

# A+M Data Center Activities in National Fusion Research Institute (2015~2017)

**DCPP**플라즈마물성데이터센터

Mi-Young Song with PFTR team

Plasma Technology Research Center  
National Fusion Research Institute

# CONTENTS

- A+M Database
- AMBDAS update.
- International Group Data Evaluation Activities
- Activities to Product of Fundamental Electron Scattering Data
- Summary and Future Plan



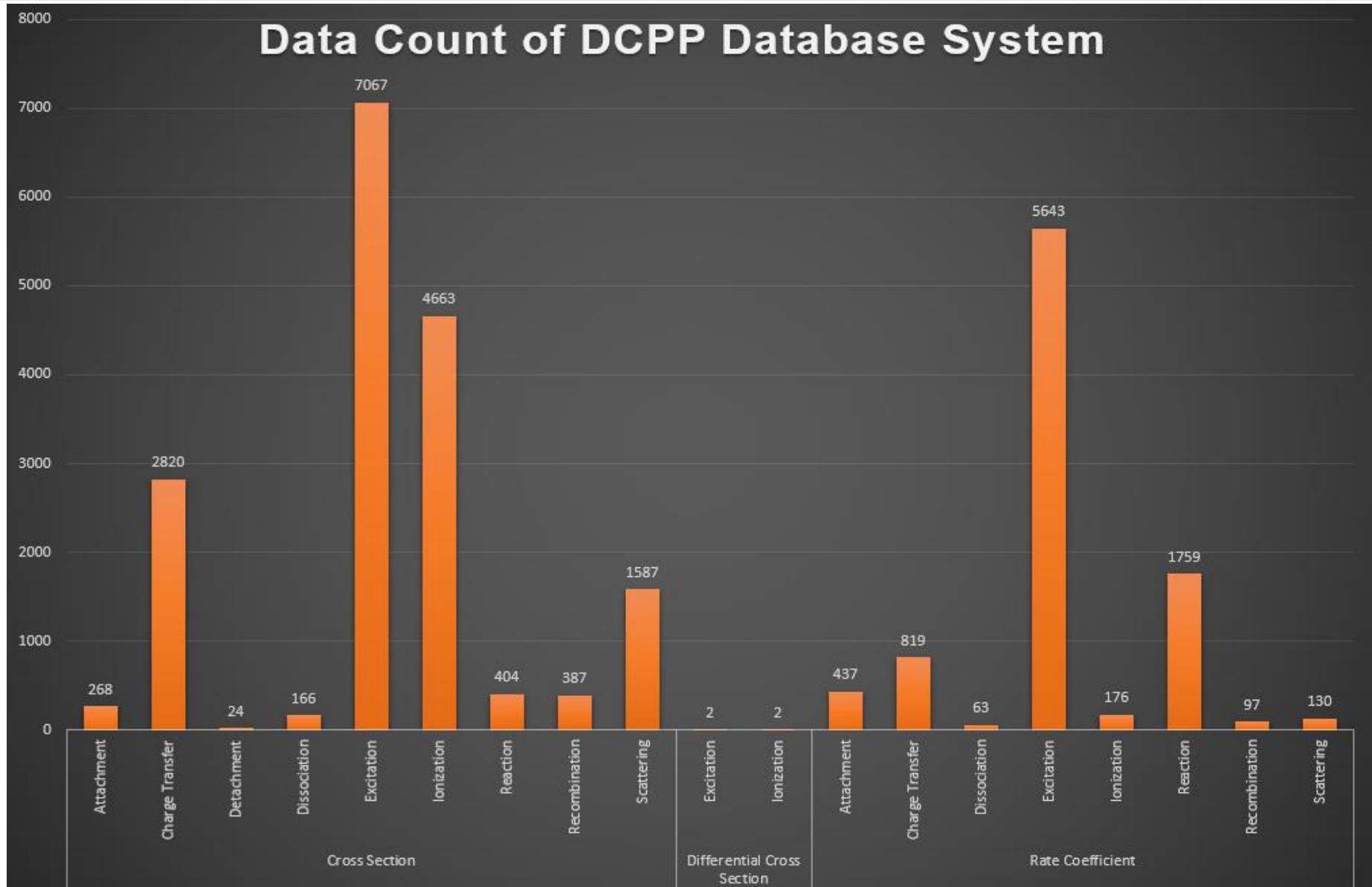
# A+M Database

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# DCPP Web Database System

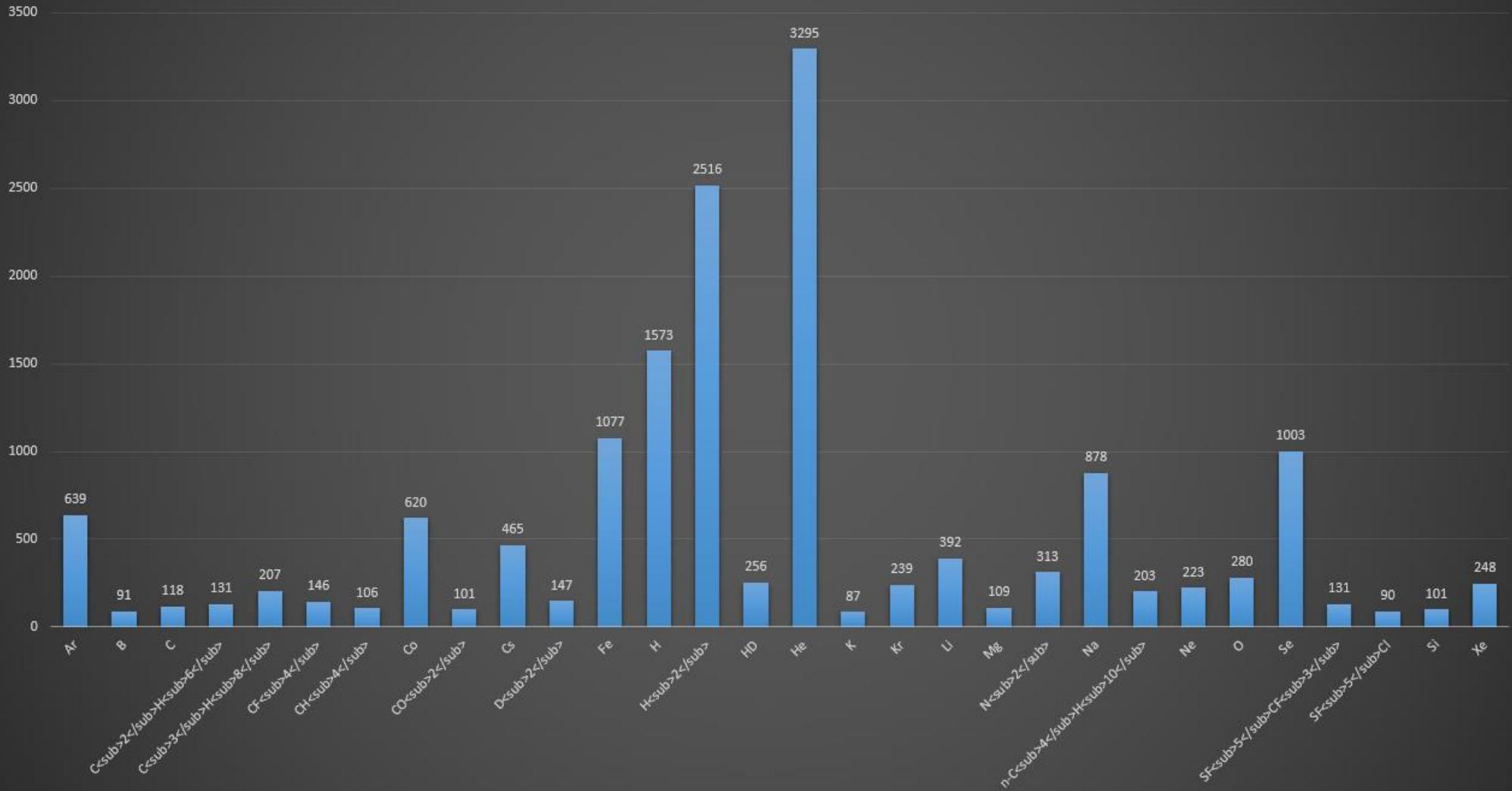
- <http://dcpp.nfri.re.kr>
- Web content
  - Collision cross sections
  - Rate coefficient
  - Electron collision
  - Heavy particle reactions
  - numerical and bibliographic data
  - Evaluation process
- Total amount of data : 26,518 records.
- DCPP web database system is improved by **a new system** that focuses on user convenience.
- We will plan to add plasma-surface reaction data end of this year.

# Data Statistics (1)



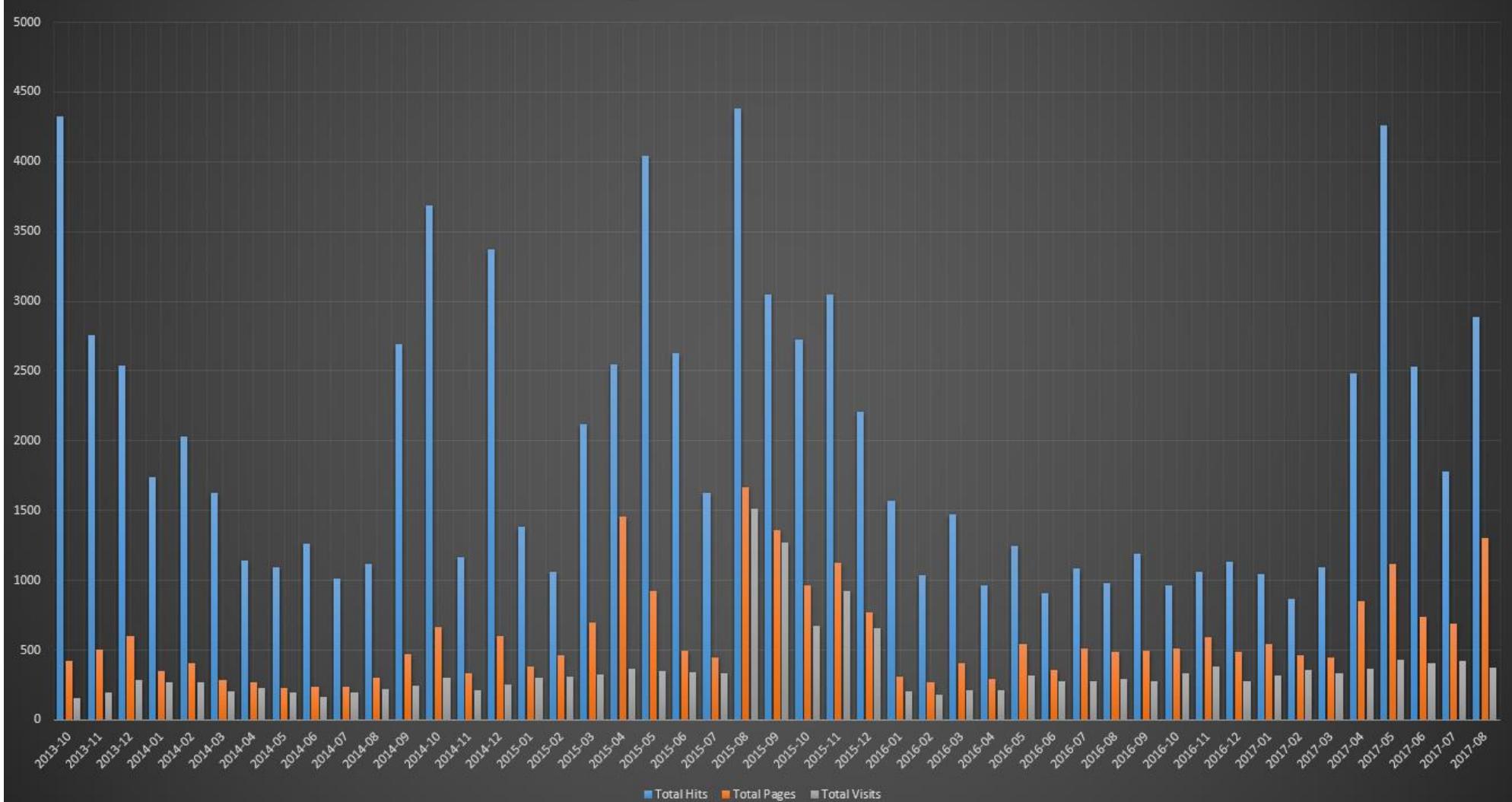
# Data Statistics (2)

## Number of Particles (Top Count 30)



# Access Statistics (Monthly)

## DCPP Web Database System Access Statistics (2013~2017)

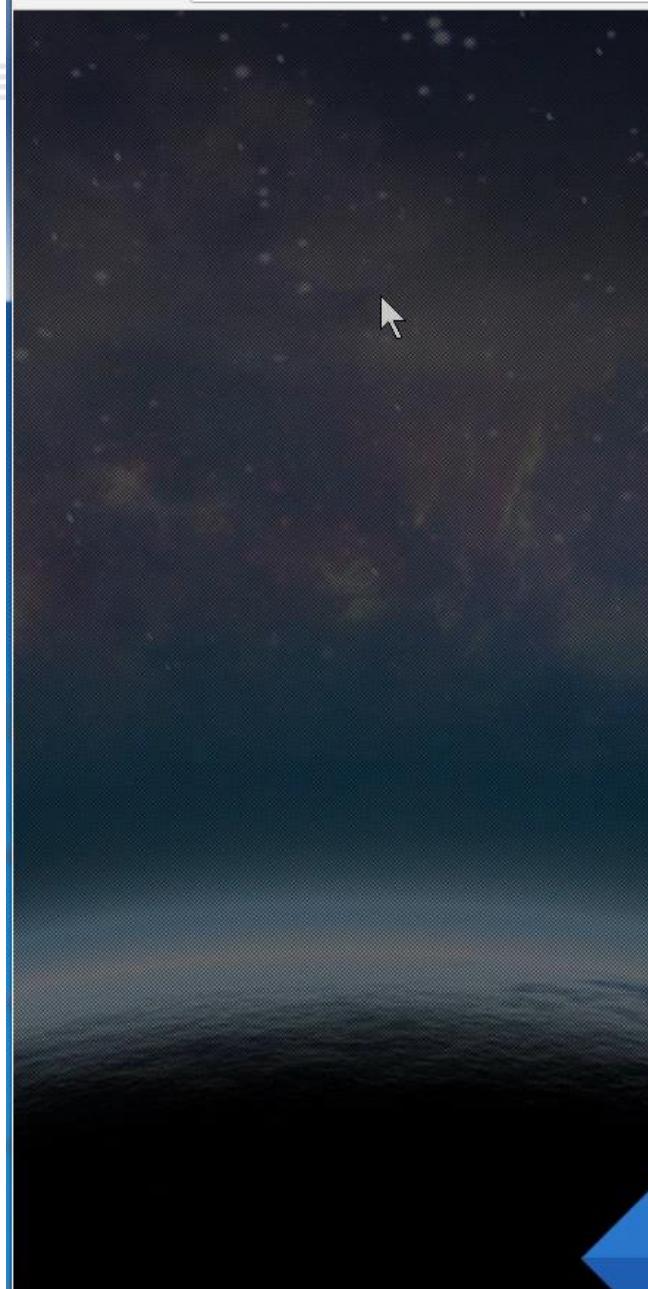


# Evaluated Data (~2017)

Total species : 90

Very small amount data

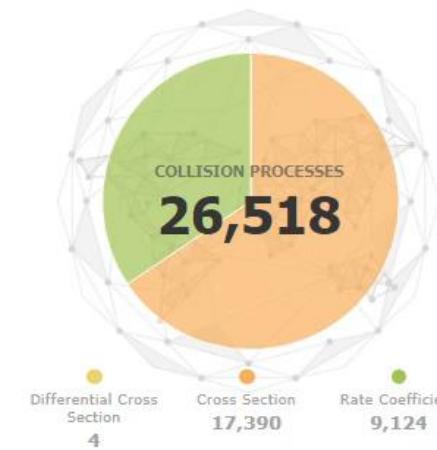
Species	TCS	ES	MT	DCS	TICS	PICS	TDCS	NDCS	TACS	DACS	VI	RO	EX
Atoms	9	2	2	2	2	9	21	0	0	0	0	0	0
2 Atoms	10	6	5	4	4	7	29	2	0	4	4	11	7
3 Atoms	7	4	4	3	3	7	35	1	0	2	9	3	0
4 Atoms	4	4	2	2	2	4	9	0	0	1	2	1	1
5 Atoms	7	7	1	1	2	4	18	0	0	0	0	0	0
CxFy (x=0~4, y=1~8)	28	5	6	5	103	8	45	4	1	4	1	1	0
CHxFy, CClxFy (x=1~3, y=1~3)	4	2	2	2	15	4	34	1	0	1	2	2	0
NFx, SFy (x=1~3, y=1~6)	7	3	2	2	2	3	20	0	0	0	3	0	0
SixYz (x=1~2, Y=Cl, F, H, D, z=1~6)	14	4	2	2	4	10	57	2	4	0	0	0	0
total	90	37	26	23	137	56	268	10	5	12	21	18	8
													28



Data Center for Plasma Properties



SEARCH



SEARCH Collision



SEARCH Surface



SEARCH Thermodynamic



ABOUT Plasma Properties



# **AMBDAS Update**

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# AMBDAS – Journal Collection

- Maintenance of Bibliographical Data on Collisional Processes (AMBDAS).

**NFRI key**

TI=(collision OR excitation OR ionization OR "electron impact" OR ("electron impact" AND excitation) OR ("electron scattering" AND calculations) OR ("cross sections" AND "ionization") OR ("rate" AND ionization) OR (electron AND collisions) OR excited OR (excitation AND D state) OR collisions) AND TS=(collision strengths OR "collisional excitation" OR ("cross sections" AND electron AND impact) OR ("cross sections" AND scattering AND electron) OR ("electron impact" AND excitation) OR ("electron scattering" AND calculations))

TI=(dielectronic recombination OR dissociative recombination OR dissociative attachment OR electron affinity OR electron transport cross-section OR Dirac-Fock calculation OR electron-impact ionization OR electron-impact excitation OR triple differential cross section OR oscillator strength distribution OR Dirac-Fock OR R-matrix OR Born approximation OR distorted-wave approximation OR close-coupling OR electron elastic scattering OR vibrational excitation)

TI=(atomic data OR momentum transfer OR configuration OR scattering) AND TS=(collision strengths OR "collisional excitation" OR ("cross sections" AND electron AND impact) OR ("cross sections" AND scattering AND electron) OR ("electron impact" AND excitation) OR ("electron scattering" AND calculations))

TS=(differential cross section AND (electron ionization OR electron excitation)) OR, (TI=(line measurement) AND TS=(electron excitation)) OR TS=(electron impact detachment OR dissociative electron attachment) OR TI=(electron emission)

Calculation of cross sections of simultaneous ionization and collisional excitation transfer between Cs+2(B(1)Pi(u)) and Cs+(2P(3/2))

Computation of resonance energies and widths in e+/-

Electron excitation of hydrogen atom by ions impact in comet

Electron impact excitation of carbon monoxide in comet

ELECTRON-IMPACT DOUBLE IONIZATION OF TUNGSTEN

Electron-Induced Desorption of Physisorbed H2 on Res

Excitation of (3) F (o) levels of nickel atom by collisions

Experimental differential investigation of state-selective s

Inelastic electron collisions with Rydberg atoms

K-Shell Ionization of Atoms and Ions by Relativistic Pro

Nightside ionosphere of Mars: Modeling the effects of cr

On the hydrogen loss from protonated nucleobases after

A	B	C	D	E	F	G	H
파일명	Title	Authors	Title of Th Volume	Page	Year	DOI	
2009							
<a href="#">Aas_493_687_2009</a>	Rotational excitation Troscon Astronomie A&A 493 687-691				2009	10.1051/	
<a href="#">Aas_493_697_2009</a>	Breit-Pauli R-matrix Hudson Astronomie A&A 493 697-711				2009	10.1051/	
<a href="#">Aas_494_729_2009</a>	Breit-Pauli R-matrix Hudson Astronomie A&A 494 729-733				2009	10.1051/	
<a href="#">Aas_497_911_2009</a>	Rotational excitation Dubern Astronomie A&A 497 911-921				2009	10.1051/	
<a href="#">Aas_498_915_2009</a>	CHIANTI - an atom Dere, K. Astronomie A&A 498 915-921				2009	10.1051/	
<a href="#">Aas_499_943_2009</a>	R-matrix electron-LLiang, C. Astronomie A&A 499 943-951				2009	10.1051/	
<a href="#">Aas_500_1253_2009</a>	Electron-impact ex Burgos, C. Astronomie A&A 500 1253-1.				2009	10.1051/	
<a href="#">Aas_500_1263_2009</a>	R-matrix electron-LLiang, C. Astronomie A&A 500 1263-1.				2009	10.1051/	
<a href="#">Aas_501_619_2009</a>	Cosmic-ray Ionizat Padova Astronomie A&A 501 619-631				2009	10.1051/	
<a href="#">Aas_505_195_2009</a>	Excitation and abu Staebu Astronomie A&A 505 195-201				2009	10.1051/	
<a href="#">Aas_506_955_2009</a>	Ionization process Granoff Astronomie A&A 506 955-961				2009	10.1051/	



**AMBDAS**

Atomic and Molecular Bibliographic Data System

Search Clear

Available Reactant/Surface Codes	Reactant Code	Ion Charge
Reactant 1	H, Na, H <sub>2</sub> O, HF	2, 26, -1
Reactant 2	H, Na, H <sub>2</sub> O, HF	
Isoelectr. Sequence	H, Be, Ca	
Surface	Mg, Ag <sub>2</sub> O, Metal	

Attention: the codes are case-sensitive, i.e., 'Hf' is Hafnium and 'HF' is Hydrogen-Fluorine

Examples are given in green

Category	Process
Structure and Spectra	— Structure and Spectra —
Photon Collisions	Line Shapes and Shifts
Electron Collisions	Structure, Spectra
Heavy Particles Collisions	Interatomic Potentials
Surface Interactions	Polarizabilities, Electric moments
Beam Heating and Fueling of Plasmas	Energy Levels, Wavelengths

Bibliography

Author's name	Mott, N+Mott, Stein*	2 <sup>nd</sup> author's name
Keywords/Patterns	resonance, "electron impact"	Exp vs Theory
Years	98, 1998, 02, 2002	Reference Type

Sort by Year:  | Abstract/Comment:  | Search Case Sensitive:  The maximal allowed number of references is 200.

AMBDAS ALADDIN Comments Home

Job Time	2014	2015	2016	2017
Search period	2009 ~2012	2013	2014	2015
Number of searches	2 weeks	3631	1138	1181
Filtering (1 <sup>st</sup> )	2 weeks	2993	739	814
Original paper collections	2~3 months	2863	527	627
Expert Reviews & update	1 months		433	407
				248

- 
- Key word searching
  - Additional filtering ( only figure or table)
  - Number of journals retrieved : 170 ~ 150
  - Too many papers collected before experts see data
- There is a need to change the filtering method or collection method.

120

## Journal Statistics (TOP 5)

100

80

60

40

20

0

Phys. Rev. A

J. Chem. Phys.

Eur. Phys. J. D

J. Phys. B

Phys. Rev. C

Plasma Sources  
Sci. Technol

■ 2014(814) ■ 2015(751)



# **International Group Data Evaluation Activities**

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# Activities of Data Evaluation

- ❖ Group Data Evaluation project (since 2013)
- ❖ Our purpose
  - To establish and to generate the internationally agree standard reference data library for AM/PMI data
- ❖ Group Members:
  - Grzegorz P. Karwasz (Nicolaus Copernicus University)
  - J. Tennyson (University College London)
  - Viatcheslav kokouoline (University of Central Florida)
  - H. Cho (Chung-Nam National University)
  - Y. Nakamura (Tokyo Denki University)
  - J.-S. Yoon, M.-Y. Song (National Fusion Research Institute)



2014

- 8–9 January 2014, Seoul, South Korea
- 4 –5 July 2014, Cumberland Lodge, UK
- 14 December 2014, Deajeon, South Korea



2015

- 14–15 May 2015, University College London, UK
- 17–19 November 2015, Seoul, Korea



2016

- 13–16 May 2016, University College London, UK
- 27 September 2016, NFRI, South Korea



2017

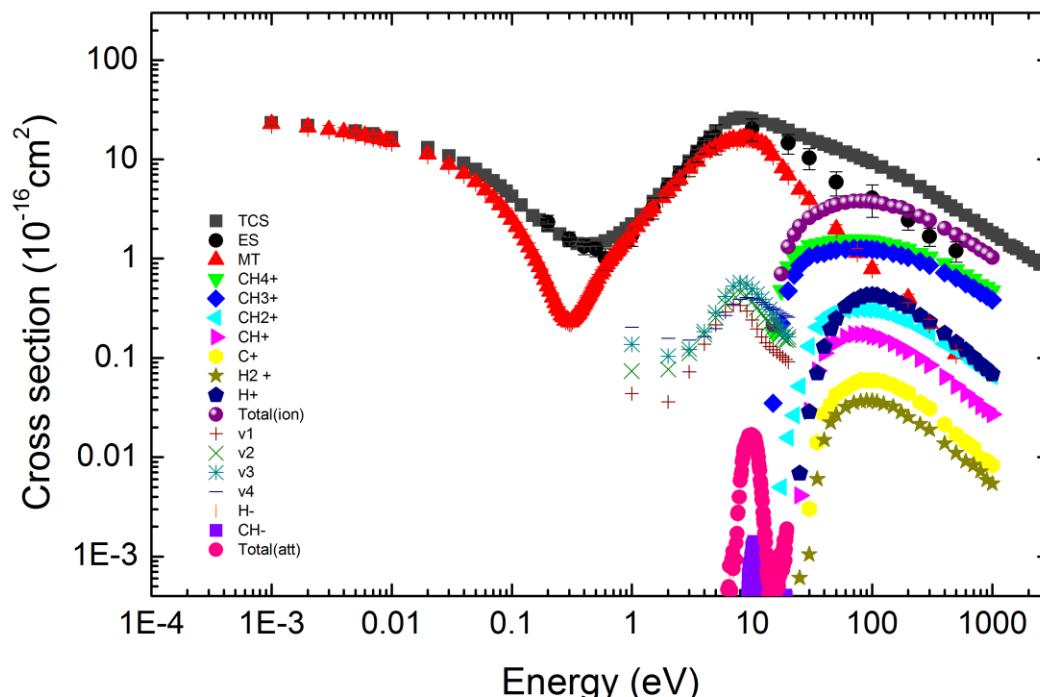
- 16~17 May 2017, Seoul, South Korea
- 13 ~ 14 September, Jeju, South Korea.

# Cross section for electron collisions with Methane

2013 ~ 2014 : review and assessment

2014.12 : submitted article. (J. Phys. Chem. Ref. Data, 44 ,023101, 2015)

- Presentation : 9th International Conference on Atomic and Molecular Data and Their Applications, 21 ~ 25 September 2014, Jena, Germany

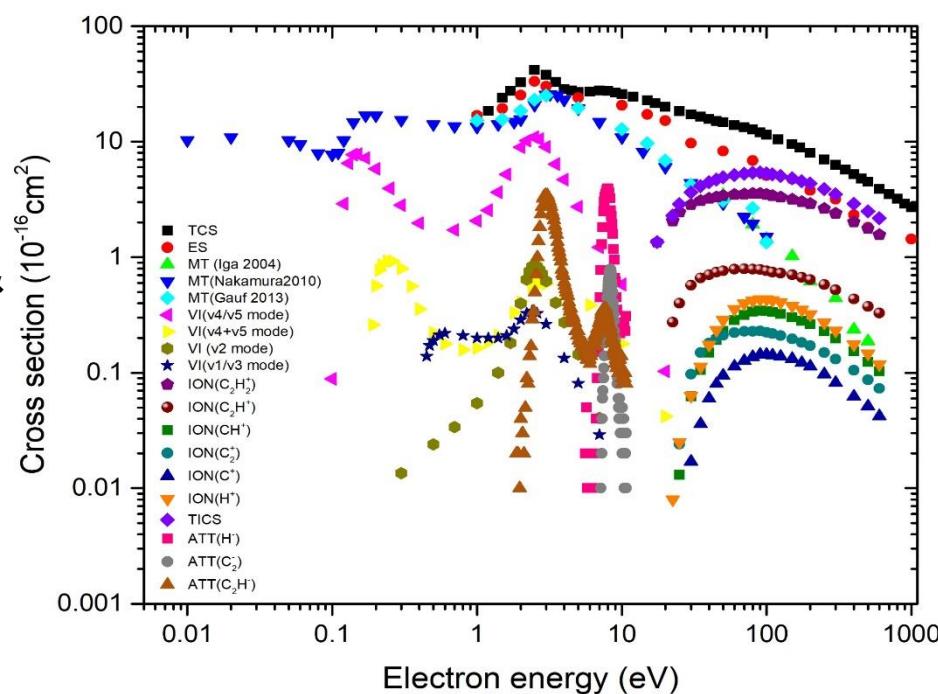


# Cross section for electron collisions with Acetylene

2014 ~2016 : review and assessment

2016.11 : submitted article (J. Phys. Chem. Ref. Data, 47 ,013106, 2017)

- Key evaluation procedures
  - ✓ Swarm method (MTCS, VICS)
- Presentation :
  - ✓ XVIII International Workshop on Low-Energy Positron and Positronium Physics & the XIX International Symposium on Electron-Molecule Collisions and Swarms, 17 - 20 July 2015, Lisboa, Portugal
- Results derived from this project :
  - ✓ Kamil Fedusa and Grzegorz P. Karwasz, "Electron scattering on molecules: search for semi-empirical Indications" Eur. Phys. J. D (2017) 71: 138

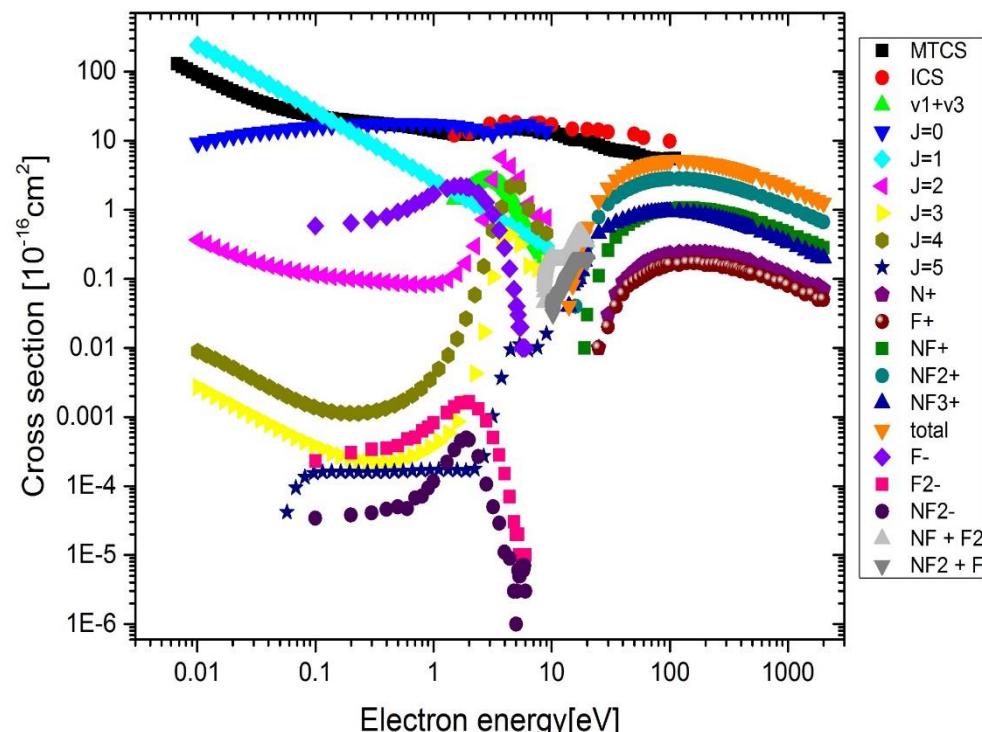


# Cross section for electron collisions with NF<sub>3</sub>

2015 ~2016 : review and assessment

2017.07 : submitted article (J. Phys. Chem. Ref. Data)

- Key evaluation procedures
  - ✓ Swarm method (MTCS, VICS)
  - ✓ New study (rotational excitation, electronic excitation)
- Results derived from this project :
  - ✓ James R Hamilton, Jonathan Tennyson, Shuo Huang and Mark J Kushner, "Calculated cross sections for electron collisions with NF<sub>3</sub>, NF<sub>2</sub> and NF with applications to remote plasma sources" Plasma Sources Sci. Technol. 26 (2017) 065010.



- Five years of team composition, 3 evaluation papers published
- The evaluation group tried to **provide the data set as complete as possible.**
- We are suggesting other researchers to study it , if we don't find any data
- The important data for evaluation is **the total scattering cross-section, and swarm data** is required to verify the dataset
- We plan to make the Group data evaluation project for continuous activity.
- Using know-how, it is possible to evaluate molecular data related to the fusion research.



# **Activities to create Fundamental electron, ion, neutral species Scattering Datasets**

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	A&M	Year	total scattering	scat elastic s cattering	momentum transfer	DCS	total ionization	partial ionization	TDCS	Neutral dissociation	Total attachment	Dissociative attachment	vibration	rotational excitati on	electronic excitation
			TCS	ES	MT	DCS	TICS	PICS	TDCS	NDCS	TACS	DACS	VI	RO	EX
1	H2	2007, 2008	C	V	V	D	Q	Q					V	Q	Q
2	O2	2008	Q	Q	Q	D	Q	V	Q			V	Q	V	
3	N2	2008	Q	Q	V	D	Q	V	Q			Q	Q	Q	Q
5	Xe	2008	V	Q	Q	D	V	V							
6	CF4	2009, 2014	V	V	V	V	V	Q	Q	Q	Q				
7	C2F6	2009, 2015	V	Q	Q	V	V	V	Q	Q	Q				
8	C3F8–2013	2009, 2013, 2015	V	Q	Q	V	V	Q	Q		Q				
9	C4F8–2013	2009, 2013, 2015	V	V	V	V	Q	Q	Q		Q				
10	CF3I–2013	2009, 2013	V			D	Q	Q							
11	CHF3	2009, 2013		V	V	D	V	Q		Q					
12	CCl2F2	2009	Q	Q		D	V	Q							
13	SF6	2009	V	Q	Q	D	Q	Q							
14	CCl4	2010	V			D	V	V							
15	SiF4	2010	V			D	Q	Q							
16	SiF3	2010						Q	Q						
17	SiF2	2010						Q	Q						
18	SiF	2010						Q	Q						
19	Si	2010						Q	Q						
20	SiH4	2010	V	Q	Q	D	V	V	Q						
21	Si2H6	2010	Q	Q	Q	D			Q						
23	NH3	2010	V	Q	Q	D	Q	Q							
27	C	2011						Q	Q						
28	O	2011						Q	Q						
29	N	2011						Q	Q						
30	F	2011						Q	Q						
31	Cl	2011						Q	Q						
32	Br	2011						Q	Q						
33	I	2011						Q	Q						
34	CFx	2011, 2014				Q		Q							
35	NFx	2011						Q							
36	SFx	2011					Q	Q							
37	C2F4	2011, 2015	Q	Q	Q	V	Q	Q				Q			
38	F2	2011						Q	Q			Q			
39	Cl2	2011	V					V	Q						
40	BCl3	2011	Q				Q	Q							

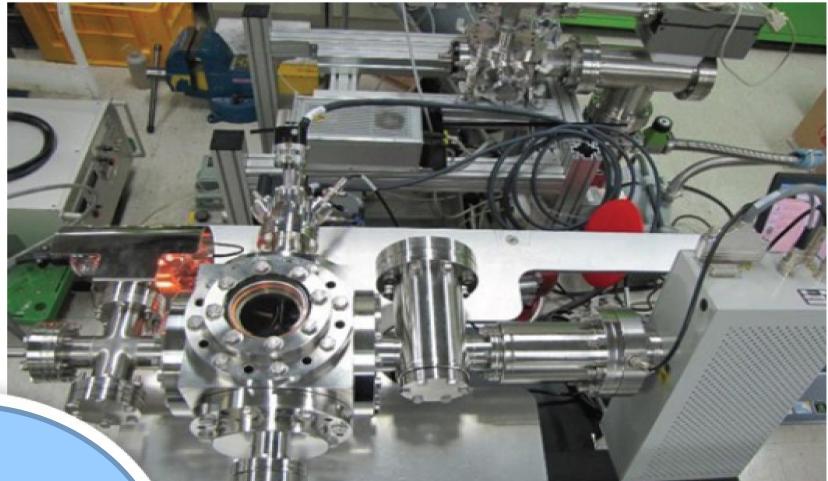
- Insufficient data set  
(excitation, dissociation, ...)

# Experimental measurement



## Total Cross Section

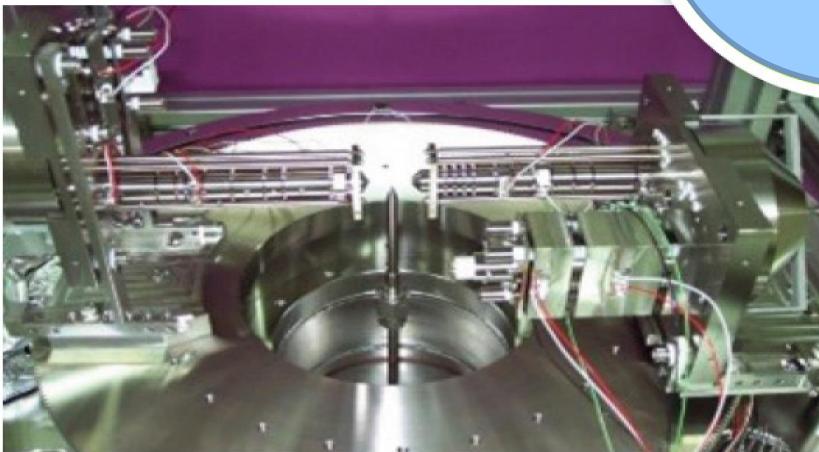
Measurement of total cross sections for electron scattering on atomic and molecules using magnetized electron beam



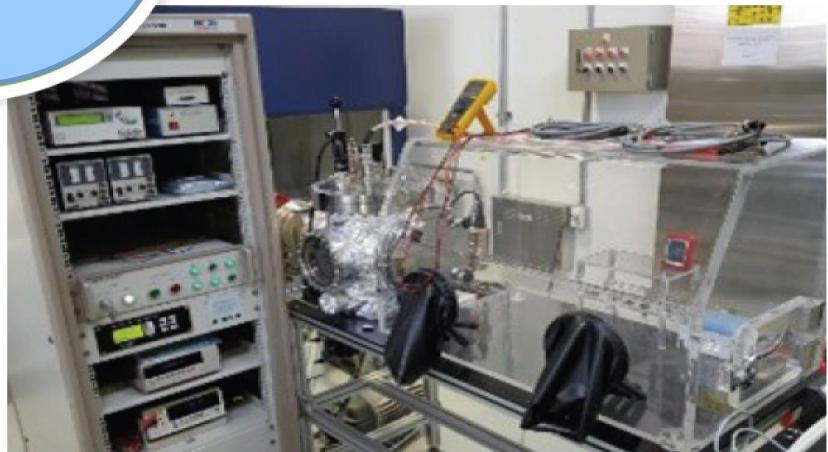
## Dissociation Cross Section

Ionization threshold spectroscopy method

Experimental  
apparatus

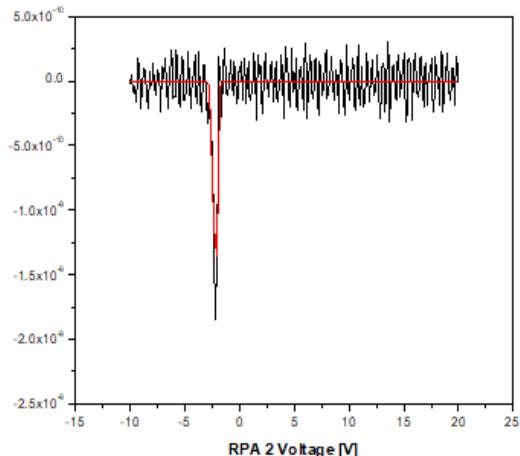


## Elastic Differential Scattering Cross Section

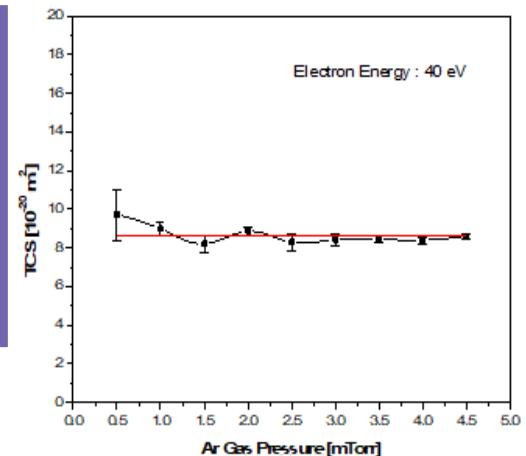


## Biomolecule-Electron Collision Data

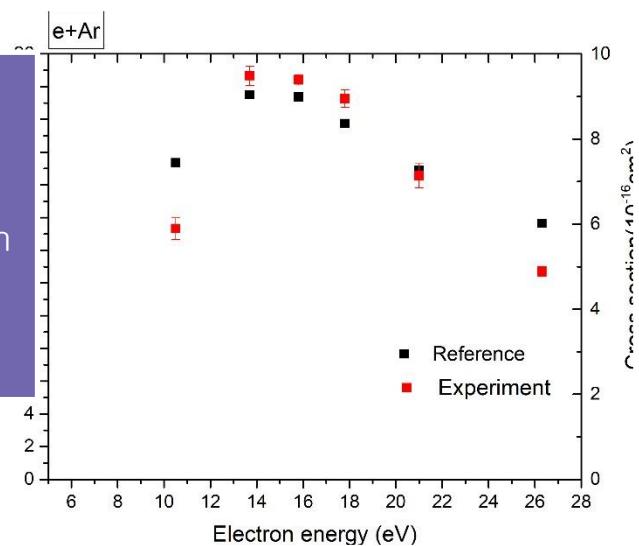
at electron  
energy 1 eV  
DC mode, 500  
Gauss  
FWHM : 0.38 eV



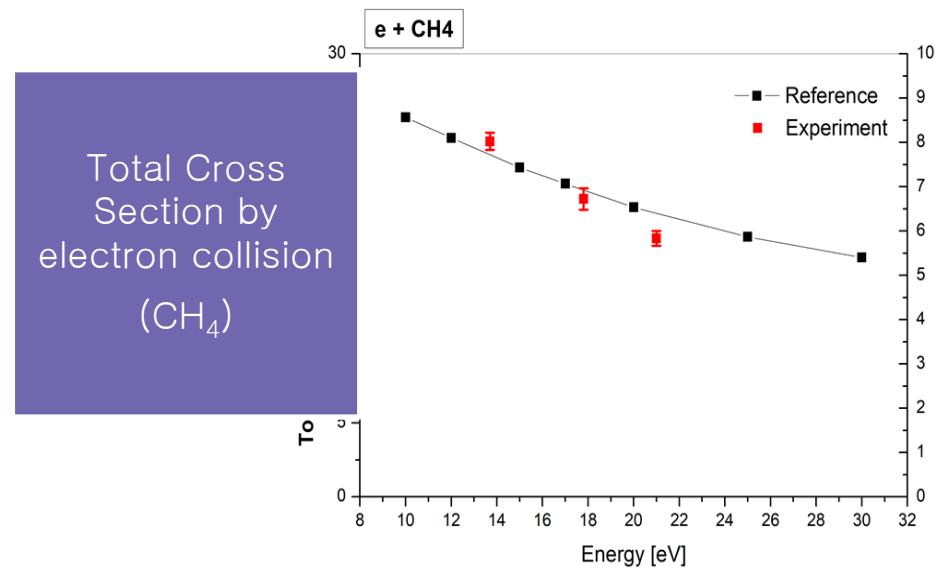
Electron TCS for  
Argon plotted  
against gas  
pressure



Total Cross  
Section by  
electron collision  
(Ar)



Total Cross  
Section by  
electron collision  
(CH<sub>4</sub>)



# Theoretical Calculations

- Total ionization cross section (BEB Model)

$$t = T / B, u = U / B, S = 4 \pi a_0^2 N (R / B)^2$$

$$a_0 = 0.5292 \text{ \AA}, \quad R = 13.60 \text{ eV}$$

at the HF// $\omega$ B97X-D/avtz level

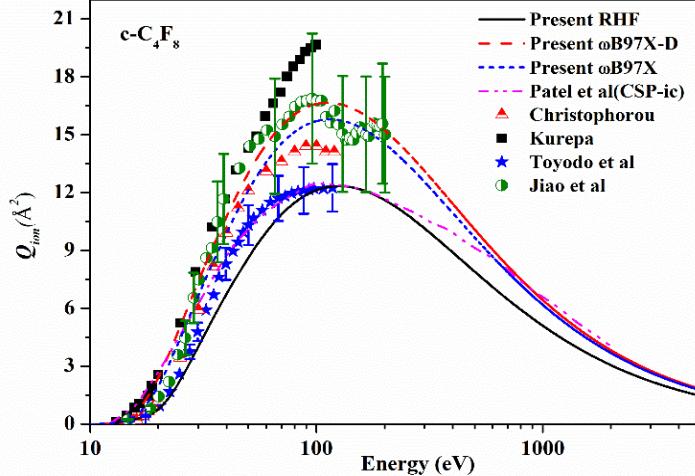
$$\sigma_{\text{BEB}} = \frac{S}{t+u+1} \left[ \frac{\ln t}{2} \left( 1 - \frac{1}{t^2} \right) + 1 - \frac{1}{t} - \frac{\ln t}{t+1} \right]$$

by using the BEB model

$B$  = electron binding energy, eV  
 $U$  = average kinetic energy, eV  
 $N$  = electron occupation number



C<sub>2</sub>F<sub>x</sub> (x=1~6), C<sub>3</sub>F<sub>x</sub> (x=1~8), C<sub>4</sub>F<sub>x</sub> (x=1~8)



DOI 10.1007/s00330-012-7090-6  
 PHYSICAL JOURNAL D  
 Regular Article

## Electron impact ionization cross section studies of C<sub>2</sub>F<sub>x</sub> (x = 1 – 6) and C<sub>3</sub>F<sub>x</sub> (x = 1 – 8) fluorocarbon species\*

Elmano Gupta\*, Hieckil Choi, Mi-Nyeon Song\*, Gyeongsoo F. Kwon† and Jungsik Yoo‡  
 \* Plasma Technology Research Center, National Fusion Research Institute, 37 Donghangan-ro, Gwangju,  
 South Korea; †KAIST, Daejeon, South Korea

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Published online: 22 April 2012 © EDP Sciences, Società Italiana di Fisica, Springer Verlag 2012

Abstract. The total ionization cross section in C<sub>2</sub>F<sub>x</sub> (x = 1 – 6) and C<sub>3</sub>F<sub>x</sub> (x = 1 – 8) fluorocarbon species are studied with the Hartree-Fock (HF) and Density Functional Theory (DFT) methods. All the targets were prepared by their various structures and energies with several electronic methods with the same basis set. The calculated ionization cross sections are compared with the present experimental results with the experimental results for stable targets C<sub>2</sub>F<sub>6</sub>, C<sub>3</sub>F<sub>8</sub> and C<sub>4</sub>F<sub>8</sub>. The results show good agreement with the present experimental results for C<sub>2</sub>F<sub>6</sub>, C<sub>3</sub>F<sub>8</sub> and C<sub>4</sub>F<sub>8</sub>. The present results for C<sub>2</sub>F<sub>6</sub>, C<sub>3</sub>F<sub>8</sub> and C<sub>4</sub>F<sub>8</sub> are in good agreement with the present experimental results for C<sub>2</sub>F<sub>6</sub>, C<sub>3</sub>F<sub>8</sub> and C<sub>4</sub>F<sub>8</sub> reported by Christophorou [1], Kurepa [2] and Toyodo et al. [3]. The present results for C<sub>2</sub>F<sub>6</sub>, C<sub>3</sub>F<sub>8</sub> and C<sub>4</sub>F<sub>8</sub> are compared for the first time in the present study. We have also compared the various ionization potentials and ionization cross sections of C<sub>2</sub>F<sub>6</sub>, C<sub>3</sub>F<sub>8</sub> and C<sub>4</sub>F<sub>8</sub> with the present experimental results [1–3]. A good agreement is found between the present and the previous results. The various ionization potentials in C<sub>2</sub>F<sub>6</sub>, C<sub>3</sub>F<sub>8</sub> and C<sub>4</sub>F<sub>8</sub> are computed for the first time in the present study. The ionization cross sections of C<sub>2</sub>F<sub>6</sub>, C<sub>3</sub>F<sub>8</sub> and C<sub>4</sub>F<sub>8</sub> are computed for the first time in the present study. The ionization cross sections of C<sub>2</sub>F<sub>6</sub>, C<sub>3</sub>F<sub>8</sub> and C<sub>4</sub>F<sub>8</sub> are compared among them, confirming the consistency and reliability of the present data.

\* This article is part of the Special Collection "Cross Sections for Ionization and Ion-Ion Reactions"

† Present address: Institute of Future Materials, Korea Maritime University, Pusan, Korea

‡ Present address: Korea Electric Power Research Institute, Daejeon, Korea

Received: 1 December 2011 / Accepted: 20 April 2012  
 DOI 10.1007/s00330-012-7090-6  
 PHYSICAL JOURNAL D  
 Regular Article

## Electron impact ionization cross section studies of C<sub>2</sub>F<sub>x</sub> (x = 1 – 6) and the isomers of C<sub>3</sub>F<sub>x</sub> and C<sub>4</sub>F<sub>x</sub>

Dhanu Gupta, Hieckil Choi, Deok-Chin Kwon, Jung-Sik Yoon and Mi-Young Song\*  
 Plasma Technology Research Center, National Fusion Research Institute, 37 Donghangan-ro, Gwangju,  
 South Korea; †Jeonju National Institute of Science and Technology, Jeonju, South Korea

Received: 1 December 2011 / Accepted: 20 April 2012  
 DOI 10.1007/s00330-012-7091-7  
 PHYSICAL JOURNAL D  
 Regular Article

Abstract. In the present article, the Binary Encounter Bethe (BEB) method is used for the

calculation of total ionization cross section ( $Q_{\text{ion}}$ ) for C<sub>2</sub>F<sub>x</sub> (x=1~6) fluorocarbon species and the isomers of C<sub>3</sub>F<sub>x</sub> and C<sub>4</sub>F<sub>x</sub> molecules from ionization threshold to 5 keV. The targets are fully atomized using the Hartree-Fock (HF) and Density Functional Theory (DFT). We have obtained a good agreement between the present results and the experimental data using the HF parameters for 1,3-C<sub>2</sub>F<sub>6</sub>, 2-C<sub>2</sub>F<sub>6</sub>, 2-C<sub>2</sub>F<sub>7</sub> and 1-C<sub>2</sub>F<sub>7</sub>. On the other hand, the DFT based  $Q_{\text{ion}}$  shows a good agreement with the present experimental data for C<sub>2</sub>F<sub>6</sub> and C<sub>2</sub>F<sub>7</sub>. The present  $Q_{\text{ion}}$  for C<sub>3</sub>F<sub>8</sub> with HF parameters showed good agreement with the experimental data of Toyoda et al. [4]. Toyoda, M. Ito, and H. Sugai, *Jpn. J. Appl. Phys.*, **36**, 3739 (1997) and the  $Q_{\text{ion}}$  from DFT presented with that of Jiao et al. [5], Q. Jiao, A. Gorczyca, and P. D. Hershaw, *Phys. Plasmas*, **19**, 123301 (2012) are also compared with the present results for C<sub>3</sub>F<sub>8</sub>. The present  $Q_{\text{ion}}$  for C<sub>3</sub>F<sub>8</sub> is in good agreement with the present experimental data. The  $Q_{\text{ion}}$  for the isomers of C<sub>3</sub>F<sub>x</sub> and C<sub>4</sub>F<sub>x</sub> were computed for the first time in the present study. The  $Q_{\text{ion}}$  for the isomers of C<sub>3</sub>F<sub>x</sub> and C<sub>4</sub>F<sub>x</sub> showed very less deviation among each other. The present cross section data are important quantity for low temperature plasma modeling especially related to the fluorocarbon plasmas.

### 1. Introduction

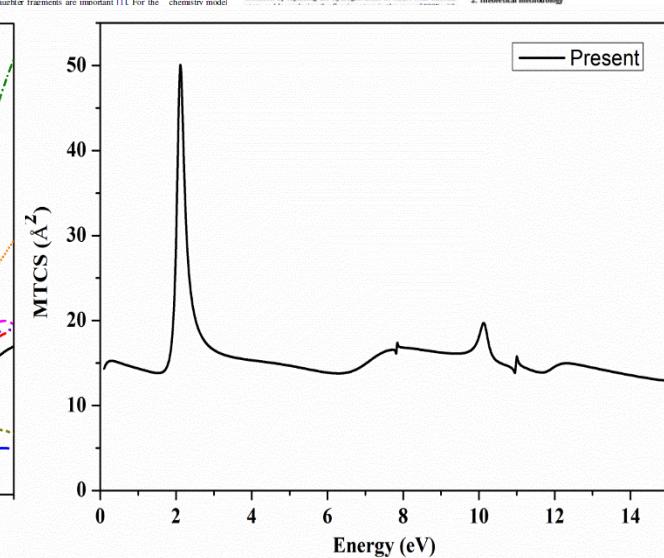
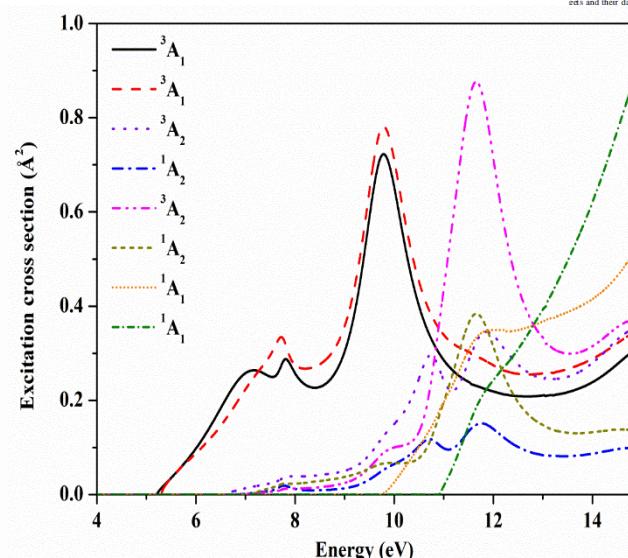
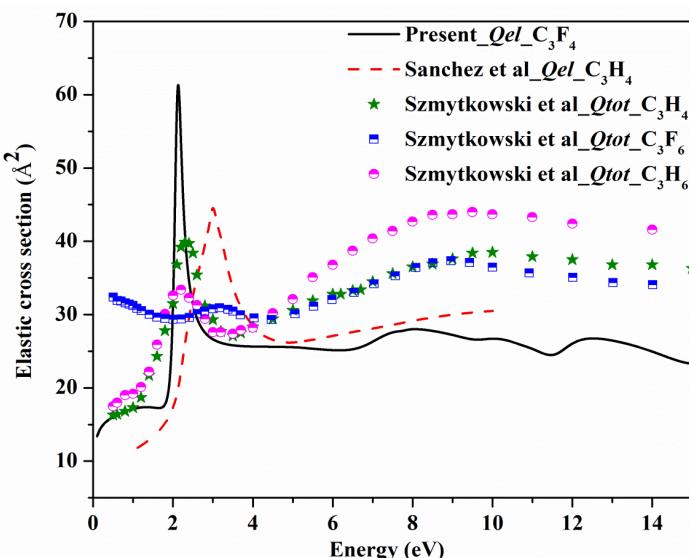
An electron-impact ionization of molecules is the main process for the production of positive ions and free electrons, which is of primary importance for generating and sustaining plasma. The ionization of molecules due to the electron impact leads to the creation of reactive mixture comprised of original gas and secondary active species like radicals and ions used for various plasma based applications [2, 3]. In recent times, C<sub>2</sub>F<sub>6</sub> and C<sub>3</sub>F<sub>8</sub> molecules have been widely used for plasma processing and etching applications in the semiconductor industry. For instance, C<sub>2</sub>F<sub>6</sub> is used for dry etching gas for selective etching of silicon dioxide (SiO<sub>2</sub>) on Si and Si<sub>3</sub>N<sub>4</sub> layers [6, 7]. C<sub>3</sub>F<sub>8</sub> is used in microelectronics fabrication for plasma etching of dielectrics such as SiO<sub>2</sub> and Si<sub>3</sub>N<sub>4</sub> [6, 7]. The electron impact on C<sub>2</sub>F<sub>6</sub> and C<sub>3</sub>F<sub>8</sub> molecules can easily lead to the dissociation of these molecules forming various polymerizing fragments and radicals that increases etch selectivity. The unassisted fluorocarbons (UFCs) (1,3-C<sub>2</sub>F<sub>6</sub> and C<sub>2</sub>F<sub>7</sub>) gases have been investigated considerably due to the Kyoto Protocol's requirement for reduced emission of perfluorocarbons (PFCs) such as C<sub>2</sub>F<sub>6</sub>, C<sub>3</sub>F<sub>8</sub> and C<sub>4</sub>F<sub>8</sub> which has been extensively used for plasma etching applications [8, 9]. The UFCs gases with low global warming potential (GWP) has been

## ● Theoretical Methodology

- ✓ The well-known *ab initio* R-matrix method through Quantemol-N

## ● Target models

- ✓ We have optimized the structure of  $C_xF_y$  using the Density Functional Theory DFT (wB97X-D/aug-cc-pVTZ) using the Gaussian 09



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### Cross sections for electron collision with difluoroacetylene

Dhanoj Gupta<sup>1</sup>, Heechol Choi<sup>1</sup>, Deuk-Chul Kwon<sup>1</sup>, Jung-Sik Yc  
Antony Mi-Young Song<sup>1</sup>

<sup>1</sup>Plasma Technology Research Center, National Fusion Research Institute, 37 Dongjung-Jeonbuk-ro 540-600, Republic of Korea

<sup>2</sup>Atomic and Molecular Physics Laboratory, Department of Applied Physics, Indian Institute of Technology (ISM) Dhanbad, JH 826004, India

E-mail: myoung@nifi.re.kr

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#### Abstract

We report a detailed calculation of total elastic, differential elastic, momentum elastic and excitation for electron impact on difluoroacetylene (C<sub>2</sub>F<sub>2</sub>) molecules. R-matrix method at low energies. After testing many target models, the final result for the target model gave the best target properties and predicted the lowest shape resonance. The shape resonance is detected at 5.36 eV and 6.49 eV with the same intensity. The total excitation cross section is calculated for the C<sub>2</sub>F<sub>2</sub> molecule. The polarization becomes prominent at low energies below 4 eV, decreasing the momentum elastic cross section systematically as it increases for C<sub>2</sub>F<sub>2</sub>. We have also computed the differential, excitation and ionization cross sections by comparing the present results with the available experimental data. The present results are in good agreement with the available experimental data.

A comparison is made between the present results and the available theoretical results for the C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>F<sub>2</sub> and C<sub>2</sub>H<sub>4</sub> with a similar model and compared with the existing available experimental data. The present results are in good agreement with the available experimental data. This comparison shows the reliability of the present results for the cross section for C<sub>2</sub>F<sub>2</sub>. The calculation of elastic scattering cross extended to higher energies up to 53 eV using the spherical complex-potential polarized basis function. The total cross section is calculated for the C<sub>2</sub>F<sub>2</sub> molecule. Finally we report the total ionization cross section using the binary Bethe method for C<sub>2</sub>F<sub>2</sub>. The performance effect in the shape and magnitude of momentum transfer and ionization cross sections when compared with C<sub>2</sub>H<sub>2</sub> trend to the C<sub>2</sub>H<sub>2</sub>-C<sub>2</sub>F<sub>2</sub> and C<sub>2</sub>H<sub>4</sub>-C<sub>2</sub>F<sub>2</sub> systems. The cross-section data article could be an important input for the development of a C<sub>2</sub>F<sub>2</sub> plasma mask etching fluorine atoms have a great environmental impact and hence the understanding of their properties is important. The present results for the impact cross sections are important. Giles et al. [2] first conducted ion-photon coincidence spectroscopy to determine the various spectroscopic properties of monohaloacetylene, HCCl and HCF. They also observed the resonance in HCCl and HCF. Hence, they various applications in atmospheric chemistry, combustion and ultrafast chemistry [1]. Recently, HCCl has been used as a precursor to synthesize HCCH<sub>n</sub> and HNCCH<sub>n</sub> molecules by UV photolysis and the formation of HCCl<sub>n</sub> and HNCCH<sub>n</sub> molecules is a molecule similar to acrylene (HCCH) and difluoroacetylene (HCCF) and offers a very good opportunity to study the effect of fluorination by replacing the hydrogen atom in HCCl with fluorine.

#### 1. Introduction

Functional electron-molecule collisions and molecular dynamics are one of the major physical interactions that help to determine the behavior of plasmas. In developing models of plasma reactors and testing their success for various plasma processing gases, the absolute electron scattering cross sections for molecular targets and their daughter fragments are important [1]. For the

equations and to cross section of colliding partial plasma particle interact plasma properties particle similar plasma properties chemistry model

have been soft-surface and characterized both experimentally [6–8] and theoretically [9–12]. In our previous work, we characterized the  $\pi^+$  resonance for FCFC and found that it lies at higher energy compared to HCCl. Hence, it is of great interest to compare the  $\pi^+$  resonance for HCCl with HCCF and FCCF. Such electron scattering cross sections are important for the development of collisional processes that are less apparent in the studies of a single target. There are some theoretical calculations of the  $\pi^+$  resonance [13] for HCCl using the RBB method. It is quite surprising to see that such simple approach is fundamentally important for use, there are no theoretical calculations of the  $\pi^+$  resonance for FCCF for getting cross sections to the best of our knowledge.

In this paper, we report the total cross section ( $Q_{tot}$ ), momentum transfer cross section (MTCS), differential cross section (DCS), excitation cross section ( $Q_{exc}$ ) and total ionization cross section ( $Q_{ion}$ ) for the electron impact on difluoroacetylene (C<sub>2</sub>F<sub>2</sub>). The present results for the cross sections of HCCl and FCCF. Such study is important to understand the fluorination effect in the cross section and resonance present at low energies.

#### 2. Theoretical methodology

— Present

# Summary and Future Plan

- Our DCPP web database system reorganization
  - ✓ Electron collision data : ~26,000 recodes
  - ✓ Change to user friendly system
  - ✓ Evaluated data: ~700 recodes
- AMBDAS update. (supporting IAEA)
  - ✓ AMBDAS Updated from 2009 to 2016.
  - ✓ Need to change the data searching method to shorten the time required.
- Group Data Evaluation Project
  - ✓ Completed evaluation of CH<sub>4</sub> and C<sub>2</sub>H<sub>2</sub> molecules by operating an evaluation group
  - ✓ Find next evaluation data
    - Possible to evaluate fusion data and related molecular data
- Data product
  - ✓ Measurement of total scattering cross section for e – Ar, CH<sub>4</sub> collisions at low electron energies.
  - ✓ Calculation of total ionization cross section for e - C<sub>x</sub>F<sub>y</sub> collisions





# Thank you very much for your attention!



# **Demonstrate of DCPP WEB**

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## **2003. 01. Plasma Properties Information System**

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- with KISTI (Korea Institute of Science, Technology and Information)
- A+M DB for Industrial Plasma Applications

## **2006. 12. Launch of DCPP Project**

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- Supported by Ministry of Knowledge Economy
- making Standard Reference Data for Low Temperature Plasmas
- making USER Network
- ISO 9001:2000 / KSA 9001:2001 (Quality Management System)

## **2008. 09. Construction of APAN Network**

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- APAN : Asia-Pacific Atomic data Network
- Korea, Japan, Australia, India, China

## **2010. 05. ADAS Project Steering Committee**

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- IDL – ADAS Program install & committee activity

## **2010. 06. Construction of Data User Network**

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- 3 major Company join DUN, 30 small and medium company
- University-Industry-Institute value chain for Data Business
- 2 Technology Transfer



**2011. 05. IAEA- Co-ordinated Research Project**

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- Evaluation of Cross Section for Electron Impact with Hydrogen and Helium and Their Combination Molecules in Fusion Plasma

**2012. 09. NFRI-IAEA-Technical Meeting**

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- The Joint IAEA-NFRI Technical Meeting (TM) on Data Evaluation for Atomic, Molecular and Plasma Material Interaction Processes in Fusion

**2013. 01. Organization of Evaluator group**

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- Group Meeting on Procedures for Evaluation of CH<sub>4</sub> Collision Processes

**2014. 12. NFRI-IAEA-Technical Meeting**

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- Decennial IAEA Technical Meeting on Atomic, Molecular and Plasma-Material Interaction Data for Fusion Science and Technology

**2015. 11. IAEA Data Center Network**

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- The Joint IAE Data Center Network Meeting in the world

**2016. 09. ICAMDATA , ADAS WORKSHOP**

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- International Conference for atomic and molecular data



# Missions

## 1. Research of plasma Fundamental data

- Molecular structure, Physical and Chemical parameters
- Electron collision processes with Molecules
- Plasma characteristics diagnostic studies
- Surface reactions related data necessary to study the plasma process analysis
- Data evaluation

## 2. Development of plasma modeling and simulator

- Developing a multi-dimensional simulator for low-temperature plasma analysis
- Development of plasma fluid model based on multi-dimensional simulator for analysis equipment
- Development S / W for the data optimization.

## 3. Activities for the dissemination of data

- Date collection and dissemination
- International collaboration for data evaluation and production
- Developing user-friendly web system

# Chemical properties

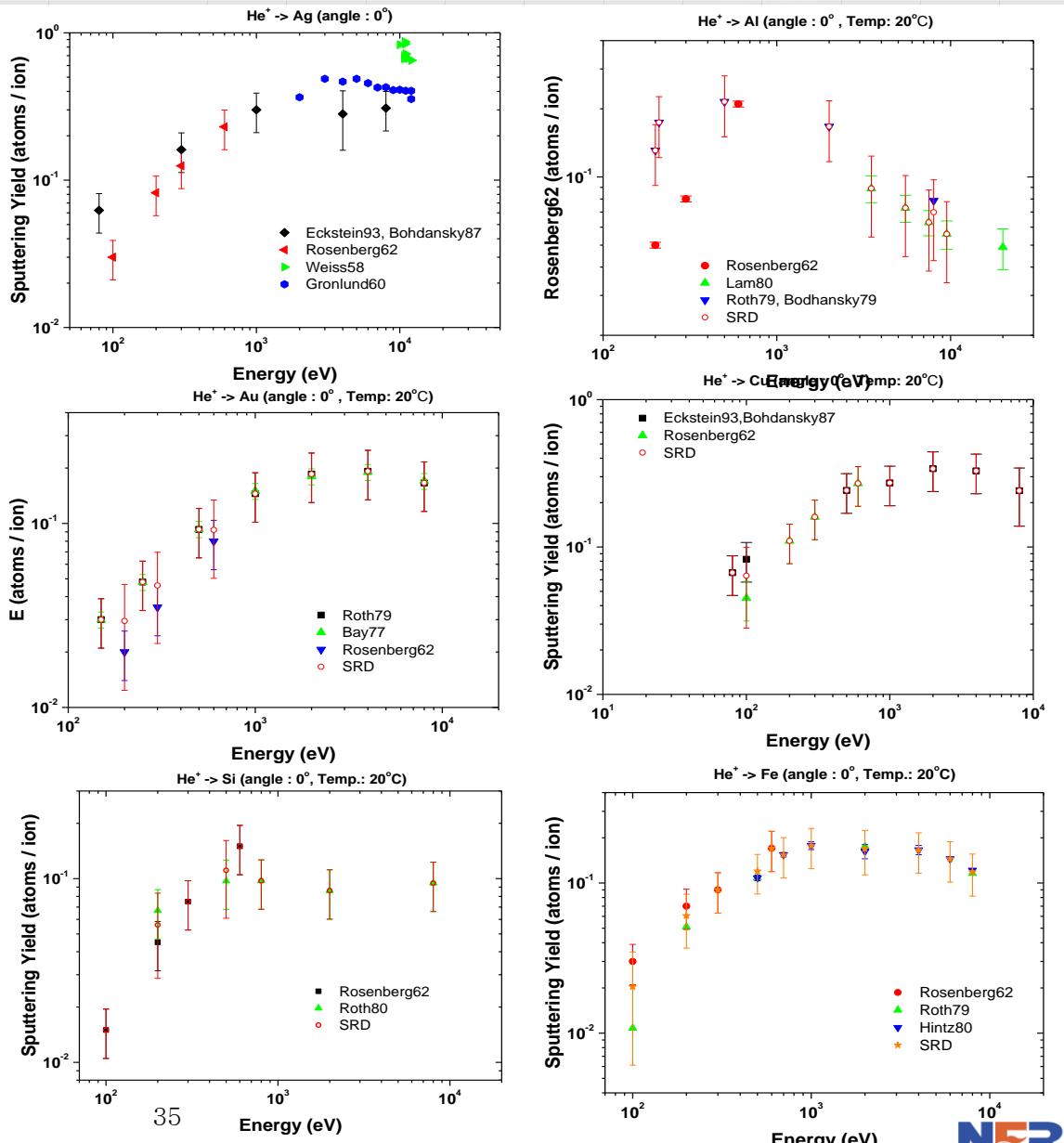
2012 ~2017 , 73 species

Group	Molecules	ion	EA	IP	$\alpha$	L-J ( $\sigma$ , $\epsilon/k_B$ )	Thermodynamics
Noble gas	1	(2)	1	1	1	1	2
	Ex) Ar	neutral		15.76 eV	1.64 Å <sup>3</sup>	4.66 Å, 134 K	
CxFy	52	(86)	43	52	76	13	28
(x=0~4, y=1~8)	Ex) c-C <sub>4</sub> F <sub>8</sub>	neutral	0.60 eV	11.79 eV	7.80 Å <sup>3</sup>		
CxHyFz	9	(15)	9	9	14	7	15
(x=0~1, y=1~2, z=1~2)	Ex) CH <sub>2</sub> F <sub>2</sub>	neutral	-0.56 eV	13.04 eV	2.63 Å <sup>3</sup>	3.70 Å, 730 K	
CxOyFz	8	(10)	3	3	3	4	10
(x=0~1, y=1~3, z=0~2)	Ex) CO <sub>2</sub>	neutral			2.91 Å <sup>3</sup>	3.94 Å, 195 K	
NFx	3	(3)	2	3	3	0	0
(x=0~3)	Ex) NF <sub>3</sub>	neutral	1.39 eV	13.14 eV	2.74 Å <sup>3</sup>	4.08 Å, 277 K	
Recodes	73	(116)	59	68	97	25	55

# Evaluated Sputtering Yield data

2007 ~2017 , 70species

- Starting : 2016
- Sputtering yield (angle, energy)
- Projectile ion  
H, He, D
- Target  
Ag (4), Al (3), Au (6), Cu (9), Fe(5), Si(5)

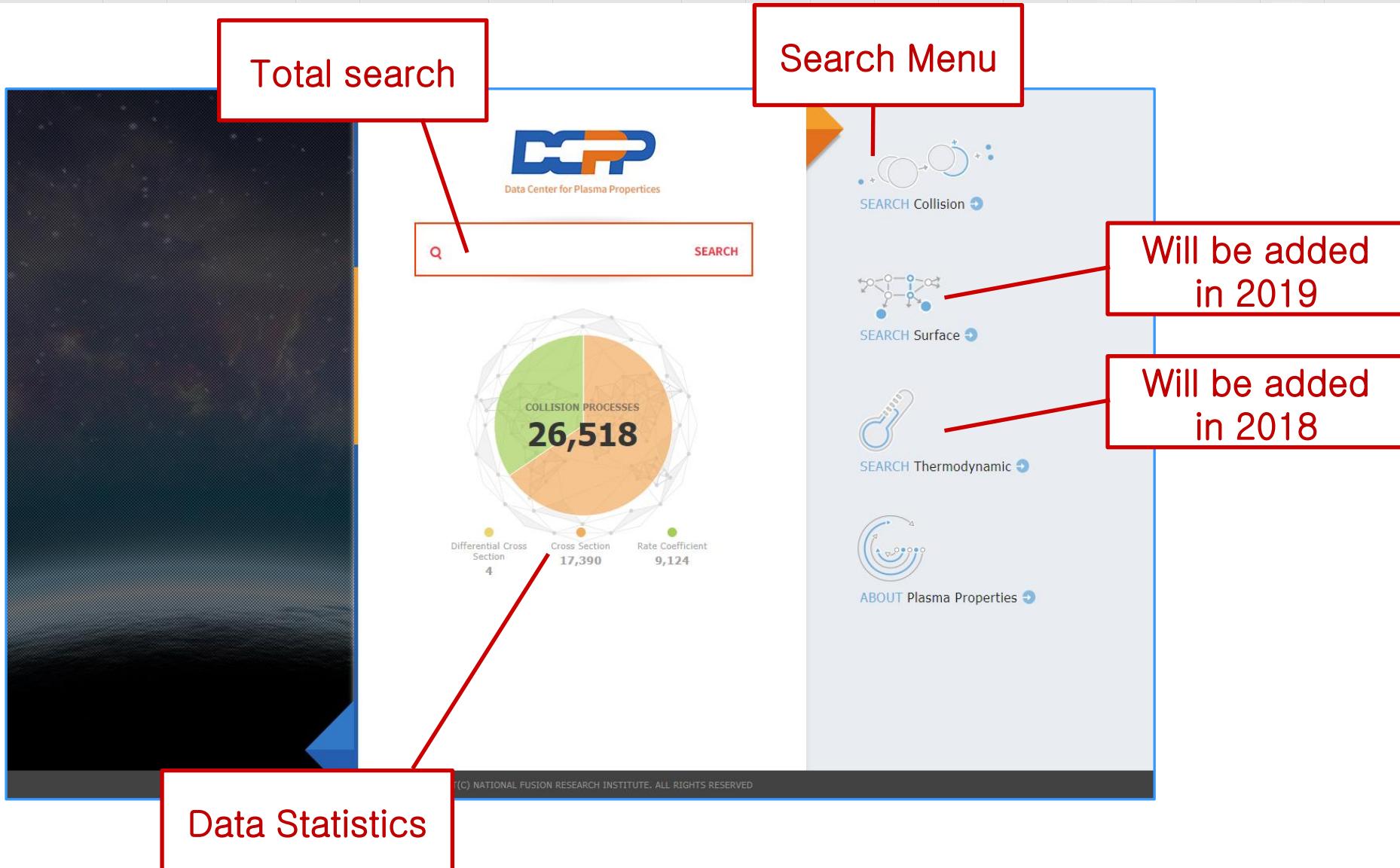




# **Demonstrate of DCPP WEB**

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# New DCPP Web Database System (1)



# New DCPP Web Database System (2)

**DCPP**  
Data Center for Plasma Properties

Search Collision

SEARCH Collision   SEARCH Surface   SEARCH Thermodynamic   ABOUT Plasma Properties

Cross Section PROCESSES

Scattering DATA : 36   Ionization DATA : 106   Excitation DATA : 19   Charge Transfer DATA : 14   Dissociation DATA : 9

Rate Coefficient PROCESSES

Excitation DATA : 3   Charge Transfer DATA : 6   Reaction DATA : 12

총 : 186건 (1 / 2page)

총 : 217건 (1 / 1page)

**17,390**

Scattering 1,589   Ionization 4,665   Excitation 7,067  
Recombination 387   Charge Transfer 2,820   Dissociation 166  
Attachment 268   Reaction 404   Detachment 24

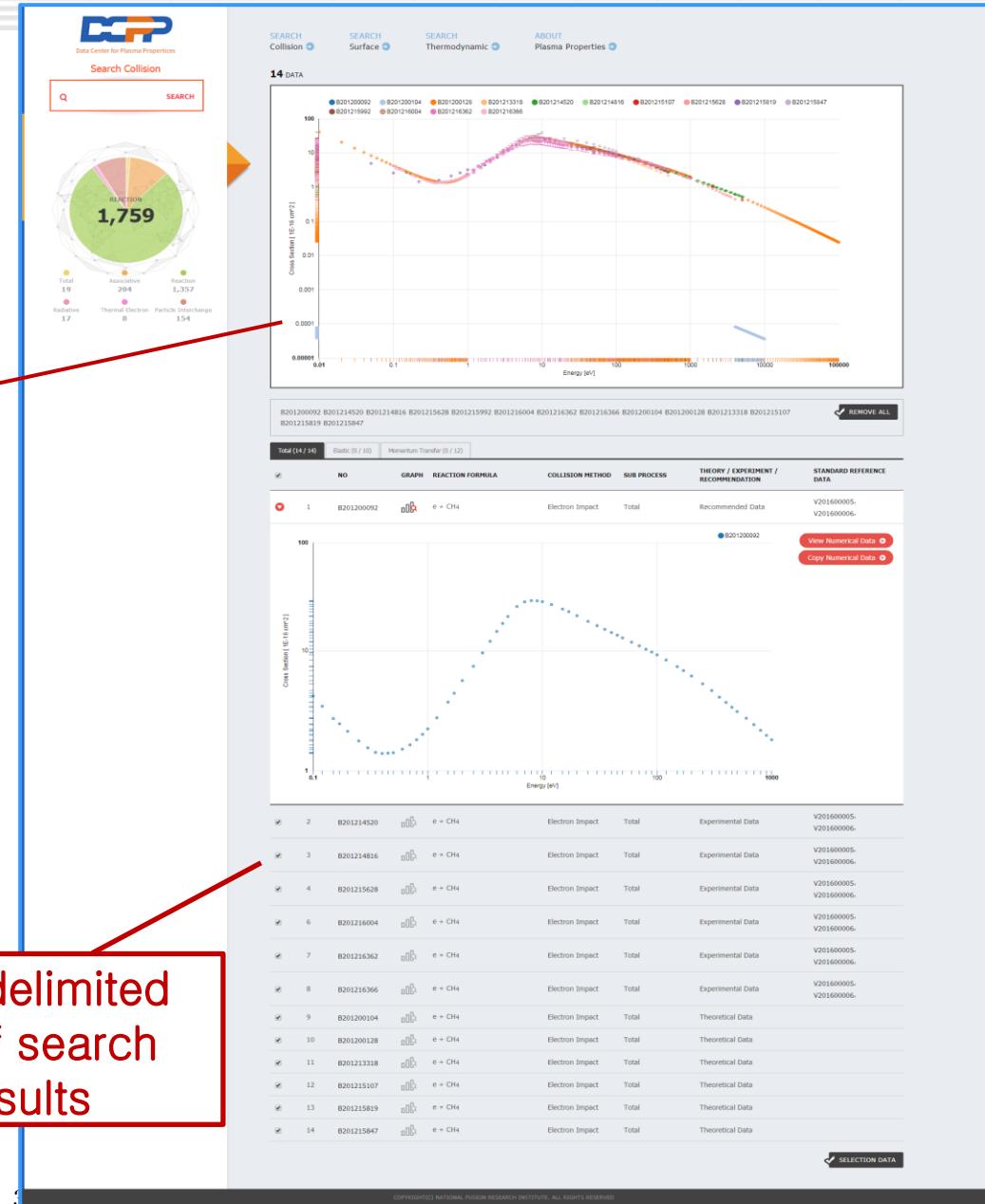
**Displays the number of processes according to the retrieved result**

# New DCPP Web Database System (3)

Graph showing search results



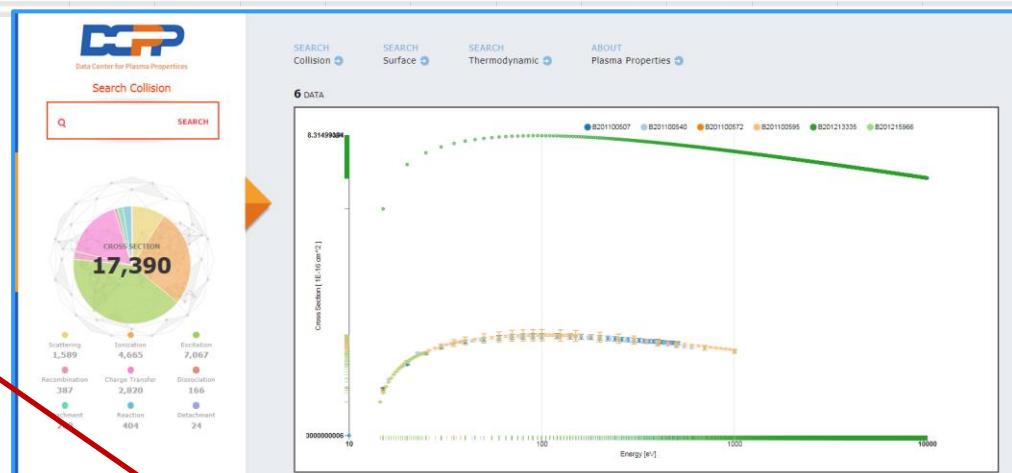
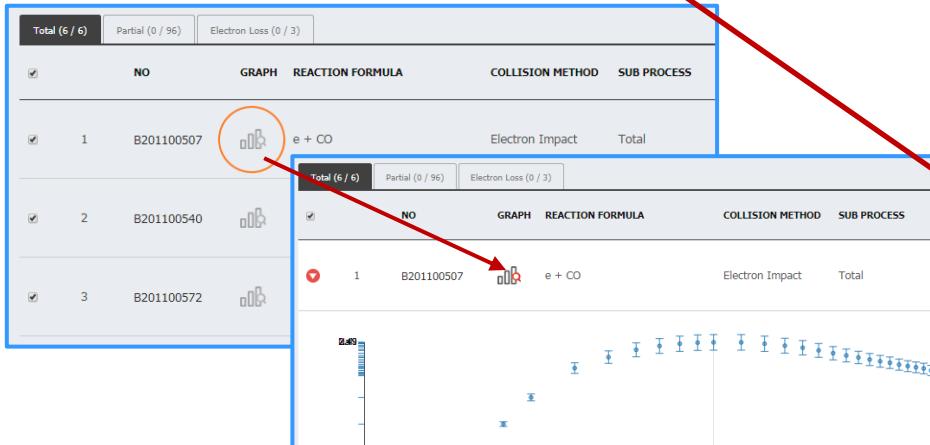
Data can be removed from selection list with just one click



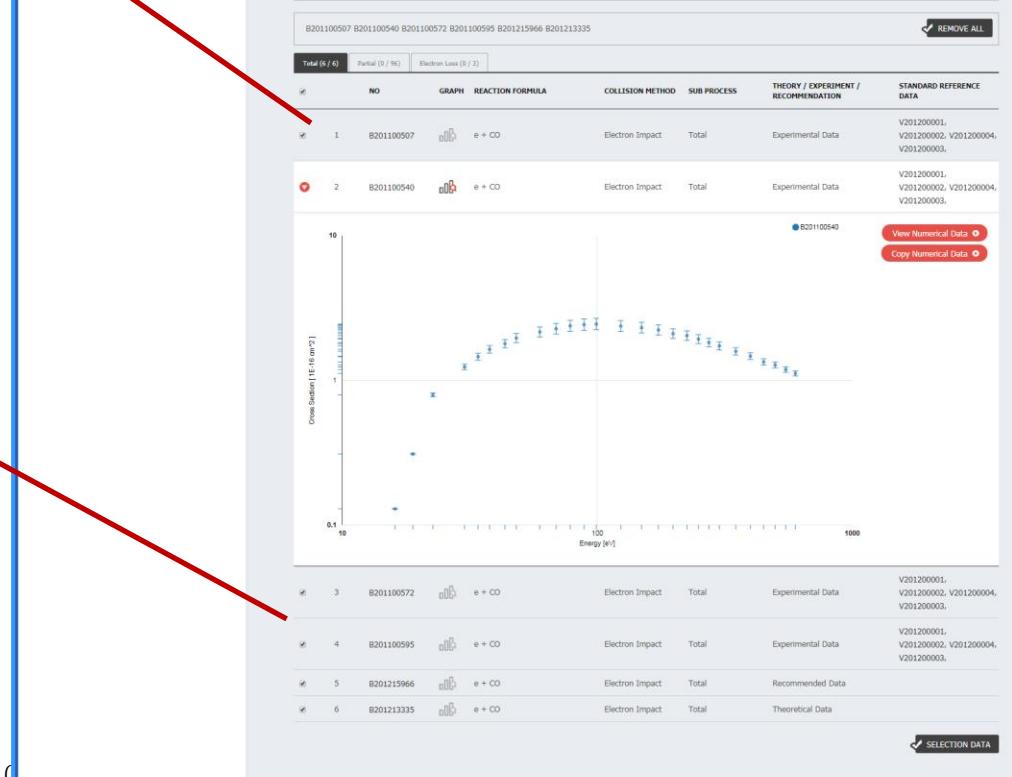
Tab-delimited list of search results

# New DCPP Web Database System (4)

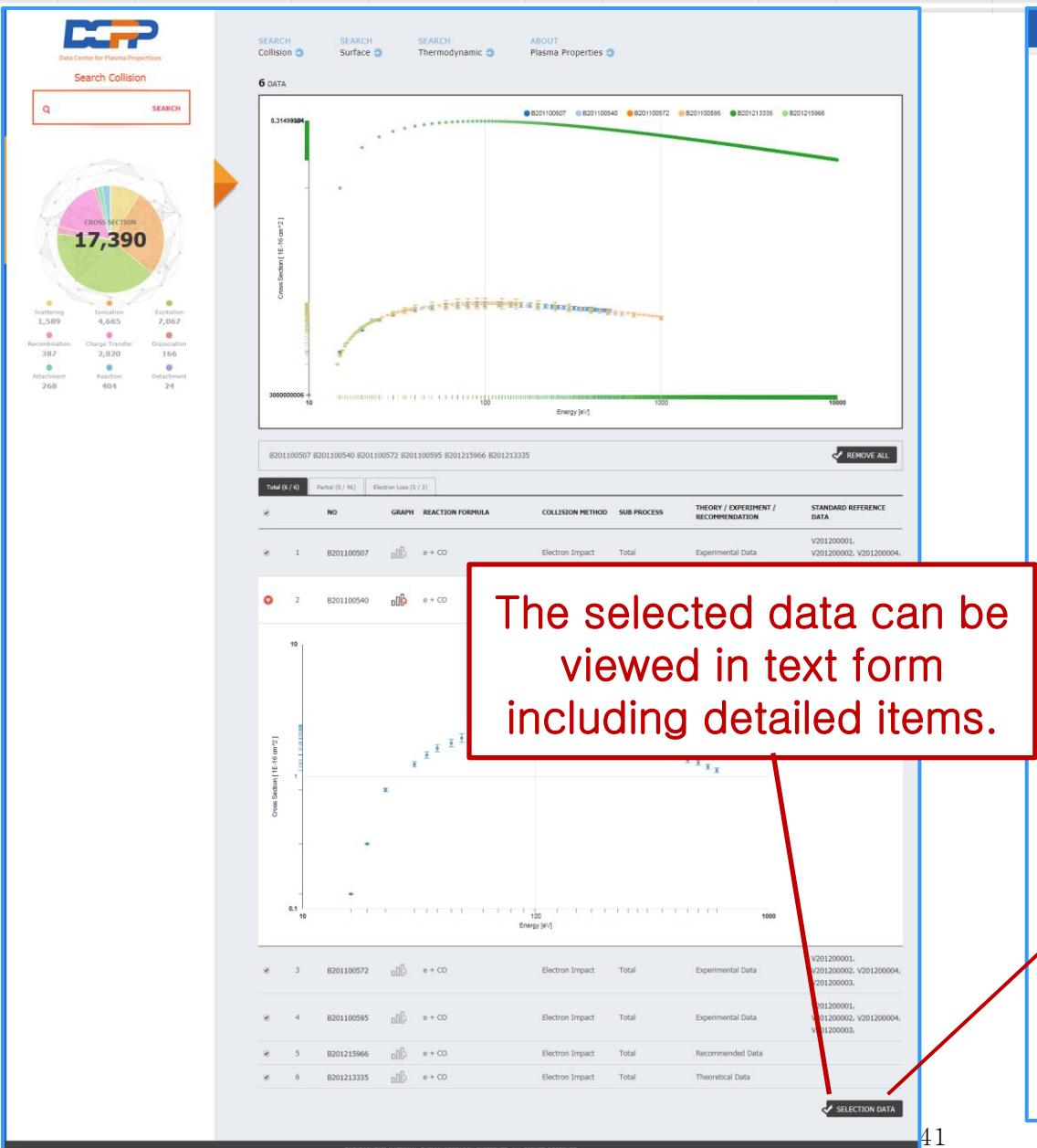
subgraph using  
wrapping method



You can select all of the  
data and select individual  
data for viewing the graph.



# New DCPP Web Database System (4)

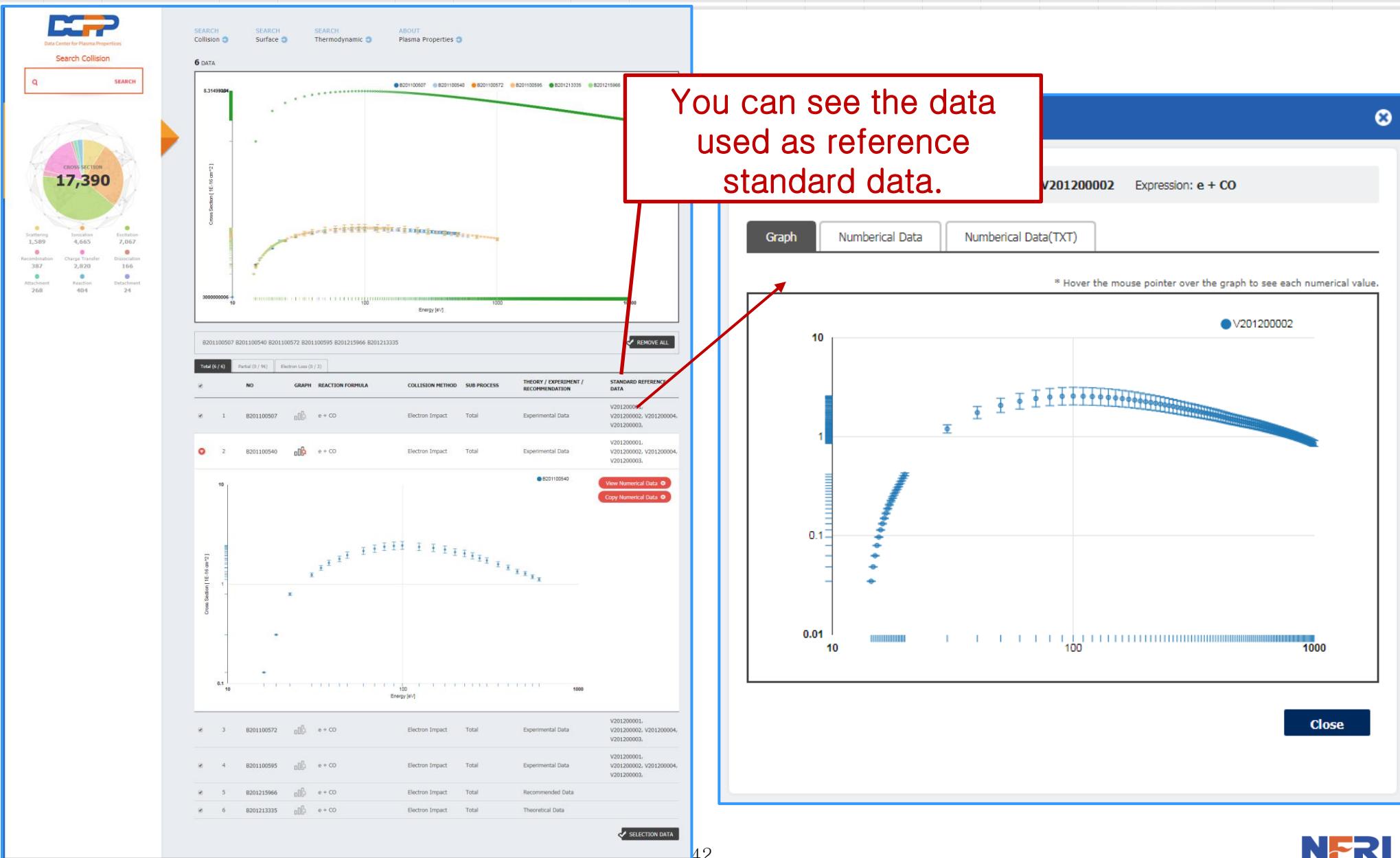


The selected data can be viewed in text form including detailed items.

Plasma Properties TEXT View	
Total Count: 1	
Properties Number:	B201219352
Expression	$\text{He} + \text{CO} \rightarrow \text{He} + \text{CO} + \text{e}$
Title	Measurement of charge-changing cross sections in collisions of He and $\text{He}^+$ with $\text{H}_2$ , $\text{O}_2$ , $\text{CH}_4$ , $\text{CO}$ and $\text{CO}_2$
Author(s)	M. Satake, A. Yagisita, Y. Nakai
Journal Name	J. Phys. B
Publication Year	1990
Volume	23
Issue No	
Page	
Categorize	
Collision data categorize	
Collision process	Ionization
Sub process	Electron Loss
Collision type	Heavy Particle Impact
THEORY / EXPERIMENT / RECOMMENDATION	Experimental Data
XSAMS Doc.	<a href="#">Download</a>
X	Y
300000.0	4.29
400000.0	4.52
500000.0	4.58
600000.0	4.67
700000.0	4.59
800000.0	4.41
900000.0	3.97
1000000.0	3.64
1200000.0	3.35
1400000.0	3.06
1600000.0	2.75
1800000.0	2.61

The XSAMS Document can be downloaded.

# New DCPP Web Database System (4)



# New DCPP Web Database System (5)

## Other functions (Support for plasma properties experts)

### • Data Insert

물성정보

물성 기본 정보 입력

\* 물성 기본 정보는 반드시 선택해야 하는 필수입니다.

물성정보 번호 : 자동으로 선택됩니다.      참고문학

대상	Select	제작자	Select
주제코드	Select	YXXXXX	Select
총점계	Select	00000	Select

반응식 정보 (물성반응식 정보, 입자정보)입력

물성반응식 표정 :

입자종	입자종
이온화	이온화
전기해지	전기해지
미네우드	미네우드
입자종	입자종
이온화	이온화
전기해지	전기해지
미네우드	미네우드
입자종	입자종
이온화	이온화
전기해지	전기해지
미네우드	미네우드

Select      00000

### • Data Evaluation

데이터평가

1차 평가 정보 입력

물성정보번호 : B201225982      물성표시번호 : Levy1999f

구분	내용	평가 내역	구분	내용	평가 내역
1. 속성 대상 명시	데이터 구분	Cross Section	2. 측정 방법 명시	검증구분	Experimental Data
	프로세스	Heavy Particle Impact, Ionization, Partial		측정방법	
	반응식	$CD5+ + Ar \rightarrow CD52+ + Ar + e^-$		실험근거 제시	
X단위	X단위		판단	● 적절    ○ 부적절	
	Y단위			● 적절    ○ 부적절	
3. 소급성	판단	● 적절    ○ 부적절	4. 정확도 제시	방식의 함께	
	판단	● 적절    ○ 부적절		실험변수 제시	
5. 재현성	데이터 분석		불확도 제시		
	판단	● 적절    ○ 부적절	판단	● 적절    ○ 부적절	
6. 일관성	간접평가		판단	● 적절    ○ 부적절	
	직접평가		판단	● 적절    ○ 부적절	
	1차 평가 내용		1차 평가 결과	● 유효한 데이터    ○ 기각    ○ 평가유보	

평가하기      나가기

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### • Report (PDF)

