phys. B, **48** 205202 (2015)
18	Dichloromethane CH_2Cl_2	0.5 - 800	10 - 130	Hlousek et al. J. Phys. B, 52 25206 (2019)
19	Chloroform $CHCl_3$	0.5 - 800	10 - 130	Hlousek et al. Phys. Rev. A accepted.
20	Furan C_4H_4O	1 - 50	10 - 130	Khakoo et al. Phys. Rev. A, **81** 062716 (2010).
21	Tetrahydrofuran $(CH_2)_4O$	0.75 - 30	10 - 130	Gauf et al. Phys. Rev. A, **85** 052717 (2012)
22	Toluene $C_6H_5CH_3$	1 - 20	10 - 130	Sakaamini et al. Phys. Rev. A, **93** 042704 (2016)
23	o-Xylene $C_6H_4(CH3)_2$	1 - 30	10 - 130	Sakaamini et al. Phys. Rev. A, **95** 022702 (2017)
24	p-Xylene $C_6H_4(CH3)_2$	1 - 30	10 - 130	Sakaamini et al. Phys. Rev. A, **95** 022702 (2017)
25	m-Xylene $C_6H_4(CH3)_2$	1 - 30	10 - 130	Sakaamini et al. Phys. Rev. A, **95** 022702 (2017)
26	Chlorobenzene C_6H_5Cl	1 - 50	10 - 130	Done
27	Acetonitrile $CH_3C{\equiv}N$	0.7 - 30	10 - 130	Zawadzki and Khakoo, J. Chem. Phys. **149** 124304 (2018)
28	Acrylonitrile $C_2H_3C{\equiv}N$	1 - 30	10 - 130	Done; Zawadzki et al.
29	Benzonitrile $C_6H_5C{\equiv}N$	1 - 30	10 - 130	Done; Zawadzki et al.
30	Dimethyl Ether CH_3OCH_3	1 - 30	10 - 130	Done; Tatreau et al.
31	Diethyl Ether $C_2H_5OC_2H_5$	1 - 30	10 - 130	Done; Tatreau et al.
4	Acetylene $HC{\equiv}CH$	1 - 100	5 - 130	Gauf et al. Phys. Rev. A, **87** 012710 (2013)
32	Propyne $HC{\equiv}C\text{-}CH3$	1 - 30	10 - 130	Done; Tatreau et al.
33	1-Butyne $C_2H_5C{\equiv}CH$	1 - 30	10 - 130	Done; Tatreau et al.
34	2-Butyne $H_3CC{\equiv}CCH_3$	1 - 30	10 - 130	Done; Tatreau et al.

Elastic Electron Scattering (cont-d).

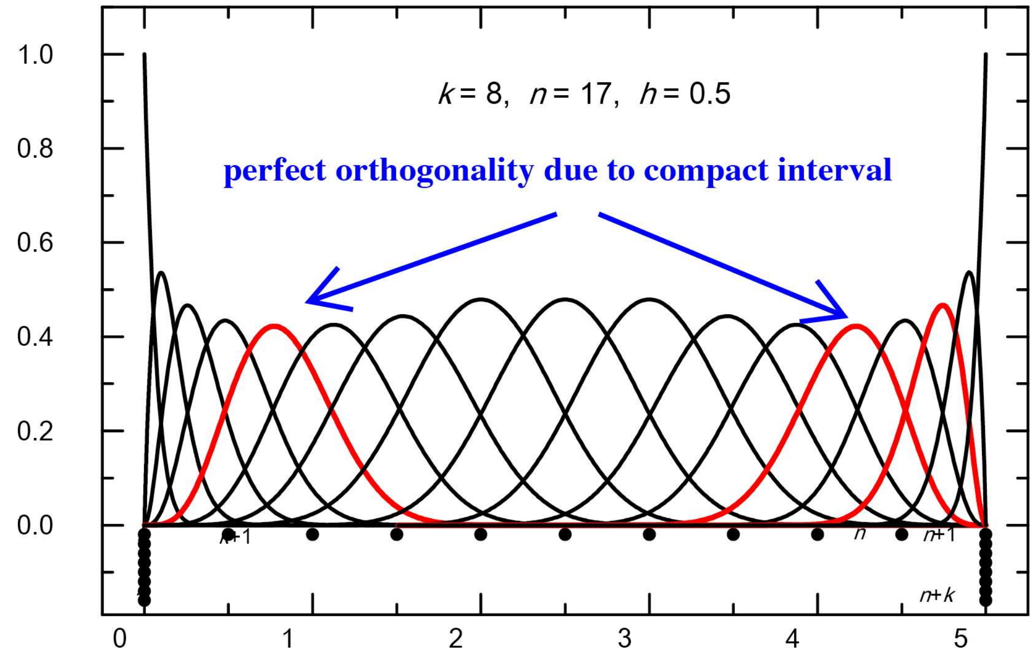
	Elastic to do			
1	Formic H-(C=O)-OH	1 - 30	10 - 130	2020
2	Acetic CH_3-(C=O)-OH	1 - 30	10 - 130	2020
3	PropionicC_2H_5-(C=O)-OH	1 - 30	10 - 130	2020
4	Butyric C_3H_7-(C=O)-OH	1 - 30	10 - 130	2020
5	Methyl Amine CH_3NH_2	1 - 30	10 - 130	2020
6	Ethyl Amine $CH_3CH_2NH_2$	1 - 30	10 - 130	2020
7	Dimethyl Amine CH_3NHCH_3	1 - 30	10 - 130	2020
8	Trimethyl Amine $(CH_3)_3N$	1 - 30	10 - 130	2020

Inelastic Electron Scattering.

	Inelastic Scattering			
1	H_2O Vibrational	1 - 100	10 - 130	Khakoo et al. Physical Review A, **79** 052711 2009
2	Ethylene Vibrational	1.5, 1.75, 2.0, 3.0, 5.0 eV, 8.0, 15	10 - 130	Khakoo et al. Physical Review A, **93** 012710 (2016)
3	Furan Vibrational	5, 6, 7.5, 10, and 15	10 - 130	Hargreaves et al. Phys. Rev. A, **84** 062705 (2011)
4	Furan Electronic	5, 6, 7.5, 10, and 15	10 - 130	da Costa et al. Phys. Rev. A, **85** 062706 (2012)
5	Methanol Electronic	9, 10, 15, 20	10 - 130	Varela et al.J. Phys. B, **48** 115208 (2015)
6	Ethanol Electronic	10, 12.5, 15, 17.5, 20	15 - 130	Hargreaves et al. Phys. Rev. A, **84** 062705 (2011)
7	H_2 Electronic	14, 15, 16, 17.5, 20	15 - 130	Hargreaves et al. J. Phys. B **50**, 225203, (2017)
8	N_2 Electronic	10, 12.5, 15, 17.5, 20, 30, 50, 100	10 - 130	Khakoo et al., Phys. Rev. A, **71**, 062703 (2005)
	Ne, Ar, Kr, Xe	10, 12.5, 15, 17.5, 20, 30, 50, 100	10 - 130	Khakoo et al., Phys. Rev. A 1998-2011 (6 papers)
9	CO Electronic	6.3, 6.5, 7, 8, 9, 10,12.5, 15, 17.5, 20	15 - 130	Zawadzki et al. Phy. Rev A in preparation (2019 or 2020).
	Inelastic to do			
1	NO	Electronic; threshold - 20 eV		2021 - 2022 ?
2	Acetylene $HC\equiv CH$	Vibrational and Electronic; 1 eV to 20 eV		2021 - 2022 ?

General B-Spline R-Matrix (Close-Coupling) Programs (D)BSR

- **Key Ideas:**
  - Use ***B*-splines as universal basis** set to represent the continuum orbitals
  - Allow **non-orthogonal orbital sets** for bound and continuum radial functions



- **Consequences:**
  - **Much improved target description possible with small CI expansions**
  - **Consistent description of the *N*-electron target and (*N*+1)-electron collision problems**
  - No "Buttle correction" since *B*-spline basis is effectively complete
- **Complications:**
  - Setting up the Hamiltonian matrix can be very complicated and lengthy
  - Generalized eigenvalue problem needs to be solved
  - Matrix size typically 10,000 and higher due to size of *B*-spline basis
  - Rescue: Excellent numerical properties of *B*-splines; use of (SCA)LAPACK *et al.*

List of calculations with the BSR code (rapidly growing)

hν **+ Li**	Zatsarinny O and Froese Fischer C *J. Phys. B* **33** 313 (2000)
hν **+ He^{-}**	Zatsarinny O, Gorczyca T W and Froese Fischer C *J. Phys. B.* **35** 4161 (2002)
hν **+ C^{-}**	Gibson N D *et al.* Phys. Rev. A **67**, 030703 (2003)
hν **+ B^{-}**	Zatsarinny O and Gorczyca T W Abstracts of XXII ICPEAC (2003)
hν **+ O^{-}**	Zatsarinny O and Bartschat K *Phys. Rev. A* **73** 022714 (2006)
hν **+ Ca^{-}**	Zatsarinny O *et al. Phys. Rev. A* **74** 052708 (2006)
e + He	Stepanovic *et al. J. Phys. B* **39** 1547 (2006)
	Lange M *et al. J. Phys. B* **39** 4179 (2006)
e + C	Zatsarinny O, Bartschat K, Bandurina L and Gedeon V *Phys. Rev. A* **71** 042702 (2005)
e + O	Zatsarinny O and Tayal S S *J. Phys. B* **34** 1299 (2001)
	Zatsarinny O and Tayal S S *J. Phys. B* **35** 241 (2002)
	Zatsarinny O and Tayal S S As. J. S. S. **148** 575 (2003)
e + Ne	Zatsarinny O and Bartschat K *J. Phys. B* **37** 2173 (2004)
	Bömmels J *et al.* Phys. Rev. A **71**, 012704 (2005)
	Allan M *et al. J. Phys. B* **39** L139 (2006)
e + Mg	Bartschat K, Zatsarinny O, Bray I, Fursa D V and Stelbovics A T *J. Phys. B* **37** 2617 (2004)
e + S	Zatsarinny O and Tayal S S *J. Phys. B* **34** 3383 (2001)
	Zatsarinny O and Tayal S S *J. Phys. B* **35** 2493 (2002)
e + Ar	Zatsarinny O and Bartschat K *J. Phys. B* **37** 4693 (2004)
e + K (inner-shell)	Borovik A A *et al. Phys. Rev. A,* **73** 062701 (2006)
e + Zn	Zatsarinny O and Bartschat K *Phys. Rev. A* **71** 022716 (2005)
e + Fe^{+}	Zatsarinny O and Bartschat K *Phys. Rev. A* **72** 020702(R) (2005)
e + Kr	Zatsarinny O and Bartschat K *J. Phys. B* **40** F43 (2007)
e + Xe	Allan M, Zatsarinny O and Bartschat K *Phys. Rev. A* 030701(R) (2006)
Rydberg series in C	Zatsarinny O and Froese Fischer C *J. Phys. B* **35** 4669 (2002)
osc. strengths in Ar	Zatsarinny O and Bartschat K *J. Phys. B: At. Mol. Opt. Phys.* **39** 2145 (2006)
osc. strengths in S	Zatsarinny O and Bartschat K *J. Phys. B: At. Mol. Opt. Phys.* **39** 2861 (2006)
osc. strengths in Xe	Dasgupta A *et al. Phys. Rev. A* **74** 012509 (2006)

About the project

The **Plasma Data Exchange Project** is a community-based project which was initiated as a result of a public discussion held at the 2010 Gaseous Electronics Conference (GEC), a leading international meeting for the **Low-Temperature Plasma** community. This project aims to address, at least in part, the well-recognized needs for the community to organize the means of collecting, evaluating and sharing data both for modeling and for interpretation of experiments.

At the heart of the Plasma Data Exchange Project is **LXCat** (pronounced "elecscat"), an open-access website for collecting, displaying, and downloading electron and ion scattering cross sections, swarm parameters (*mobility, diffusion coefficient, etc.*), reaction rates, energy distribution functions, etc. and other data required for modeling low temperature plasmas. The available data bases have been contributed by members of the community and are indicated by the contributor's chosen title.

> This is a dynamic website, evolving as contributors add or upgrade data. Check back again frequently.

Supporting organizations

Laplace · cnrs · Plasmas Froids · Chatham University · Colorado Kinema · Curtin University of Technology · CERN · Técnico Lisboa · Drake University · Quantemol · Institute of Space and Astronautical Science · York · ABB · TU/e · STAE Toulouse · Australian National University · Plasma Matters.

FAST NAVIGATION

« PREV NEXT »

NEWS AND EVENTS

2018-07-10 | New links to software

Links have been added to a multi-term Boltzmann solver, and to three tools by Mikhail Benilov and co-workers. Visit the recommended software page.

RECENT PUBLICATIONS

2019-03-05 | NEW UNPUBLISHED NOTES

Data needed for modeling low-temperature plasmas by LC Pitchford … read more »

PROJECT STATISTICS

Scattering cross sections: 24 databases | 94 x 415 species | 21.1k records | updated: 30 April 2019

Differential scattering cross sections: 4 databases | 29 species | 517 records | updated: 12 March 2019

Interaction potentials: 1 database | 78 x 8 species | 646 records | updated: 30 April 2019

Oscillator strengths: 1 database | 65 species | 150 records | updated: 25 November 2013

Swarm / transport data: 15 databases | 362 x 108 species | 169.4k records | updated: 30 April 2019

Publications, notes and reports: 5 databases | 30 records | updated: 5 March 2019

BSR (Quantum-mechanical calculations by O. Zatsarinny and K. Bartschat)

PERMLINK: www.lxcat.net/BSR

DESCRIPTION: The results in this database are from a semirelativistic Breit-Pauli B-spline R-matrix (close coupling) treatment of e-Ar collisions. An individually optimized, term-dependent set of non-orthogonal valence orbitals was used to account for the strong term dependence in the one-electron orbitals. The predictions have been validated against a number of benchmark experimental data measured in crossed-beam setups. Particularly good agreement was achieved in the near-threshold resonance regime, where the excitation process is dominated by negative-ion resonances.

CONTACT: O. Zatsarinny and K. Bartschat
Drake University
Des Moines, Iowa 50311, USA
e-mails: oleg_zoi@@yahoo.com and klaus.bartschat@@drake.edu

HOW TO REFERENCE: O. Zatsarinny and K. Bartschat 2004 J. Phys. B: At. Mol. Opt. Phys. 37 4693 and
M. Allan, O. Zatsarinny, and K. Bartschat 2006 Phys. Rev. A 74 030701 (R).

SCATTERING CROSS SECTIONS

Species: e + **Ar {30}** , **Be {19}** , **C {63}** , **F {8}** , Kr [70], **N {27}** , Ne [34], Xe [76]

Updates: 2011-06-28 … 2017-09-09

Downloads: 5020 times from 2010-11-21

DIFFERENTIAL SCATTERING CROSS SECTIONS

Species: e + Ar [62]

Updates: 2013-11-06 … 2016-05-29

Downloads: 1219 times from 2013-11-07

Conclusions

- The non-orthogonal orbital technique allows us account for **term-dependence** and **relaxation** effects practically to full extent. At the same time, this reduce the size of the configuration expansions, because we use **specific non-orthogonal sets of correlation orbitals** for different kinds of correlation effects.
- ***B***-spline multi-channel models allow us to treat entire Rydberg series and can be used for accurate calculations of oscillator strengths for states with **intermediate and high *n*-values**. For such states, it is difficult to apply standard CI or MCHF methods.
- The accuracy obtained for the low-lying states is close to that reached in large-scale MCHF calculations.
- **Good agreement with experiment** was obtained for the transitions from the ground states and also for transitions between excited states.
- **Calculations performed in this work**: s-, p-, d-, and f-levels up to ***n* = 12**.

```
Ne – 299 states  –  11300 transitions
Ar – 359 states  –  19000 transitions
Kr – 212 states  –   6450 transitions
Xe – 125 states  –   2550 transitions
```

- **All calculations are fully *ab initio*.**
- The **computer code BSR** used in the present calculations and the results for Ar were recently published:

BSR: O. Zatsarinny, Comp. Phys. Commun. **174** (2006) 273
Ar: O. Zatsarinny and K. Bartschat, J. Phys. B **39** (2006) 2145

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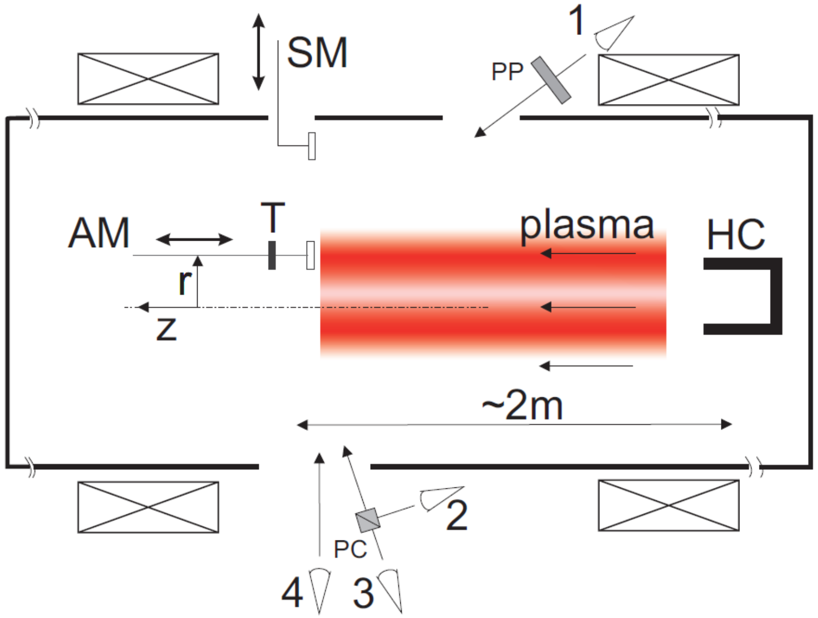
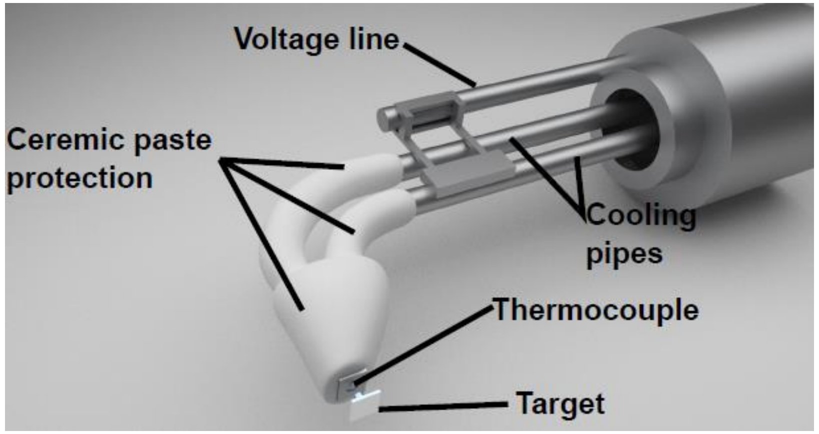
Testing the atomic data of low-temperature plasmas at the linear device PSI-2

O. Marchuk, S. Brezinsek, S. Dickheuer, S. Ertmer and Ph. Mertens

Forschungszentrum Jülich GmbH - Institut für Energie- und Klimaforschung - Plasmaphysik,
Partner of the Trilateral Euregio Cluster (TEC), 52425 Jülich, Germany

EXPERIMENTAL SETUP





- Emission and absorption spectroscopy (Ar/Kr/ArH/KrH)

- **Low-density/coronal experimental conditions**

  - Ratio of metastables (probably rather precise)
  - Absolute values of metastable (less precise)
  - Line intensities (gas / sputtered / reflected)
  - Diffusion + Abel Inversion

Plasma pressure : 0.01…0.1 Pa

Electron temperature: 3..10 eV / Ion temperature 1- 3 eV

Electron density: $10^{10}…10^{11}$ cm^{-3}

Magnetic field: 0.025…0.1 T

Ionization degree: 1-5%

Target: $13x13mm^2$

Kreter A. et al, Fusion Sci. Technol. **68**, 8 (2015)
Dickheuer S. et al, Atoms **7** **(48)** (2019)
Marchuk O. et al, Atoms 7 (**81**) (2019)

EXAMPLE

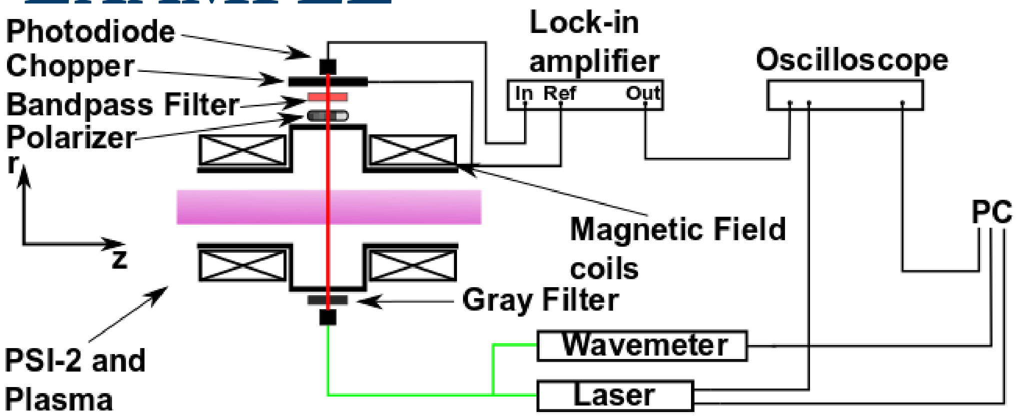


Fig. 1: Schematic setup of the TDLAS system at the PSI-2 device

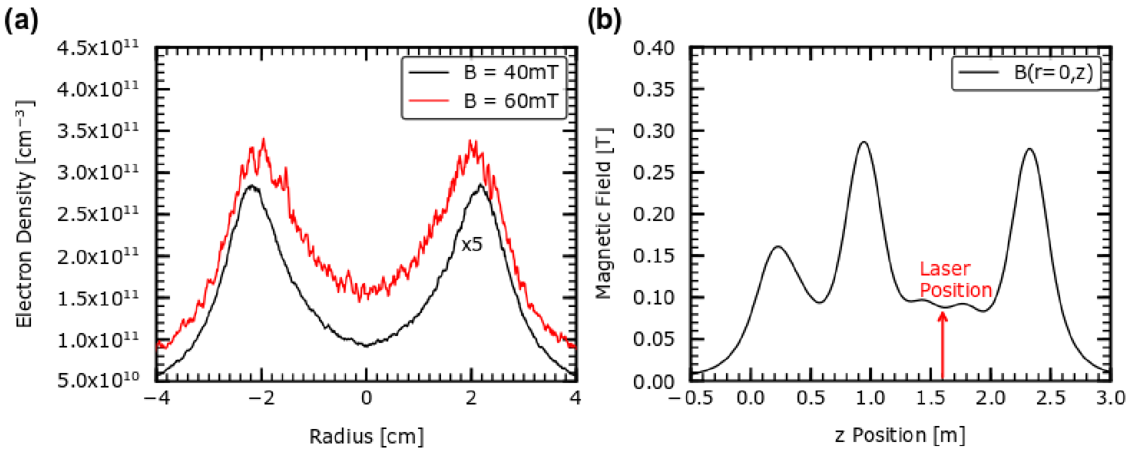
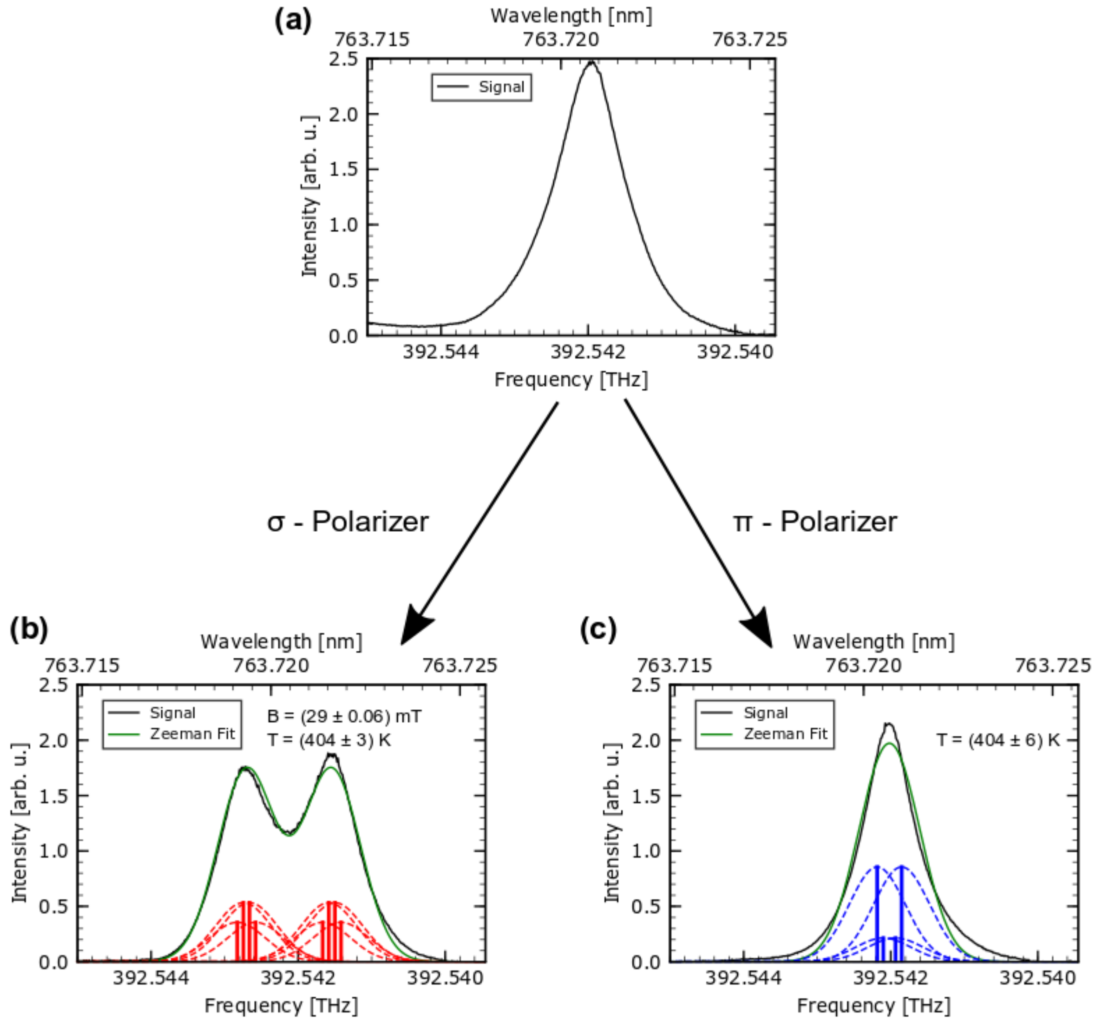


Fig. 2: (a) Measured electron density for the magnetic field configuration B = 40 mT and B = 60 mT measured with a Langmuir probe. Note that the black curve (B = 40 mT) is multiplied by a factor of five to be in the same scale. Note, a negative radius means that the langmuir probe is moving into the plasma, a positive means the probe is moving out of the plasma. (b) Calculated magnetic field of the PSI-2 device at r = 0 m along the z -axis.The position of the laser measurement is marked with the red arrow.

Dickheuer S et al, Atoms **7** (**48**) (2019)

- Measurements of Ar^m (J=2)



JÜLICH Forschungszentrum

LXCAT Data Needs and Los Alamos Data Capabilities

Mark C. Zammit[1]

[1] *Los Alamos National Laboratory, Los Alamos, United States*

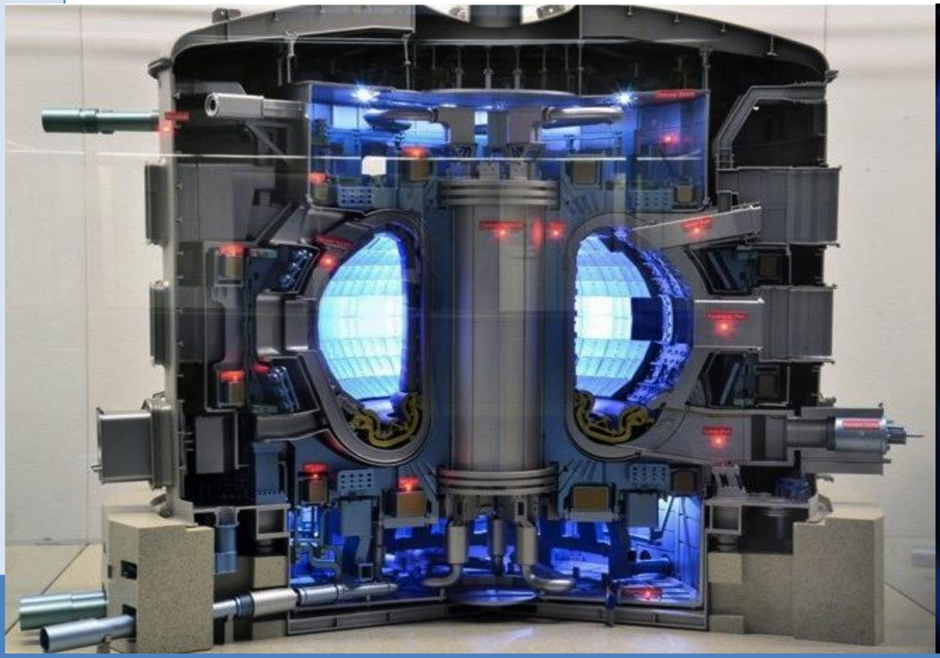
Los Alamos
NATIONAL LABORATORY
EST. 1943

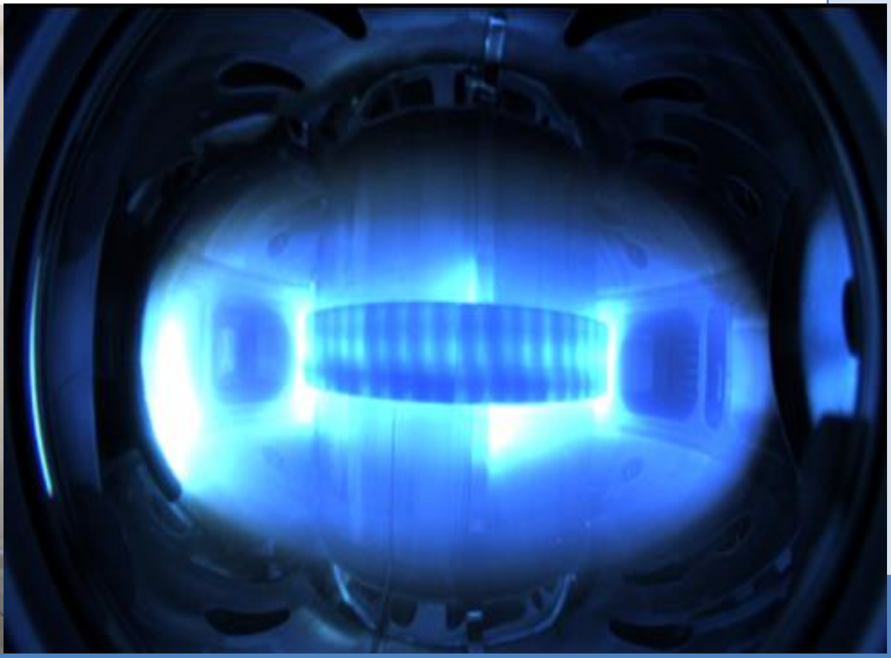
LXCAT Data Needs

Fusion Tokamak Plasma Devices:

- Electron collision **angle** and **energy differential** cross sections
  - Atoms: H, He, Li, Be, C, **N**, **Ne**, **Ar**, W.
  - Ions: for the above.
  - Molecules: H_2, D_2, T_2, DT, and other molecules of fusion tokamak interest.

- Atom+atom, atom+ion, ion+ion cross sections E=1 eV to 1 keV for the above, multi-electron targets and molecules.





Curtin University and Los Alamos National Lab

Curtin University Institute of Theoretical Physics

- Research electron (e^-) and positron (anti-electron e^+) **molecules** using *ab-initio* approaches.
- Developed convergent close-coupling (CCC) method.
- Vibrationally resolved cross sections.
- Rotationally resolved cross sections coming soon ☺

Los Alamos National Laboratory Atomic Physics Group

- Developed general codes for atomic structure, γ-, and e^--collisions (all atoms/ion stages).

  aphysics2.lanl.gov/tempweb/lanl - atomic structure and e^--collisions.

  aphysics2.lanl.gov/opacity/lanl - atomic opacities H – Zn (up to Kr coming soon ☺).
- Research LTE and non-LTE plasmas (opacities, EoS, radiation transport).
- Absorption and emission from a wide varied of plasma types

  (laser produced, ICF, magnetic fusion, and astrophysical).
- Developing *ab-initio* **photon-molecule** codes.