A+M Data Center Activities in National Fusion Research Institute (2017~2019)

Mi-Young Song with FTR Division

Plasma Technology Research Center, National Fusion Research Institute

25th Meeting of the Data Centre Network, Vienna, Austria

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National Fusion Research Institute

A World-class Institution in Fusion & Plasma R&D

that is spear-heading the way to national energy independence while countering global climate change.

- R&Ds for Core Sciences and Technologies to achieve self-sustenance of Fusion Power Plant Technologies
- R&Ds for Spin-off **Plasma Technologies** of Fusion & Plasma Science

National Fusion Research Institute

NFRI
@ Daejeon
@ Gunsan

[Headquarter (Daejeon)]

- Main building with administration
- KSTAR & ITER Project
- Construction : '10~'13
- Area : 22,035M²

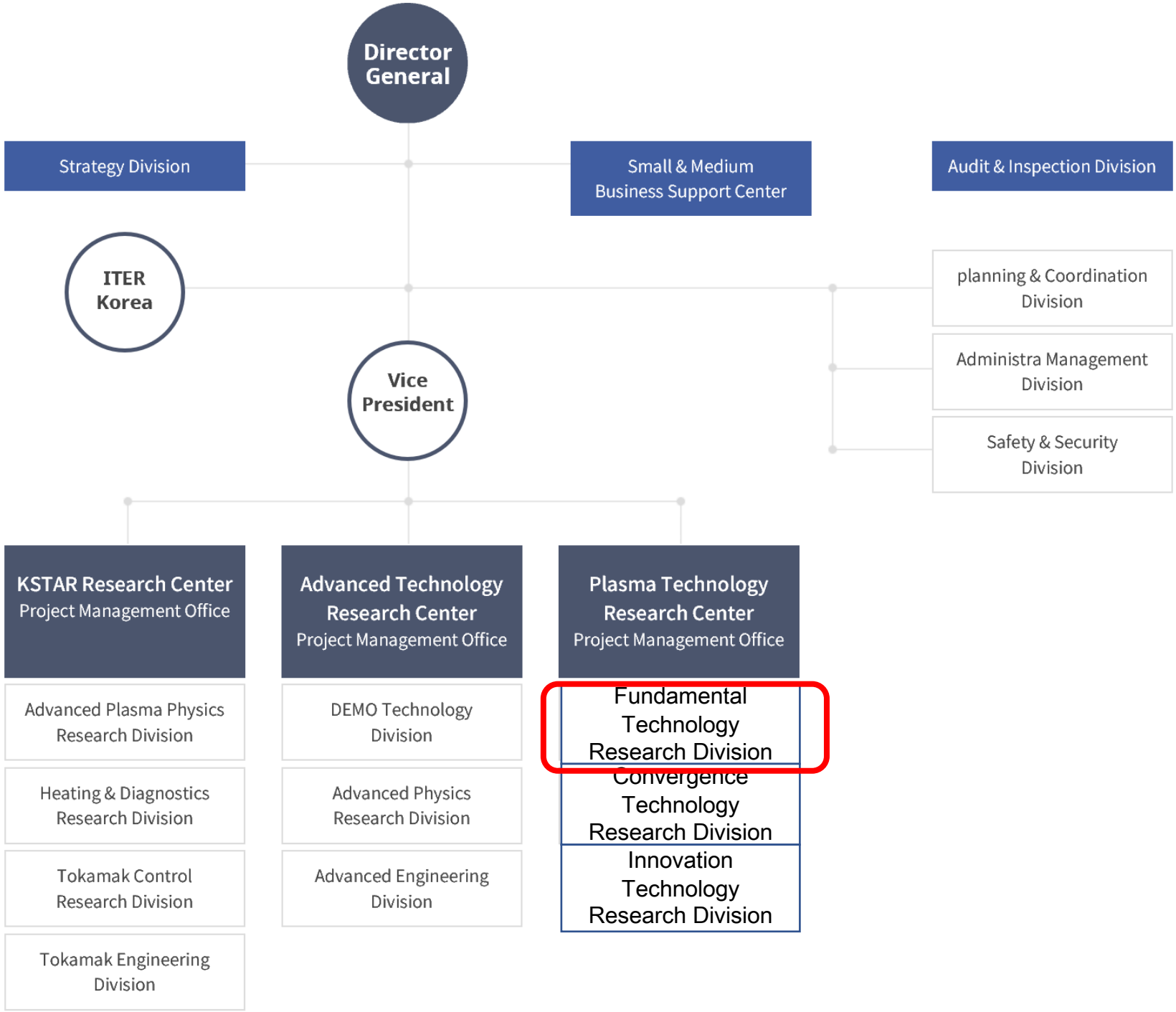
[Fusion Research Center : KSTAR(Daejeon)]

- KSTAR research facilities
- Construction : '98~'02
- Area : 22,866M²

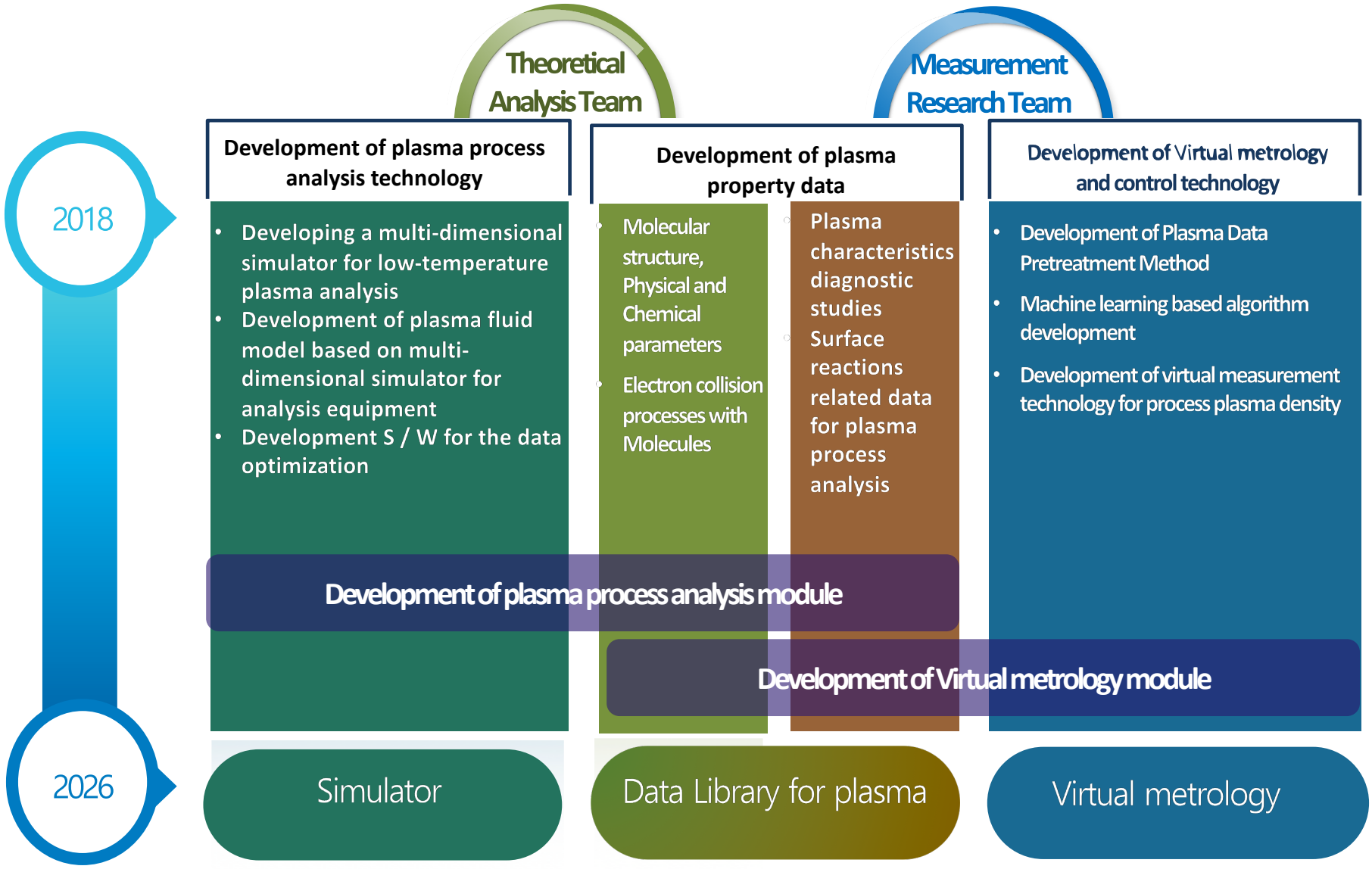
[Plasma Technology Research Center(Gunsan)]

- Research and administration
- Construction : '09~'12
- Area : building 7,535m², Land 16,500M²


Environmental Experiment Building
Main building
오식도
Dormitory
Complex Research Building (new)


Director General
Strategy Division
Small & Medium Business Support Center
Audit & Inspection Division
ITER Korea
planning & Coordination Division
Administra Management Division
Safety & Security Division
Vice President
KSTAR Research Center
Project Management Office
Advanced Technology Research Center
Project Management Office
Plasma Technology Research Center
Project Management Office
Advanced Plasma Physics Research Division
Heating & Diagnostics Research Division
Tokamak Control Research Division
Tokamak Engineering Division
DEMO Technology Division
Advanced Physics Research Division
Advanced Engineering Division
Fundamental Technology Research Division
Convergence Technology Research Division
Innovation Technology Research Division

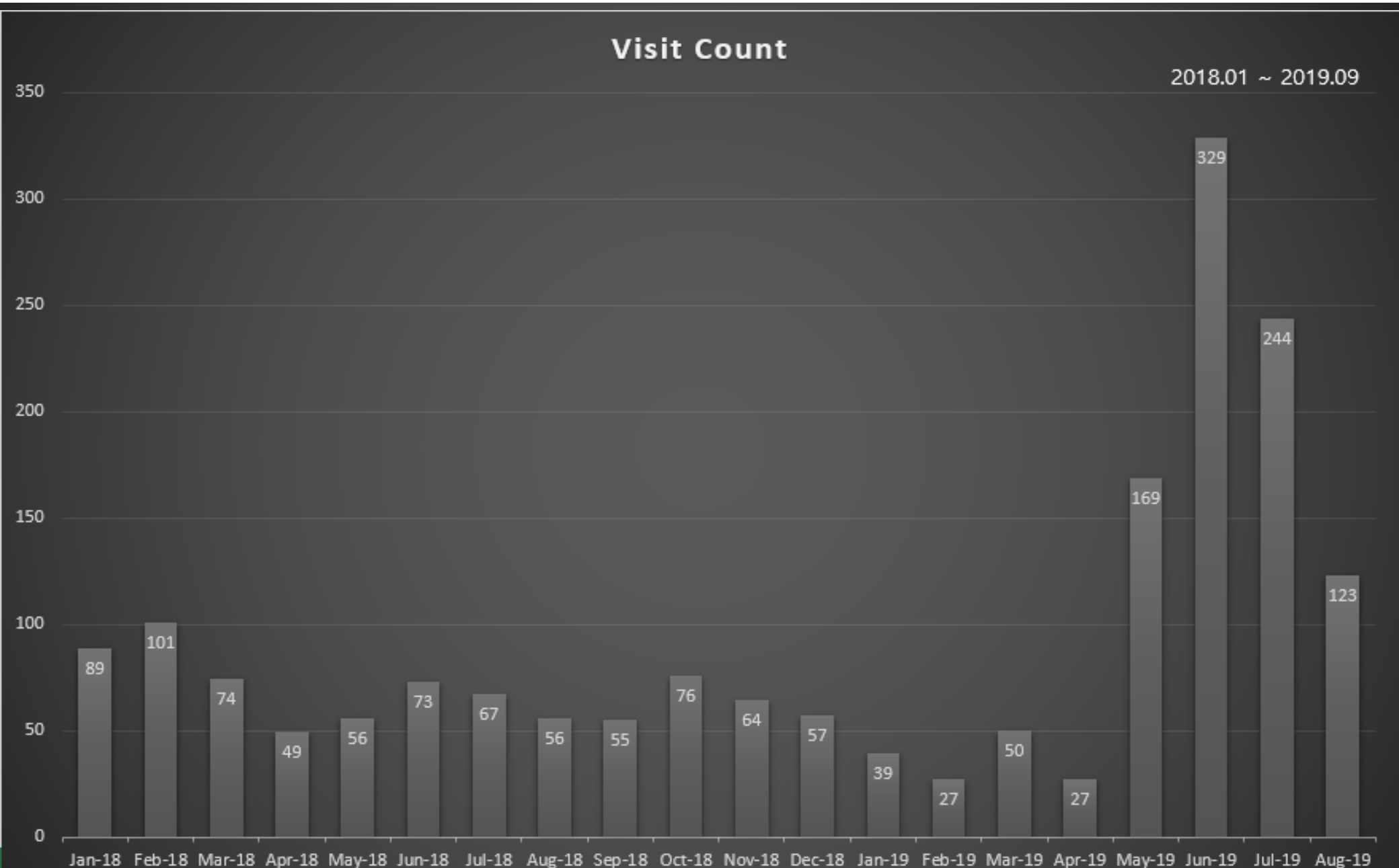
Fundamental Technology Research Division



A+M Database

- 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 recodes.
- 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.

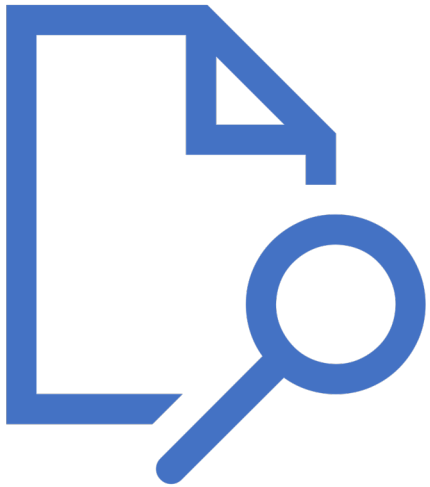
Site Statistics



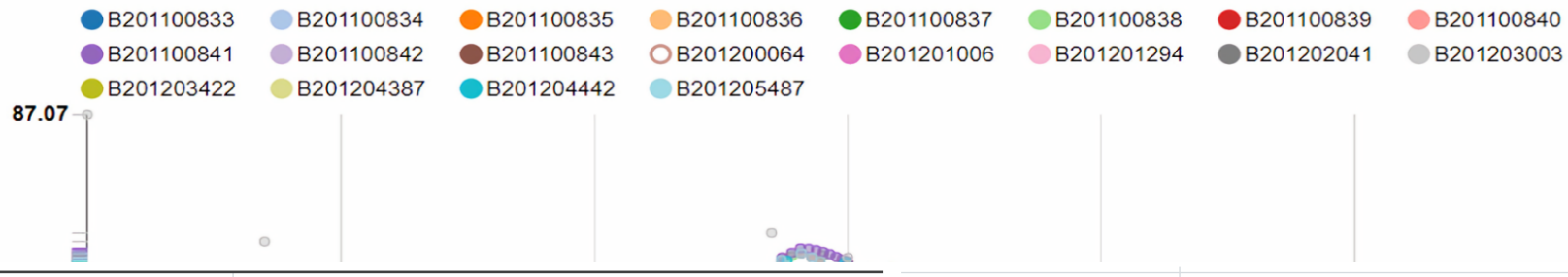
Numerical data summary

database	recode
Chemical properties	660건
Cross section	69,371건
Rate coefficient	32,230건
Evaluation	860건
Sputtering yield	60건
International group evaluation (published)	H2, D2,DH, CH4, C2H2, NF3, N2O, NO, NO2
Complete set DB	C4F6/C4F8/CH2F2/O2/Ar HBr/Cl2/Ar, NF3/Ar

Func. Total Search

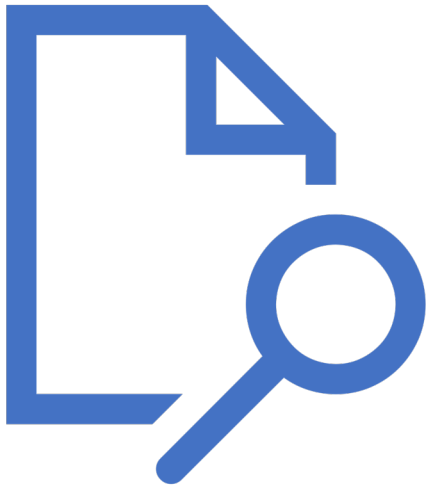


- Total Search
  - Search by species name
  - Search by specifying a specific item such as collision, surface, thermodynamic data
  - Classification of search result by process
  - Detail items
    - Chemical reaction info.
    - Graph (possible to compare the different values)
    - Numerical data
    - Article info.
    - Text type of info.
    - Xsams document download
    - Uncertainty info.



Expression	e + Xe	**THEORY / EXPERIMENT / RECOMMENDATION**	Experimental Data	
Title	Elastic electron scattering cross sections for Xe in the 1-100 eV impact energy region	**XSAMS Doc.**	Download	
Author(s)	D. F. Register, L. Vuskovic and S. Trajmar	**수치정보**	**X**	**Y**
Journal Name	J. Phys. B		1	1.65
Publication Year	1986		1.75	7.3
Volume	19		2.75	16.5
Issue No	-		3.75	26
Page	pp.1685 ~ pp.1697		4.75	35.3
Categorize	Collision Processes		5.75	40.7
Collision data categorize	Cross Section		9.75	40.4
Collision process	Scattering		14.75	37.2
Sub process	Total		19.75	35.6
Collision type	Electron Impact		29.75	21

Func. Thermodynamic data Search



- Thermodynamic Data Search
  - search results of Structured Formula
  - Data generated by quantum chemical calculations and data created by Fitting
  - Search available : C3F2, C3F3, C3F4, CF4 (45 count)
  - Detail items
    - xyz-coordinates
    - Adiabatic Electron Affinity (AEA)
    - Vertical Electron Affinity (VEA)
    - Vertical electron Detachment Energy (VDA)
    - Vertical Ionization Potential (VIP)
    - Adiabatic Ionization Potential (AIP)
    - Polarizability
    - Thermodynamic Data (Raw)
    - Thermodynamic Data (Fitted Equation)

Search Results

Collision Data | Surface Data | Thermodynamic Data

cyclo-C_3F_2(7) | $CCCF_2$(7) | FCCCF(7)

Molecular formula

1. xyz_coordinates

Molecular	Rational	Level	charge	spin state	atom	x	y	z
C_3F_2	$CCCF_2$	wB97X-D/avtz	0.0	singlet	C	-0.000002	-2.302779	0.000000
					C	-0.000002	-1.039403	0.000000
					C	0.000000	0.280488	0.000000
					F	-1.058040	1.020566	0.000000
					F	1.058042	1.020563	0.000000

2. Adiabatic Electron Affinity (AEA)

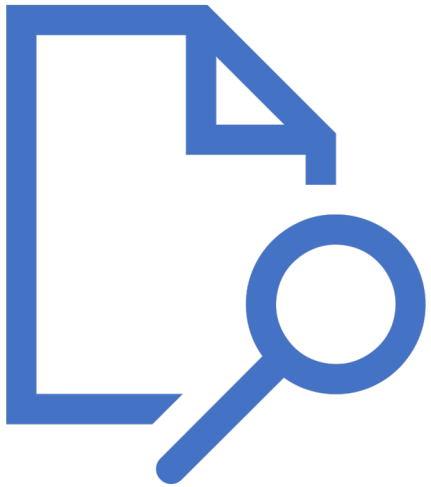
Molecular	Rational	Level	AEA(eV)	difference(eV)	error(%)	note
C_3F_2	$CCCF_2$	BHandHLYP/avdz				
		BHandHLYP/avtz				
		wB97X-D/avdz				
		wB97X-D/avtz	1.879			Recommendation
		expt.	–			

8. Thermodynamic Data (Raw)

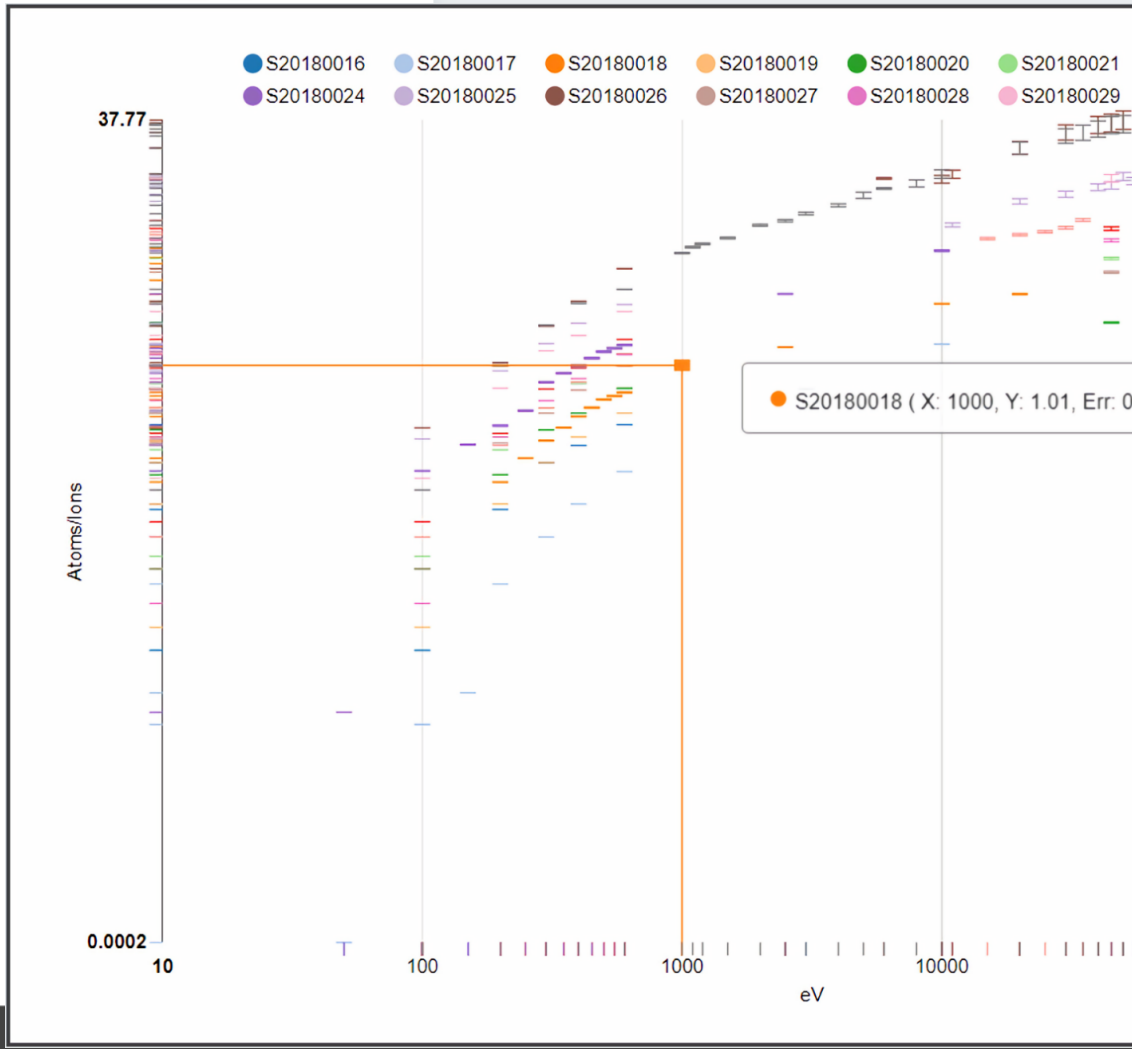
Molecular	Rational	Lavel	temperature(K)	Cv (J/mol K)	Cp (J/mol K)	H° (KJ/mol)	H°-H°298.15 (KJ/mol)	S° (J/mol K)	-(G°-H°298.15)/T" (J/molK)
C_3F_2	$CCCF_2$	wB97X-D/avtz	298.15	56.6	64.9	62.5	0.0	297.6	297.5
			298.00	56.6	64.9	62.5	0.0	297.5	297.5
			300.00	56.8	65.1	62.6	0.1	298.0	297.5
			400.00	64.8	73.1	69.5	7.1	317.8	300.2
			500.00	71.2	79.5	77.2	14.7	334.9	305.5
			600.00	76.3	84.6	85.4	22.9	349.8	311.6
			700.00	80.3	88.6	94.1	31.6	363.2	318.1
			800.00	83.5	91.8	103.1	40.6	375.2	324.5
			900.00	86.0	94.3	112.4	49.9	386.2	330.7
			1000.00	88.1	96.4	121.9	59.5	396.2	336.8
			1100.00	89.7	98.0	131.7	69.2	405.5	342.6
			1200.00	91.1	99.4	141.5	79.1	414.1	348.2
			1300.00	92.2	100.5	151.5	89.1	422.1	353.6
			1400.00	93.1	101.4	161.6	99.1	429.6	358.8
			1500.00	93.8	102.1	171.8	109.3	436.6	363.7

C3F2 (View details)

Func. Surface data Search



- Surface Data Search
  - Search by species name (Currently only Sputtering Yield possible)
  - Search available : Ar, Kr, Xe (45 count)
  - Other checkable items besides the basic search results
    - Sputtering coefficient (Theory only)
    - Surface critical energy (Theory only)
    - Incident particle energy
    - Incident particle angle
    - Sputtering yield numeric data
    - Sputtering yield uncertainty
  - Upcoming Items
    - sticking coefficient, adsorption coefficient, diffusion coefficient



Prop. No. S20180018

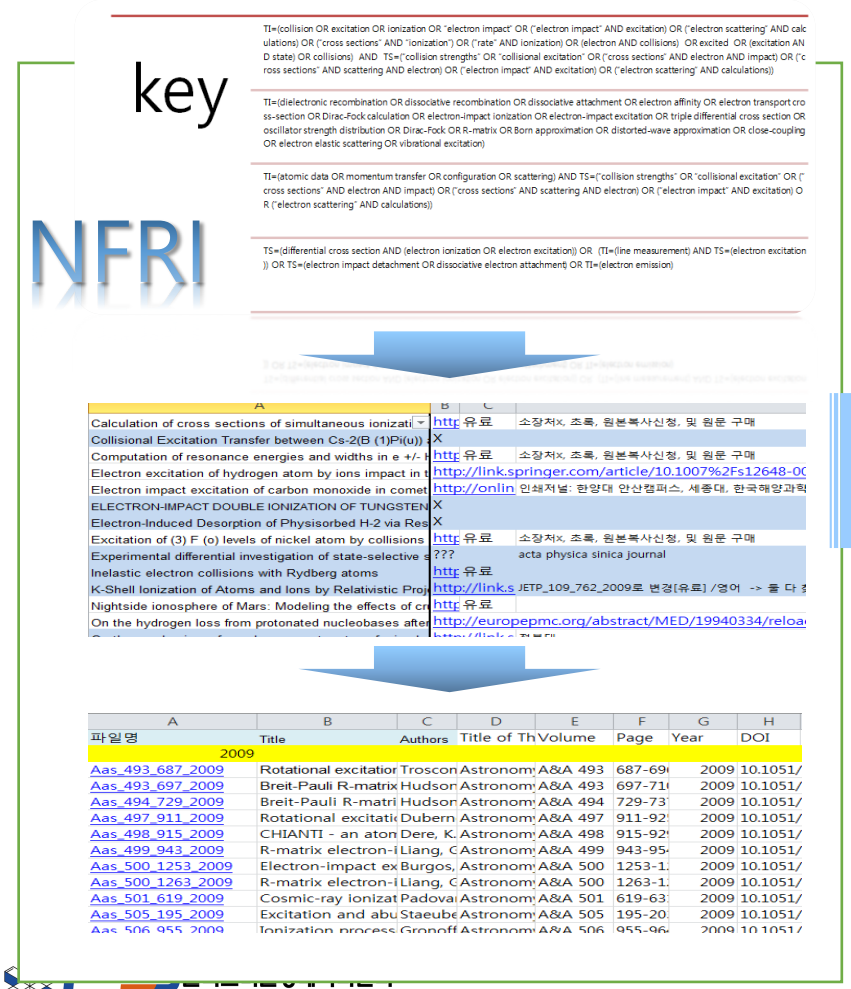
Referece Link	2019000004 2019000012 2019000014
Categorize	Surface Processes
Surface categorize	Surface Rcaction
Classisication	Sputtering Yield
Type	Evaluated
Verification	Valid Reference Data
Uncertainty	YES
Expression	Si + Xe^{+}-> Si

Prop. No. S20180018

X value	Y value	Err	Angle	Temp
200.0	0.18	0.141	0.0	--
250.0	0.256	0.157	0.0	--
300.0	0.332	0.172	0.0	--
350.0	0.403	0.194	0.0	--
400.0	0.473	0.217	0.0	--
450.0	0.54	0.245	0.0	--
500.0	0.608	0.272	0.0	--
550.0	0.642	0.254	0.0	--
600.0	0.676	0.235	0.0	--
1000.0	1.01	0.051	0.0	--

AMBDAS Update

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



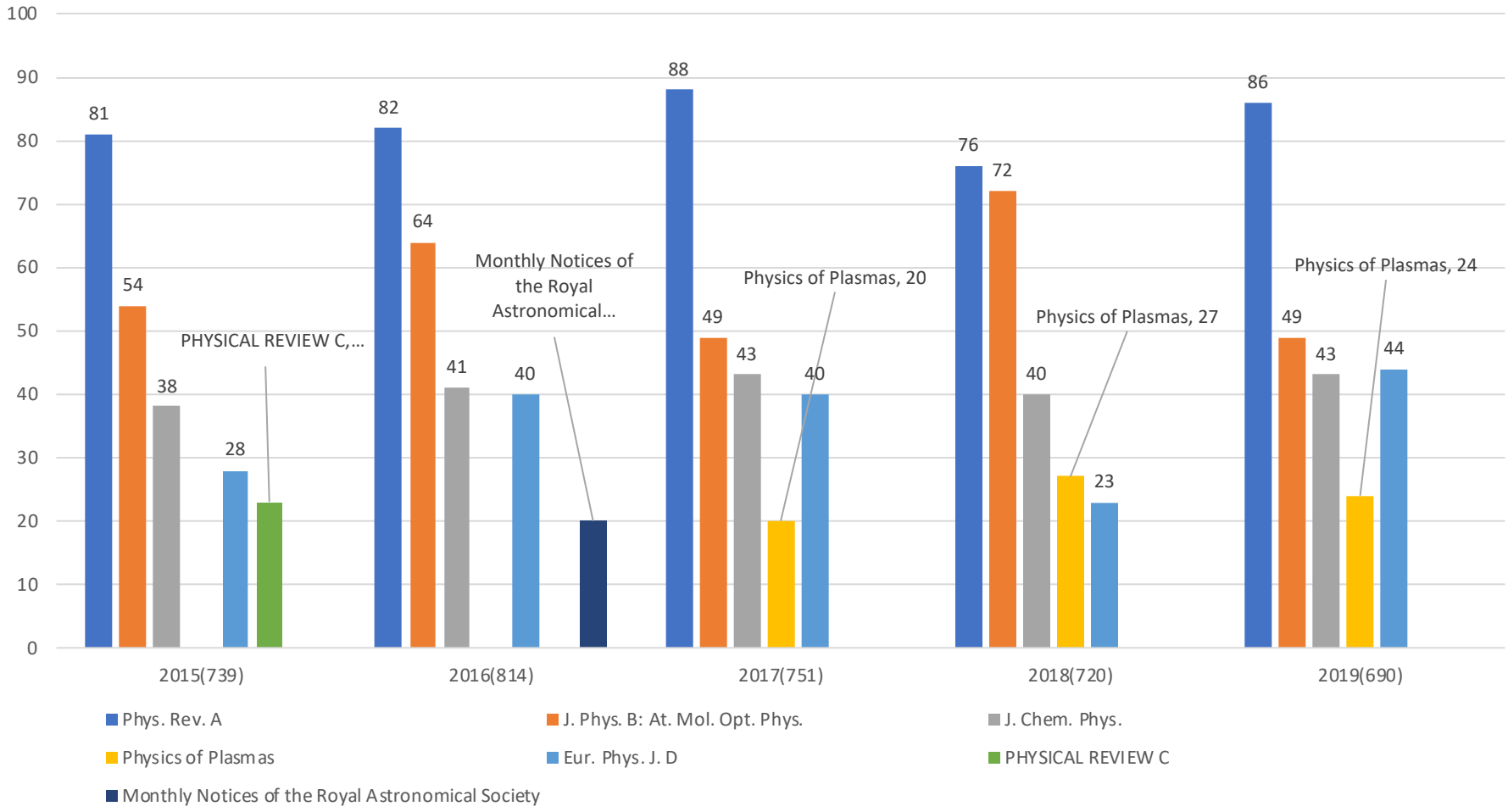
	Job Time	2014	2015		2016	2017	2018	2019
Search period		2009 ~2012	2013	2014	2015	2016	2017	2018
Number of searches	2 weeks	3631	1138	1181	1150	1054	1237	1283
Filtering (1st)	2 weeks	2993	739	814	751	844	1008	1071
Filtering(2st)	2~3 months	2863	527	627	549	600	720	690 (334)
Expert Reviews & update	1 months		433	407	248	184	293(210)	179(178)

- First we collected articles through complex keywords.
- After that, I filtered the duplicate collection and canceled it if there was no data.
- So we got the following result

	Please indicate the format of data in the paper (Figure, Table, Analytic Fit etc)	E: Electron P: Photon H: Heavy particle S: Structure/spectra M: particle-matter D: Data Compilation B: Bibliography	Please refer to ProcessClassification.pdf -pages 4-14	Please find valid energy / temperature ranges
doi	**Comments**	**IAEA Category**	**IAEA Process**	**Energy range**
	Figure	E	ETS, EEL, EX, EI	0.1 ~ 5000 eV
https://doi.org/10.1088/1361-6455/aa640b	Table	E	EEL, EMT	6, 7, 8, 10, 12
DOI: 10.1103/PhysRevA.96.042703	Figure	E	EIN	0 ~360 degree
https://doi.org/10.1140/epjd/e2017-70809-3	Figure	E	EIN	20 ~ 180 degre
https://doi.org/10.1016/j.radphyschem.2016.10.003		P		

	2018 (2017)	2019 (2018)
Electron	115	117
Photon	14	
Heavy particle	88	40
Structure/ spectra	59	21
particle-matter	.	9
Data Compilation	.	.
Bibliography	.	.
positron	12	.
Null	5	.

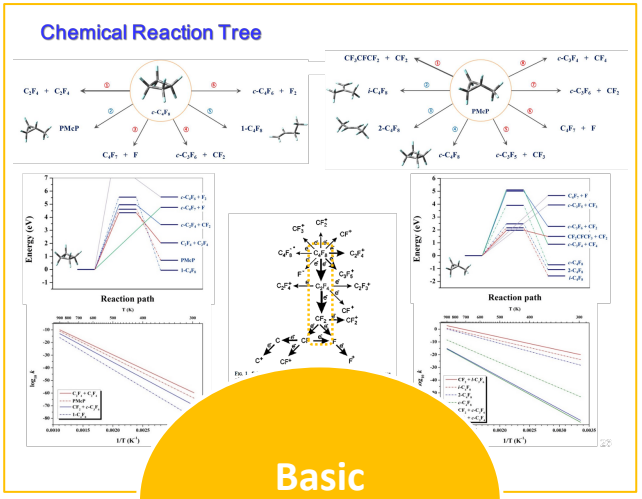
Journal Statistics (TOP 5)

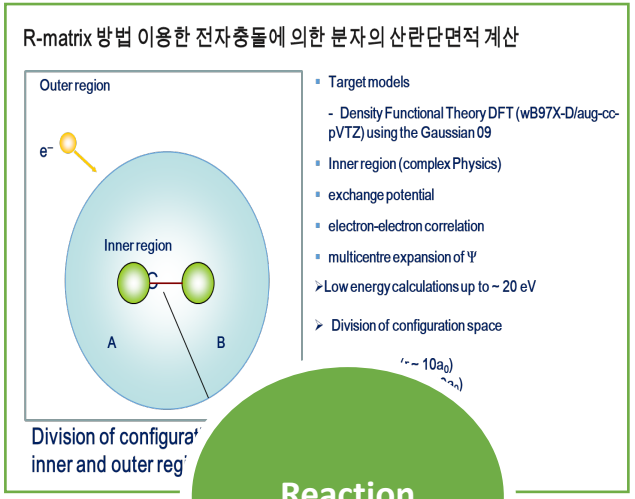


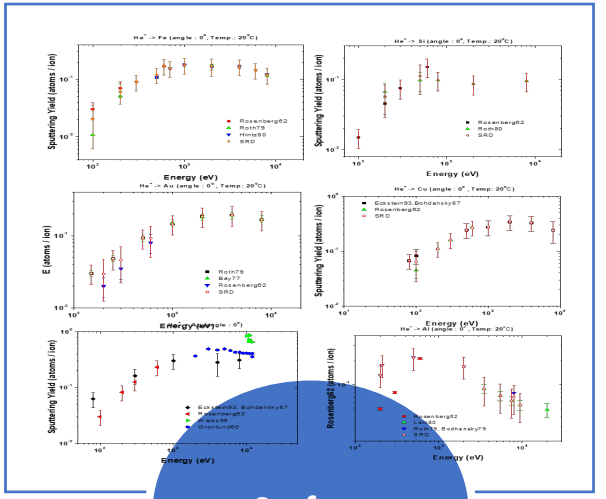
Study of Fundamental Properties about Atomic and Molecular

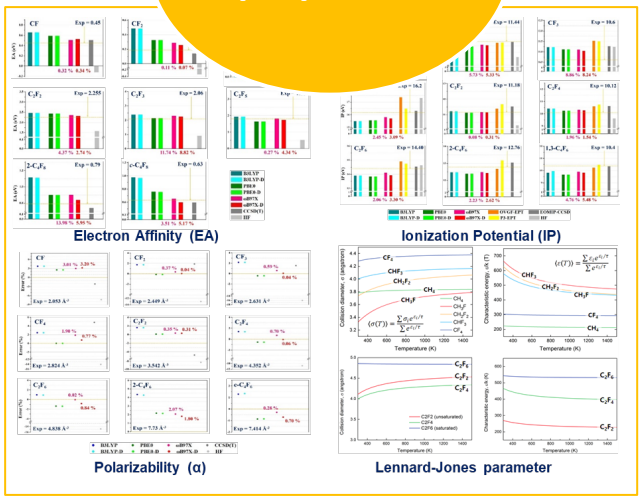
- Molecular structure, Physical and Chemical parameters
- Electron collision processes with A + M
- Plasma properties of A+M

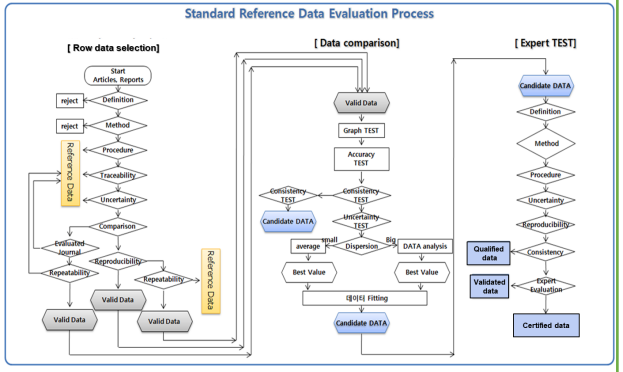
Theoretical Measurement











Basic properties

Reaction

Surface

MOLECULAR DYNAMICS (2020)

Molecular structure, Physical and Chemical parameters

- The fluorocarbon molecules (FCs) have been widely used for plasma processing in the semiconductor industry for various applications.
- The plasma assisted oxide-etch technology depends on the use of FCs to achieve the required profile control and etch selectivity to mask and etch stop layers.
- A deep understanding of all possible reaction of FCs and their fragments in plasma is required to make technological progress.

Fundamental Physical Property Data

Target Compound	C_xF_y, $C_xF_yH_z$, $C_xF_yX_z$ (X=O, Cl, Br, I), N_xF_y, …
Fundamental Physics Data	Kind of Data : Molecular geometry, Internal energy, Electron affinity, Ionization potential, Polarizability, Specific heat, Standard enthalpy, Standard entropy, Orbital energy, Electron binding energy, Total ionization cross-section Number of Data : Over 500
Chemical Reaction Data	Kind of Data : Chemical reaction path, TS geometry, Activation energy, Relative energy, Reaction rate constant Number of Data : Over 160
Level of Theory applied	Density Functional Theory (DFT), Binary Ecounter-Bethe (BEB) model, Transition State Theory (TST)
Calculation Program used	Gaussian09, GAMESS, Cfour, KiSTheIP(Kinetic and Statistical Thermo-dynamical Package)

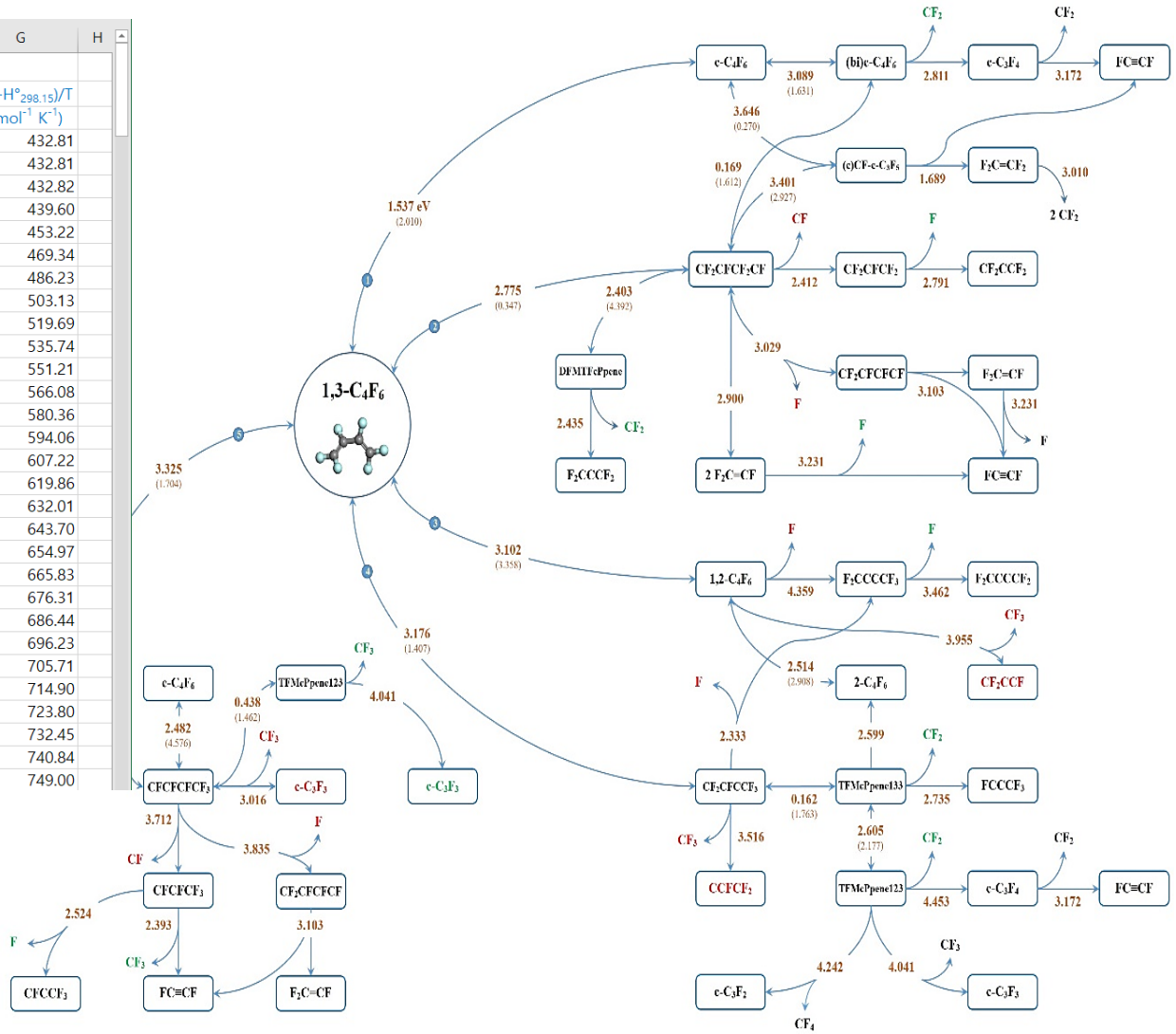
Symbol	Molecular Weight [kg/kmol]	Characteristic Energy (Lennard-Jones Parameter) [K]	Collision Diameter (Lennard-Jones Parameter) [angstroms]	Polarizability [angstroms^3]	Ionization Energy [eV]	Electron Affinity [eV]
C2F4						
C2F4	100.015	202.6	5.164	6.82 (copy of C2F6)	9.89	
C2F4+	100.015	202.6	5.164	6.82 (copy of C2F6)	-	
C2F5						
C2F5	119.013	500	5	6.82 (copy of C2F6)	12.5	
C2F5+	119.013	500	5	6.82 (copy of C2F6)	-	
C2F6						
C2F6	138.012	194.5	5.512	6.82	14.2	
C3F2						
C3F2						
C3F3						
C3F3	93.0273	500	5	6.19	10	
C3F3+	93.0273	500	5	6.19	-	
C3F3-	93.0273	500	5	6.19	-	
C3F5						
C3F4						
C3F5						
C3F5	131.043	500	5	6.014	10	
C3F5+	131.043	500	5	6.014	-	
C3F6						
C3F6						
C4F5						
C4F5	143.035	500	5	8.64 (copy of C4F7)	10.5	
C4F5+	143.035	500	5	8.64 (copy of C4F7)	-	
C4F6						
C4F6	162.033	500	5	8.64 (copy of C4F7)	10.5	
C4F6+	162.033	500	5	8.64 (copy of C4F7)	-	
C4F7						
C4F7	180.269	500	5	8.64	10.6	
C4F7+	180.269	500	5	8.64	-	
C4F7-	180.269	500	5	8.64	-	
C4F8						
C4F8	200.03	500	5	7.731	12	
C4F8-	200.03	500	5	7.731	-	

Molecule	IP (eV)		α (Å^3)		EA (eV)	
	Exp.	Theo.	Exp.	Theo.	Exp.	Theo.
CF	9.55 ± 0.01	9.725	2.053	2.119	0.45 ± 0.05	0.524
CF_2	11.445 ± 0.025	12.055	2.449	2.450	0.180 ± 0.020	0.255
CF_3	10.6	11.041	2.631	2.632	1.7 ± 0.2	1.623
CF_4	16.2 ± 0.1	15.699	2.824	2.846	-	-
C_2F	-	11.785	-	4.451	-	3.098
C_2F_2 (FC=CF)	11.18	11.145	3.542	3.553	-	0.533
C_2F_2 (C=CF_2)	-	11.201	-	3.867	2.2550 ± 0.0060	2.317
C_2F_3	-	11.738	-	4.127	2.06 ± 0.22	2.242
C_2F_4	10.12	10.276	4.352	4.349	-	-0.472
C_2F_5	10.0 ± 0.1	10.588	-	4.552	1.81 ± 0.15	1.731
C_3F_6	14.40	13.924	4.838	4.797	-	-1.541
2-C_4F_6	12.76	12.425	7.73	7.063	-	0.885
c-C_4F_6	-	11.420	7.414	7.362	-	0.566
1,3-C_4F_6	10.4	9.830	8.345	8.145	-	0.279
2-C_4F_8	11.1	11.285	-	8.466	0.79 ± 0.06	0.837
c-C_4F_8	11.6	11.795	-	7.801	0.63 ± 0.05	0.597

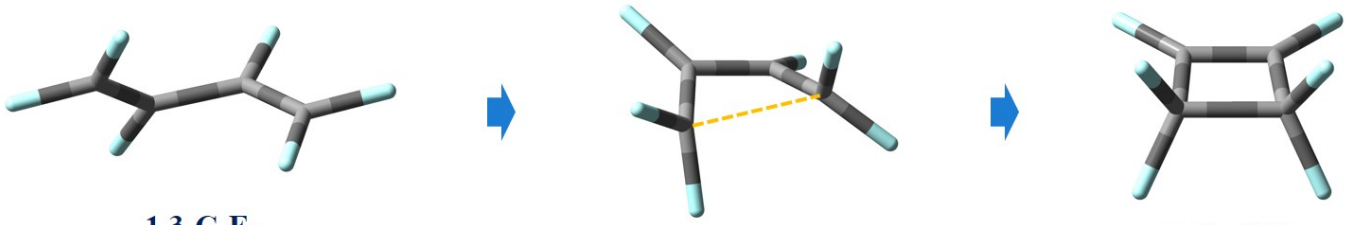
Thermodynamic Property Data

	A	B	C	D	E	F	G	H
1				c-C4F8+				
2	Temperature	C_V	C_P	H°	H°-H°$_{298.15}$	S°	-(G°-H°$_{298.15}$)/T	
3	(K)	(J mol^{-1} K^{-1})	(J mol^{-1} K^{-1})	(KJ mol^{-1})	(KJ mol^{-1})	(J mol^{-1} K^{-1})	(J mol^{-1} K^{-1})	
4	298.15	155.65	163.96	153.42	0.00	432.82	432.81	
5	298	155.61	163.92	153.40	-0.02	432.74	432.81	
6	300	156.20	164.51	153.73	0.30	433.83	432.82	
7	400	182.18	190.49	171.53	18.11	484.88	439.60	
8	500	202.18	210.49	191.63	38.20	529.64	453.22	
9	600	217.28	225.59	213.47	60.05	569.41	469.34	
10	700	228.61	236.92	236.62	83.20	605.08	486.23	
11	800	237.14	245.46	260.76	107.34	637.30	503.13	
12	900	243.64	251.95	285.64	132.22	666.60	519.69	
13	1000	248.66	256.97	311.10	157.68	693.42	535.74	
14	1100	252.60	260.91	337.00	183.58	718.10	551.21	
15	1200	255.72	264.04	363.26	209.83	740.94	566.08	
16	1300	258.24	266.56	389.79	236.37	762.18	580.36	
17	1400	260.29	268.61	416.55	263.13	782.01	594.06	
18	1500	261.99	270.30	443.50	290.08	800.60	607.22	
19	1600	263.40	271.71	470.60	317.18	818.10	619.86	
20	1700	264.58	272.90	497.83	344.41	834.61	632.01	
21	1800	265.59	273.91	525.18	371.75	850.23	643.70	
22	1900	266.45	274.77	552.61	399.19	865.07	654.97	
23	2000	267.20	275.51	580.13	426.70	879.18	665.83	
24	2100	267.84	276.16	607.71	454.29	892.64	676.31	
25	2200	268.40	276.72	635.35	481.93	905.50	686.44	
26	2300	268.90	277.21	663.05	509.63	917.81	696.23	
27	2400	269.33	277.65	690.79	537.37	929.62	705.71	
28	2500	269.72	278.03	718.58	565.16	940.96	714.90	
29	2600	270.06	278.37	746.40	592.98	951.87	723.80	
30	2700	270.37	278.68	774.25	620.83	962.38	732.45	
31	2800	270.64	278.96	802.13	648.71	972.52	740.84	
32	2900	270.89	279.21	830.04	676.62	982.32	749.00	

Chemical Reaction path



Chemical Reaction



1,3-C_4F_6 TS *cyclo*-C_4F_6

$$k^{GT} = \sigma \frac{k_b T}{h} \frac{Q^{TS}(T,s)}{N_A Q^R(T)} e^{(-V^{\ddagger}(s)/k_b T)}$$

	$V^{\ddagger}$ (kcal/mol)	Error (%)
Expt. [a]	***35.38***	
ωB97X-D / avtz	35.44	0.16
ωB97X / avtz	37.67	6.48
B3LYP / avtz	34.38	–2.83
PBE0 / avtz	32.56	–8.01
CCSD(T) // ωB97X-D / avtz	34.77	–1.73

[a] Schlag et al., *J. Am. Chem. Soc.*, 86, 1676 (1964)

T (K)	k_{expt} (s^{-1}) [a]	k (s^{-1})	Error (%)
400	5.025×10^{-8}	8.623×10^{-8}	3.213
410	1.488×10^{-7}	2.570×10^{-7}	3.478
420	4.184×10^{-7}	7.275×10^{-7}	3.767
430	1.121×10^{-6}	1.962×10^{-6}	4.085
440	2.873×10^{-6}	5.060×10^{-6}	4.435
450	7.060×10^{-6}	1.251×10^{-6}	4.823
460	1.668×10^{-5}	2.974×10^{-5}	5.254
470	3.801×10^{-5}	6.815×10^{-5}	5.737
480	8.368×10^{-5}	1.509×10^{-5}	6.280
490	1.784×10^{-4}	3.235×10^{-4}	6.896
500	3.689×10^{-4}	6.727×10^{-4}	7.599
510	7.415×10^{-4}	1.359×10^{-3}	8.410
520	1.451×10^{-3}	2.674×10^{-3}	9.355
530	2.768×10^{-3}	5.128×10^{-3}	10.470
540	5.156×10^{-3}	9.602×10^{-3}	11.803

Target	L-PFCX			L-HFC		
	CBr2F2	C4F9I	C6F12O	CHF3	C3H2F6	C5H2F10
1. 필수 기초물성 데이터						
바닥상태 구조	●	●	●	●	●	●
ZPE	●	●	●	●	●	●
IP	●	●	●	●	●	●
EA	●	●	●	●	●	●
α	●	●	●	●	●	●
2. 열역학물성 데이터						
E	●	▶	▶	●	●	▶
H°	●	▶	▶	●	●	▶
S°	●	▶	▶	●	●	▶
Cp	●	▶	▶	●	●	▶
Cv	●	▶	▶	●	●	▶
3. 전자충돌 특성 데이터						
B	●	●	●	●	●	●
U	●	●	●	●	●	●
TICS	●	●	●	●	●	●
MTCS	▶	▶	▶	▶	▶	▶
ECS	▶	▶	▶	▶	▶	▶
4. 화학반응 특성 데이터						
Reaction path	4	13	13	3	13	23
BDE	2	6	6	2	4	11
전이상태 구조	2	7	7	1	9	12
E(act)	●	●	●	●	●	●
IRC	●	●	●	●	●	▶
k	▶	▶	▶	▶	▶	○
Reaction table	◐	◐	◐	◐	◐	◐

● 확보 ◐ 미완 ○ 대기 ▶ 진행 중

Electron collision processes with Molecules

- The collision of electrons - atoms and molecules in the reactor is an important phenomenon for the generation and maintenance of plasma.
- The ionization reaction of atoms and molecules by electron collision induces the generation of electrons and ions to maintain the plasma.
- The dissociation reaction of molecules by electron collisions generates reactive radicals and ions, and the chemical reaction of the active radicals is useful for the plasma process It becomes an argument.
- Therefore, it is necessary to understand the reaction principle of atoms and molecules in plasma in order to utilize the plasma state well in the technical field.

BEB Method

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

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

at the HF//ωB97X-D/avtz level

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

by using the BEB model

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

Eur. Phys. J. D (2017) 71: 88
DOI: 10.1140/epjd/e2017-70769-6

THE EUROPEAN PHYSICAL JOURNAL D

Regular Article

Electron impact ionization cross section studies of C_2F_x (x = 1–6) and C_3F_x (x = 1–8) fluorocarbon species*

Dhanoj Gupta[1,a], Heechol Choi[1], Mi-Young Song[1], Grzegorz P. Karwasz[2], and Jung-Sik Yoon[1]

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J. Phys. D: Appl. Phys. 51 (2018) 155203 (10pp)
https://doi.org/10.1088/1361-6463/aab1e3

Electron induced ionization of plasma processing gases: C_4F_x (x = 1–8) and the isomers of C_4F_6 and C_4F_8

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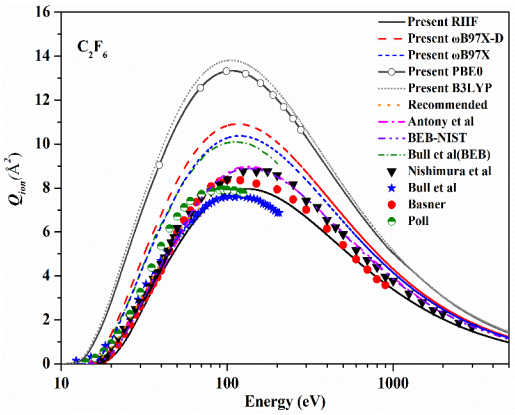
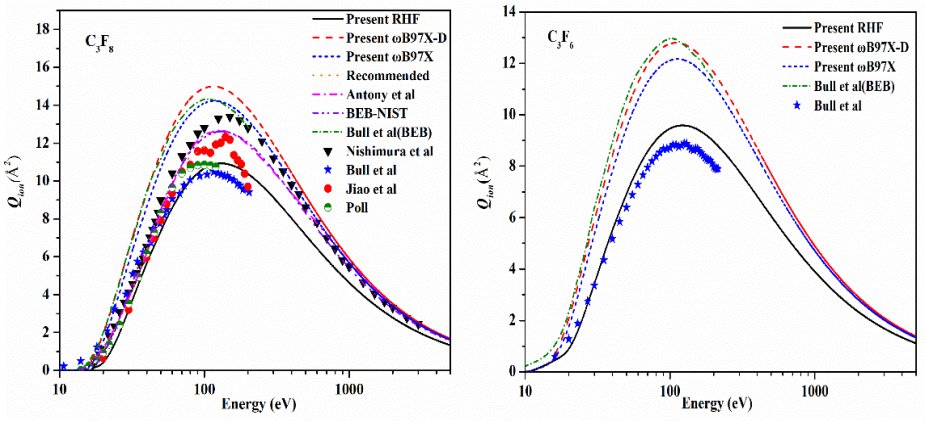
Abstract

The total ionization cross section (Q_{ion}) for C_4F_x (x = 1–8) fluorocarbons and the isomers of C_4F_6 and C_4F_8 molecules are calculated from ionization threshold to 5 keV using the binary-encounter bethe method. The targets are fully optimized using the Hartree–Fock (HF) method and density function theory (DFT) for their minimum energy structure and orbital parameters. The present Q_{ion} with HF parameters showed good agreement with the experimental data for 1,3-C_4F_6, 2-C_4F_6, 2-C_4F_8 and 1-C_4F_8. On the other hand, the Q_{ion} with DFT parameters are in good accordance with the recent theoretical results for 1,3-C_4F_6 and 2-C_4F_6. The Q_{ion} for c-C_4F_8 showed much variation among the various results. The isomer effect in Q_{ion} is negligible for the isomers of C_4F_6 and C_4F_8 molecules. The calculation of Q_{ion} for C_4F, C_4F_2, C_4F_3, C_4F_4, C_4F_5, c-C_4F_6, C_4F_7 and iso-C_4F_8 is a maiden attempt. The present cross section data are important quantities for low temperature plasma modeling especially related to the fluorocarbon plasmas.

C_2F_x(x=1-6), C_3F_x(x=1-8) and C_4F_x(x=1-8) total ionization

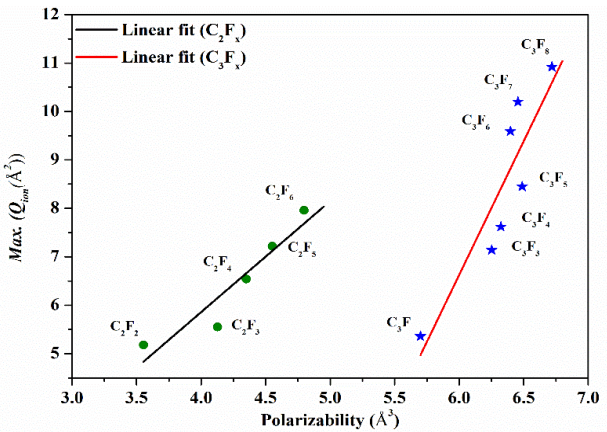


e-C_2F_6 Ionization: present study

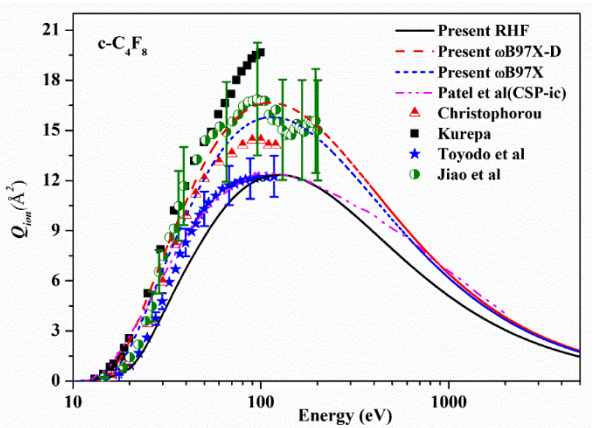


Total ionization cross section for C_3F_8 and C_3F_6

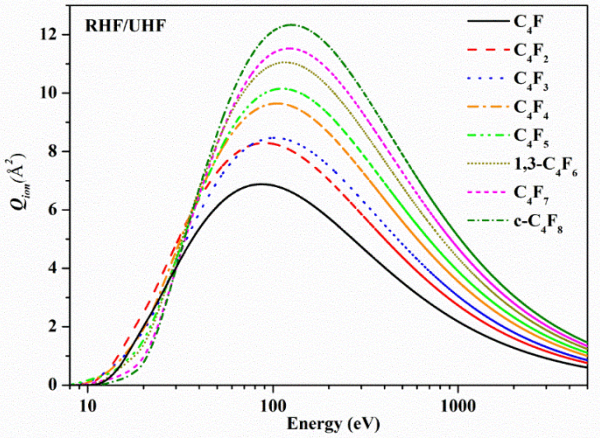
ωB97X/avtz combination in good agreement with recent theoretical data whereas HF is good with experiment, need for more investigation



Correlation plot between maximum Q_{ion} and polarizability of the targets.



Total ionization cross section for c-C_4F_8



Total ionization cross section for C_4F_x (x=1-8) in Å^2 with the RHF/UHF orbital parameters

Gupta et al, Eur. Phys. J. D (2017) 71: 88

R-matrix method

- **Theoretical Methodology**
  - ✓ The well-known *ab initio* R-matrix method through Quantemol-N
- **Target models**
  - ✓ The have optimized the structure of CxFy, BeH2, NH using the Density Functional Theory DFT (wB97X-D/aug-cc-pVTZ) using the Gaussian 09

PHYSICS OF PLASMAS **24**, 123511 (2017)

An R-matrix study of electron induced processes in BF_3 plasma

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An R-matrix formalism is used to study electron collision with the BF_3 molecule using Quantemol-N, a computational system for electron molecule collisions which uses the molecular R-matrix method. Several target models are tested for BF_3 in its equilibrium geometry, and the results are presented for the best model. Scattering calculations are then performed to yield resonance parameters, elastic, differential, excitation, and momentum transfer cross sections. The results for all the cross sections are compared with the experimental and theoretical data, and a good agreement is

PHYSICS OF PLASMAS **25**, 063504 (2018)

Electron impact elastic and excitation cross-sections of the isomers of C_4F_6 molecule for plasma modeling

Dhanoj Gupta,[1] Mi-Young Song,[1,a)] K. L. Baluja,[2] Heechol Choi,[1] and Jung-Sik Yoon[1]
[1]*Plasma Technology Research Center, National Fusion Research Institute, 37, Dongjangsan- ro, Gunsan, Jeollabuk-do 54004, South Korea*
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We report the calculations of elastic (along with its symmetry components) and electronic excitation cross sections by electron impact of the three isomers of C_4F_6, namely, hexafluoro-1,3-butadiene (1,3-C_4F_6), hexafluoro-2-butyne (2-C_4F_6), and hexafluorocyclobutene (c-C_4F_6) belonging to the point groups C_2, D_{3d}, and C_{2v}, respectively, using the R-matrix approach. The electron energy range is from 0.01 eV to 12 eV. We have employed the cc-pVTZ basis set for C and F atoms to generate self-consistent field molecular orbitals to construct the target states for all the isomers included in our calculations. All the target states are constructed by including correlation effects in a configuration interaction (CI) approach. The target properties such as vertical excitation energies and dipole moment of all the isomers are in reasonable agreement with the literature values. Differences in the cross sections of these isomers are strongly influenced by the effect of correlation and polarization effects and their geometrical extent. We have included the ground state and many excited states of each isomer in the trial wave function of the entire scattering system. The resulting elastic cross sections are compared with the available experimental results. The agreement is reasonably good for energies above 5 eV. The shape resonances detected at 2.57, 2.95, and 3.20 eV for c-C_4F_6, 1,3-C_4F_6, and 2-C_4F_6 isomers are associated with the negative anion formation of $C_3F_3^-$ as observed in the mass spectrometry experiments. We have also performed 1-state CI calculation for all the isomers that include only the correlated ground state. The position of resonances shifts to lower energies as the number of target states is increased compared to 1-state calculation for all the isomers. The elastic cross section for 2-C_4F_6 isomer is larger than the other isomers because of its larger spatial extent. The present cross section data are important for plasma simulation and modeling, especially related to fluorocarbon plasma. *Published by AIP Publishing.*
https://doi.org/10.1063/1.5037959

Physics of Plasmas ARTICLE scitation.org/journal/php

Vibrationally resolved excitation, dissociation, and rotational cross sections of NH radical by electron-impact using the R-matrix method

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J. Phys. B: At. Mol. Opt. Phys. **52** (2019) 065204 (10pp) https://doi.org/10.1088/1361-6455/aafdc4

R-matrix study for electron scattering of beryllium dihydride for fusion plasma

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Abstract
We report the integral elastic, differential, momentum transfer, dissociative electron attachment and electronic- and rotational excitation cross sections for low-energy electron impact on beryllium dihydride computed using the Quantemol-N interface for driving the UK molecular R-matrix code. The energy of the projectile electron is in the range 0.1–10 eV. The effect of multichannel coupling is investigated by calculating the cross sections with various target models by increasing the number of target states in the trial wave function of the entire scattering system. The cross sections converge for the calculation with more than 15-target states. The vertical excitation energies calculated with the present model give excellent agreement with the EOM-CCSD calculations. Collisional frequencies are determined using the momentum transfer cross section for a Maxwell–Boltzmann distribution. From the collisional frequency, the

C4F6

- The unsaturated fluorocarbons (UFCs) such as C_4F_6 gases with low global warming potential (GWP) have been a good replacement for the perfluorocarbons (PFCs) such as CF_4, C_2F_6, and C_3F_8 gases for plasma etching applications.
- The 1,3-C_4F_6 isomer can be used for fabricating contact holes in ultra large integrated circuits by selective etching processes of silicon oxide (SiO_2) on Si and silicon nitride (Si_3N_4) layers.
- The calculations of elastic (along with its symmetry components) and electronic excitation cross sections by electron impact of the three isomers of C4F6 belonging to the point groups C_2, D_{3d}, and C_{2v}, respectively, using the R-matrix approach
- We have employed the cc-pVTZ basis set for C and F atoms to generate self-consistent field molecular orbitals to construct the target states for all the isomers included in our calculations.
- All the target states are constructed by including correlation effects in a configuration interaction (CI) approach.

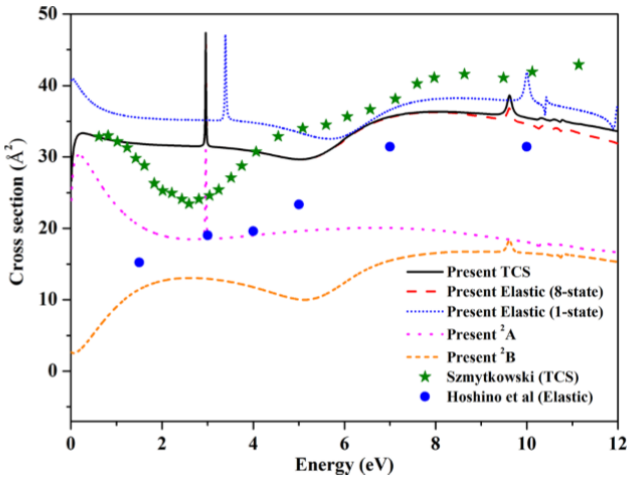


FIG. 2. Cross section of 1,3-C_4F_6 along with the available data for comparison. Solid line: present TCS; dashed line: present elastic (8-state); short dotted line: present elastic (1-state); dotted line: present ^2A symmetry; short dashed line: present ^2B symmetry; star: Szmytkowski and Kwitnewski[5] (TCS); circle: Hoshino *et al.*[9] (elastic).

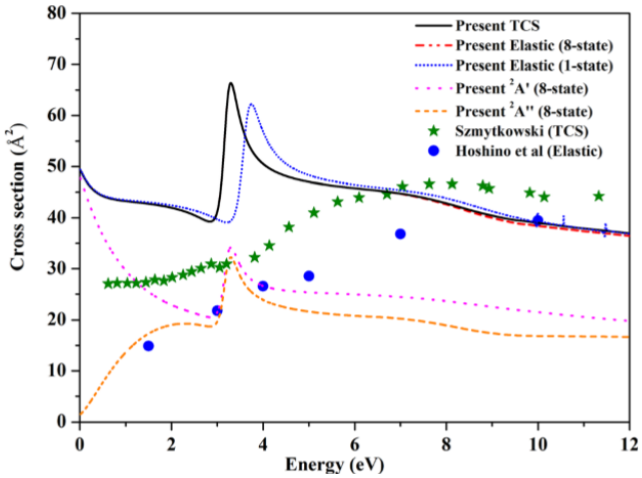
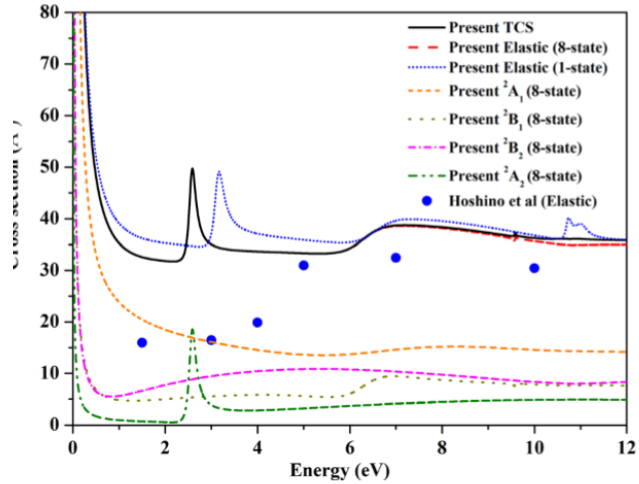


FIG. 4. Cross section of 2-C_4F_6 along with the available comparison. Solid line: present TCS; dashed line: present elastic (8-state); short dotted line: present elastic (1-state); dotted line: present $^2A'$ symmetry; short dashed line: present $^2A''$ symmetry; star: Szmytkowski and Kwitnewski[5] (TCS); circle: Hoshino *et al.*[9] (elastic).



. 6. Cross section of c-C_4F_6 along with the available comparison. Solid : present TCS; dashed line: present elastic (8-state); short dotted line: ent elastic (1-state); short dashed line: present $^2A_1$ symmetry; dotted : present $^2B_1$ symmetry; dashed-dotted line: present $^2B_2$ symmetry; ed-dotted-dotted line: present $^2A_2$ symmetry; circle: Hoshino *et al.*[9] stic).

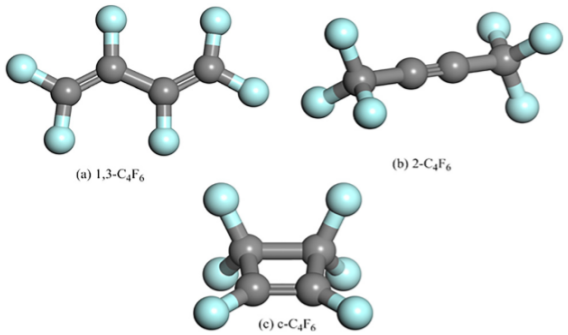


FIG. 1. Molecular structures of the targets used in the present calculation for (a) 1,3-C_4F_6, (b) 2-C_4F_6, and (c) c-C_4F_6.

- The shape resonances detected at 2.57, 2.95, and 3.20 eV for c-C_4F_6, 1,3-C_4F_6, and 2-C_4F_6 isomers are associated with the negative anion formation of $C_3F_3^-$ as observed in the mass spectrometry experiments.
- The Qexc for 1,3-C_4F_6 and c-C_4F_6 shows a broad and narrow peak at around 9.6 eV, which may be due to the Feshbach resonances detected for these targets at the same energy range.

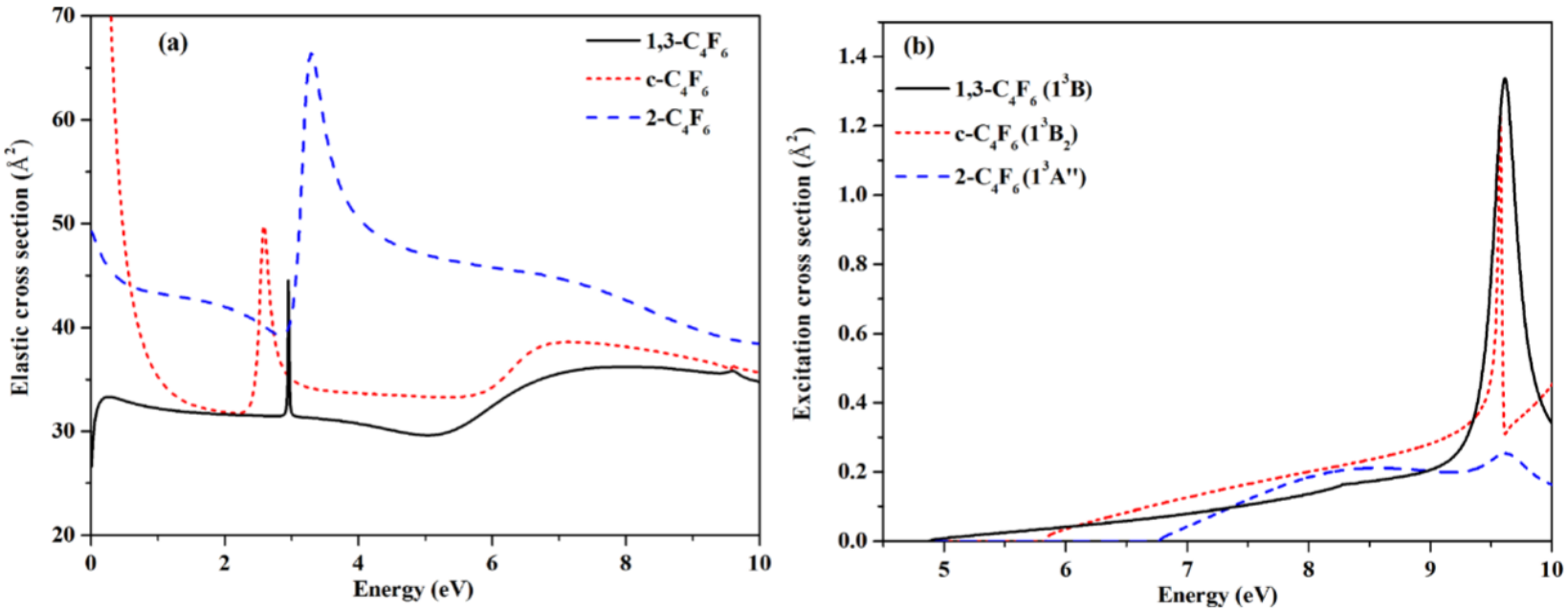
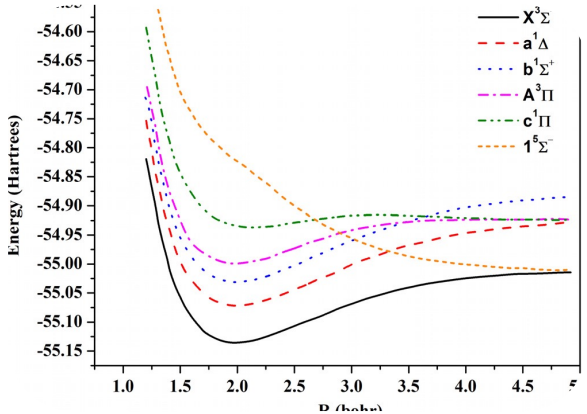


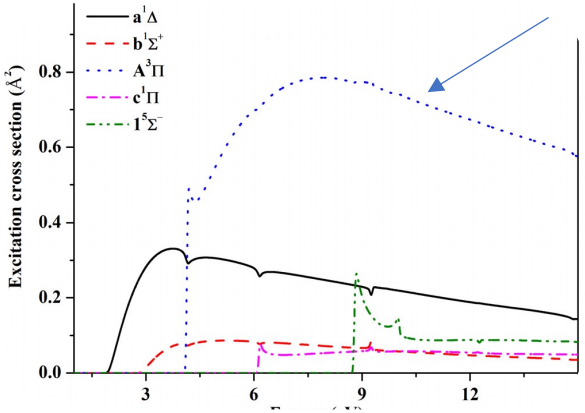
FIG. 8. Isomer effect in the (a) elastic cross section and (b) first excitation cross section of 1,3-C_4F_6, c-C_4F_6, and 2-C_4F_6 in a multistate CI calculations. Solid line: present 1,3-C_4F_6; short dashed line: present c-C_4F_6; dashed line: present 2-C_4F_6.

NH

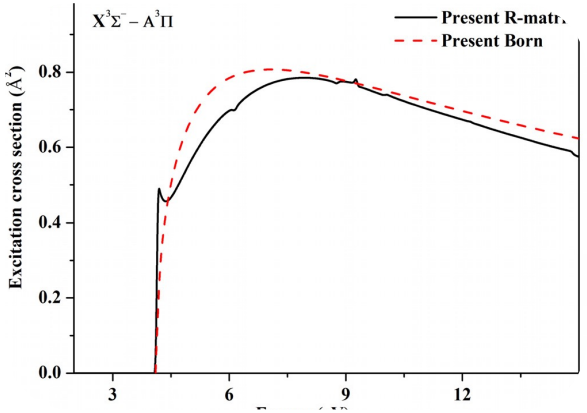
- we calculated the cross sections of low-energy electron impact on BeH_2 using the UK molecular R-matrix code(Quantemol-N).
- The open-shell radical molecule NH has a natural C_{1v} point group having a bond length of 1.958 A° in its equilibrium geometry but used the C_{2v} point group symmetry, which is an abelian, the subset of the C1v point group.
- We have used the cc-pVTZ Gaussian basis set for the N and H atoms
- The cross section for the $^3\prod$ state is maximum compared the other excited states because this is a dipole allowed transition and all other transitions are spin forbidden, it has smaller cross sections.
- The cross sections for the optically allowed transition X-A show a rather good agreement with the Born approximation cross section.



Potential energy curve of NH

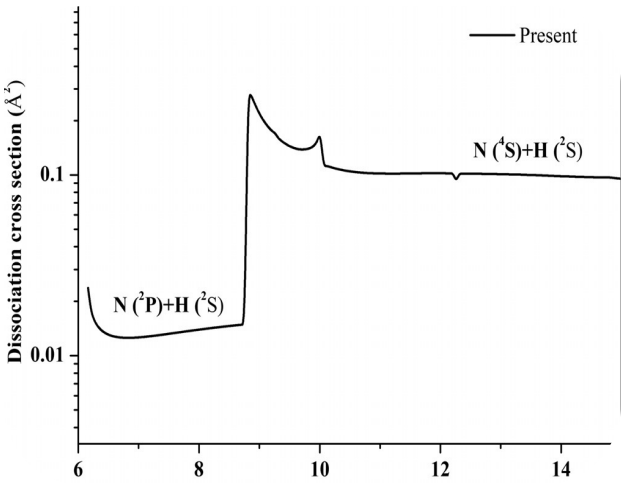


Electronic excitation cross section for the five low-lying excited states of NH

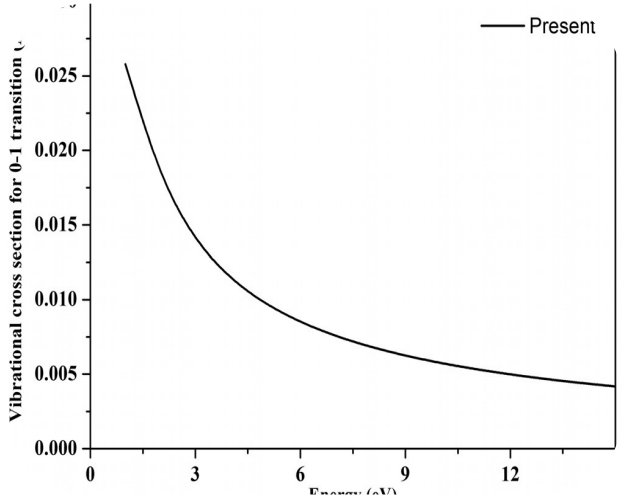


Electronic excitation cross section using the R-matrix method and the Born approximation for the dipole allowed transition.

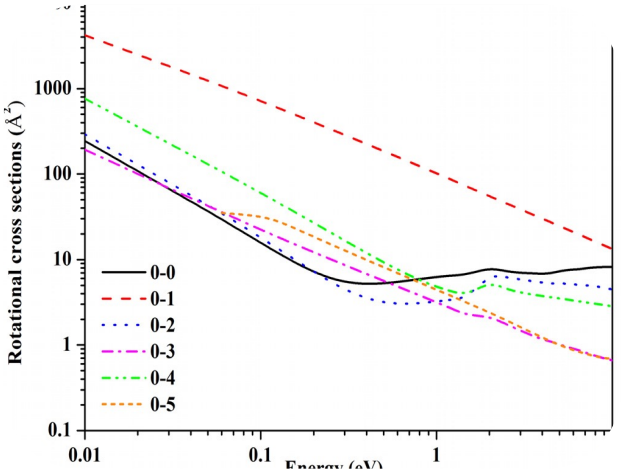
- The $^5\sum^-$ state is purely repulsive in nature, and its excitation cross section is purely dissociative yielding atomic fragments N(^{4}S) +H(^{2}S)
- Another contribution for the dissociative cross section arises from the excitation to the c $^1\prod$ state to the dissociative cross section with atomic fragments N(^{2}P) + H(^{2}S).
- The first-Born dipole approximation is used to calculate the infrared active 0–1 vibrational inelastic cross section for the NH molecule.
- Excitation of transitions with Δj =1 is the most likely process which is dipole moment induced transition.



Dissociation cross section of NH for the dissociation into fragments N and H



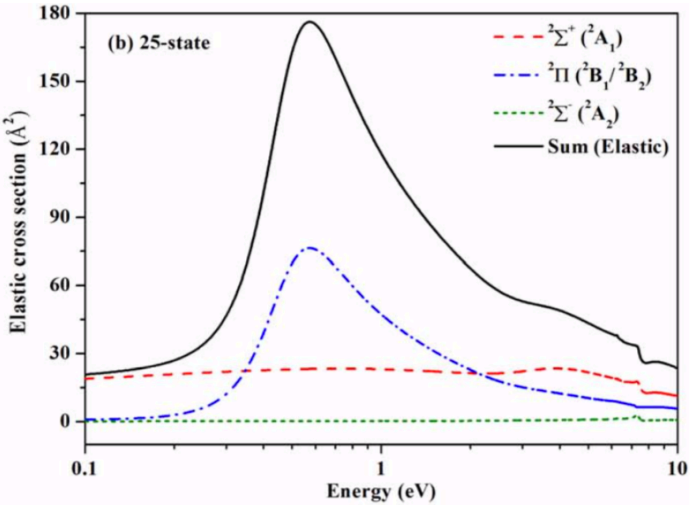
Infrared active 0–1 cross section for the NH molecule.

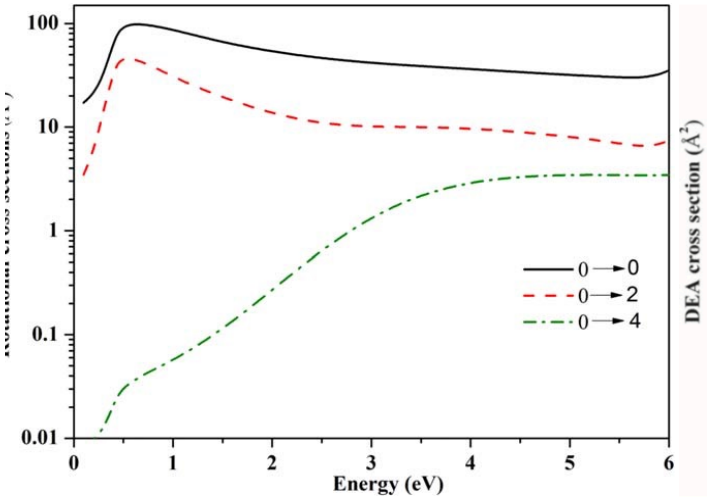


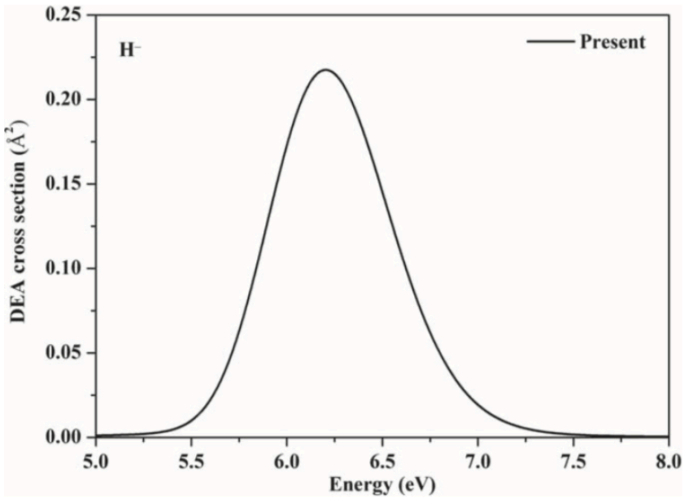
Rotational cross section of the NH radical calculated using the POLYDCS program

BeH2

- we calculated the cross sections of low-energy electron impact on BeH_2 using the UK molecular R-matrix code(Quantemol-N).
- The BeH_2 molecule is a linear, closed-shell system belonging to the C_{2v} point point group symmetry. .
- The first broad peak around 0.45 eV with a width of 0.40 eV in a 25-state calculation is a $^2\Pi_u$ shape resonance.
- BeH_2 is a symmetric molecule which does not possess a permanent dipole moment so rotational excitation only involves transitions with ΔJ even.
- The DEA cross section shows a peak at around 6.2 eV, and overlaps the threshold for the first excitation energy. This peak in the DEA cross section is due to the presence of the resonance detected in the present study at around 6.2 eV







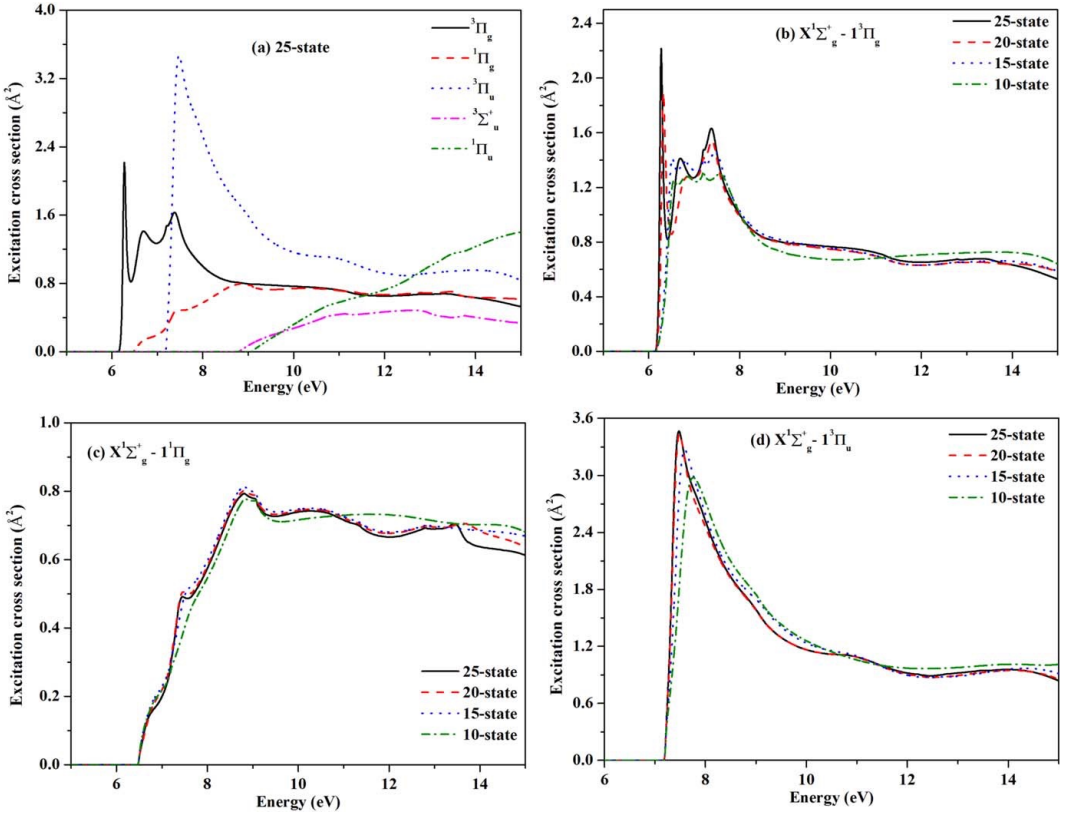


Table 1. BeH_2 vertical excitation energy computed with the CAS-CI and EOM-CCSD methods; also show are the symmetry-allowed CAS-CI dipole transition moments (and permanent quadrupole moments).

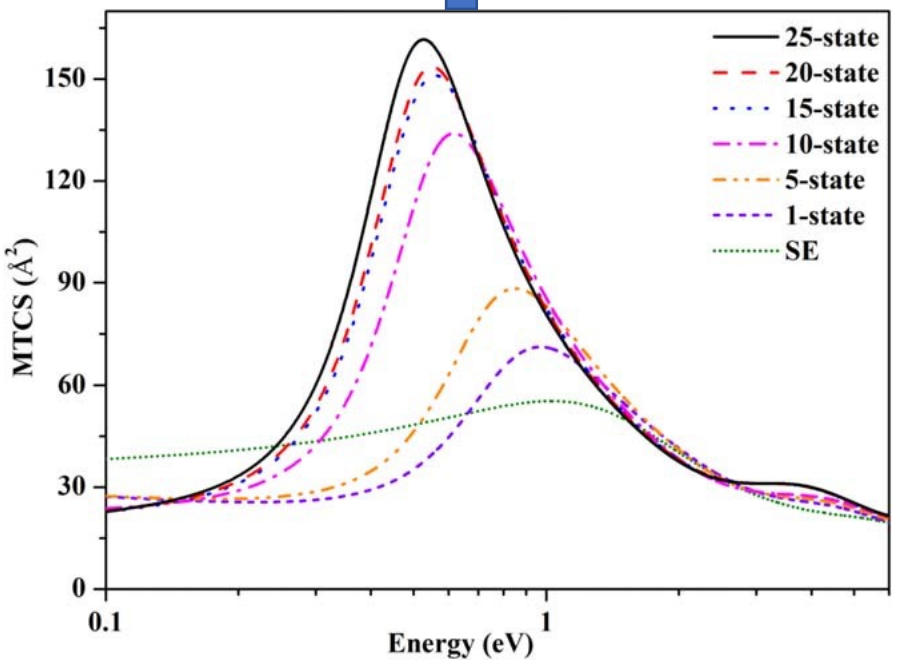
State (C_{2v})	State ($D_{\infty h}$)	Energy (eV) (CAS-CI)	Energy (eV) EOM-CCSD	Transition moments (au)
$^1A_1$	$^1\Sigma^+_g$	0.0	0.0	0.0, (3.4541)
$^3B_1/^3B_2$	$^3\Pi_g$	6.15	6.147	(−3.1708, 3.3643)
$^1B_1/^1B_2$	$^1\Pi_g$	6.48	6.548	0.0, (−3.5048, 3.4926)
$^3B_1/^3B_2$	$^3\Pi_u$	7.19	7.046	(−2.1279, 3.3201)
$^3A_1$	$^3\Sigma^+_u$	8.79	8.588	(−1.7107)
$^1B_1/^1B_2$	$^1\Pi_u$	9.08	8.717	−1.4674, (−0.0927, 3.7184)
$^3A_1$	$^3\Sigma^+_g$	10.71	9.744	(0.0872)
$^1A_1$	$^1\Sigma^+_g$	11.14	—	(−1.8157)
$^1A_1$	$^1\Sigma^+_u$	11.36	—	1.3713, (0.0267)
$^3A_2$	$^3\Sigma^-_g$	12.23	—	(−7.3653)
$^3A_1$	$^3\Sigma^+_u$	12.79	—	(2.5032)
$^3A_2$	$^3\Sigma^-_u$	13.27	—	(−7.1653)
$^1A_2/^1A_1$	$^1\Delta_g$	13.30	—	(−7.4110)
$^3A_2/^3A_1$	$^3\Delta_u$	13.32	—	(−7.3718)
$^3A_1$	$^3\Sigma^+_u$	13.40	—	(0.0600)
$^1A_1$	$^1\Sigma^+_g$	13.75	—	(0.0573)
$^1A_2$	$^1\Sigma^-_u$	14.41	—	(−6.6582)
$^3A_1$	$^3\Sigma^+_u$	14.49	—	(−3.7782)
$^1A_1$	$^1\Sigma^+_u$	14.59	—	0.0876, (3.0011)

- The vertical excitation energies calculated with the present model give excellent agreement with the EOM-CCSD calculations.
- Excitation to the triplet excited states contribute most to the total cross section compared to other electronic excited states.

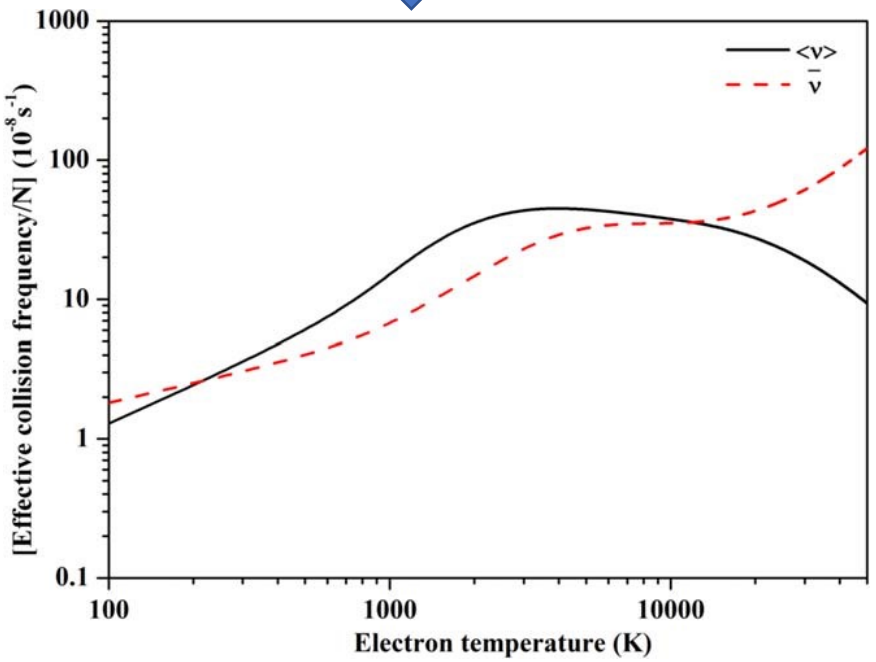
- Collisional frequencies are determined using the momentum transfer cross section for a Maxwell–Boltzmann distribution

$$\langle \nu \rangle = \frac{8}{3\pi^{\frac{1}{2}}} N \left(\frac{m_e}{2K_B T_e} \right)^{\frac{5}{2}} \int_0^{\infty} \upsilon^5 Q^m(\upsilon) \mathrm{e}^{\frac{-m_e \upsilon^2}{2K_B T_e 2}} d\upsilon,$$

$$\overline{\nu}^{-1} = \frac{8}{3\pi^{\frac{1}{2}} N} \left(\frac{m_e}{2K_B T_e} \right)^{\frac{5}{2}} \int_0^{\infty} \frac{\upsilon^3}{Q^m(\upsilon)} \mathrm{e}^{\frac{-m_e \upsilon^2}{2K_B T_e}} d\upsilon.$$



Momentum transfer cross sections for SE, 1-state, 5-state, 10-state, 15-state, 20-state and 25-state CC calculations.



Effective collision frequency of the BeH_2 molecule ground state as a function of electron temperature.

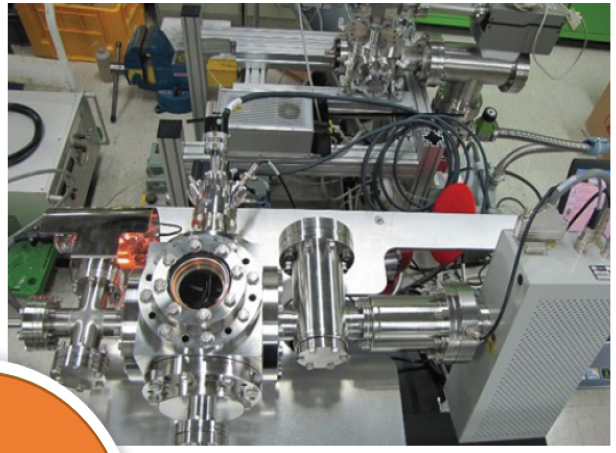
✓ Published papers

- Dhanoj Gupta, Heechol Choi, Deuk-Chul Kwon, Jung-Sik Yoon, Bobby Antony and Mi-Young Song, **"Cross sections for electron collision with Difluoroacetylene"** *J. Phys. B: At. Mol. Opt. Phys*. 50 (2017) 085202.
- Dhanoj Gupta, Kalyan Chakrabarti, Mi-Young Song, and Jung-Sik Yoon" **An R-matrix study of electron induced processes in BF_3**, *Plasma, Phys. Plasma* 24 (2017) 123511.
- Dhanoj Gupta, Heechol Choi, Mi-Young Song, Kalyan Chakrabarti and Jung-Sik Yoon "**Low energy cross sections for electron scattering from tetrafluoroallene**", *Eur. Phys. J. D* 71 (2017) 213.
- Dhanoj Gupta, Heechol Choi, Mi-Young Song and Jung-Sik Yoon "**Cross sections for electron collision with fluoroacetylene: a comparative study with acetylene and difluoroacetylene along with fluorination**", *Chem. Phys. Letts*. 684 (2017) 333
- Dhanoj Gupta, Heechol Choi, Mi-Young Song, Grzegorz P. Karwasz and Jung-Sik Yoon , **"Electron impact ionization cross section studies of C_2F_x (x=1-6) and C_3F_x (x=1-8) fluorocarbon species**", *Eur. Phys. J. D* 71 (2017) 88.
- Dhanoj Gupta, Heechol Choi, Deuk-Chul Kwon, Jung-Sik Yoon and Mi-Young Song* ,"**Study of electron induced ionization for plasma processing gases: C_4F_x (x=1-8) and the isomers of C_4F_6 and C_4F_8 for plasma modeling**", J. Phys. D: Appl. Phys. 51 (2018) 155203
- Dhanoj Gupta, Mi-Young Song, K. L. Baluja, Heechol Choi, and Jung-Sik Yoon, "**Electron impact elastic and excitation cross-sections of the isomers of C4F6 molecule for plasma modeling**", Physics of Plasmas 25, (2018) 063504
- Dhanoj Gupta, Mi-Young Song , Heechol Choi, Deuk-Chul Kwon, K L Baluja and Jonathan Tennyson, **R-matrix study for electron scattering of beryllium dihydride for fusion plasma**, J. Phys. B: At. Mol. Opt. Phys. 52 (2019) 065204
- Dhanoj Gupta , K. L. Baluja, and Mi-Young Song, "**Vibrationally resolved excitation, dissociation, and rotational cross sections of NH radical by electron-impact using the Rmatrix method**" Phys. Plasmas 26 (2019) 063503

Experimental Measurement

Total Cross Section

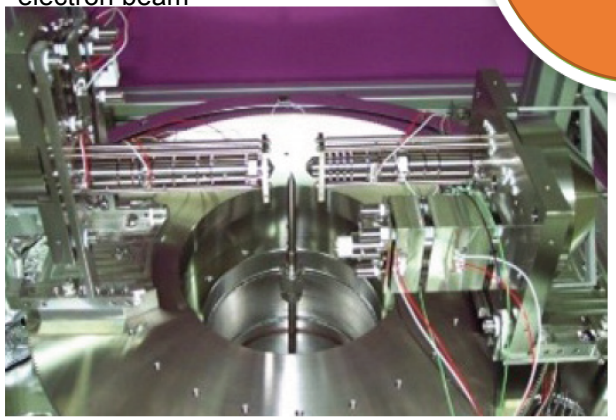
Measurement of total cross sections for electron scattering on atomic and molecules using magnetized electron beam



Dissociation Cross Section

Ionization threshold spectroscopy method

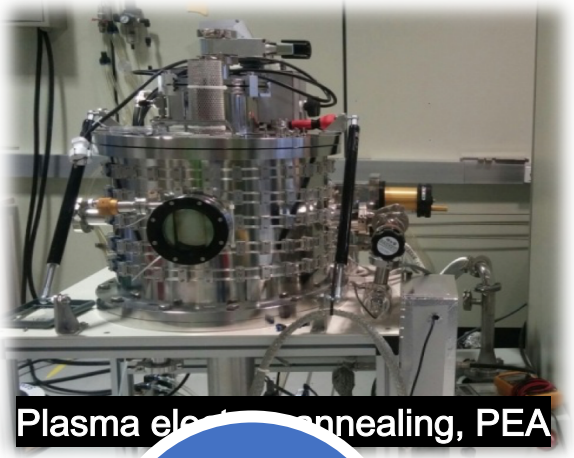
Apparatus



Elastic Differential Scattering Cross Section

(2018 ~2021)

Biomolecule-Electron Collision Data

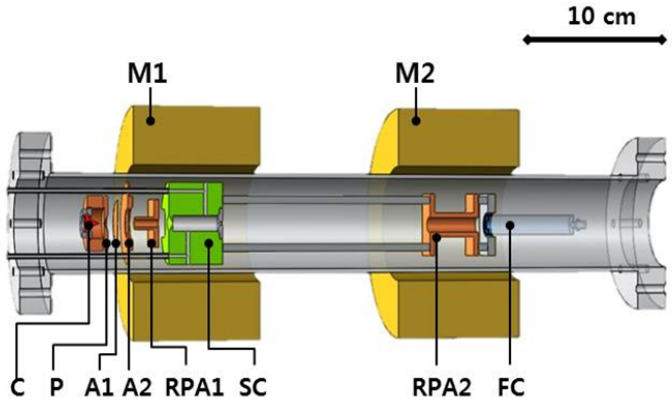


PMI

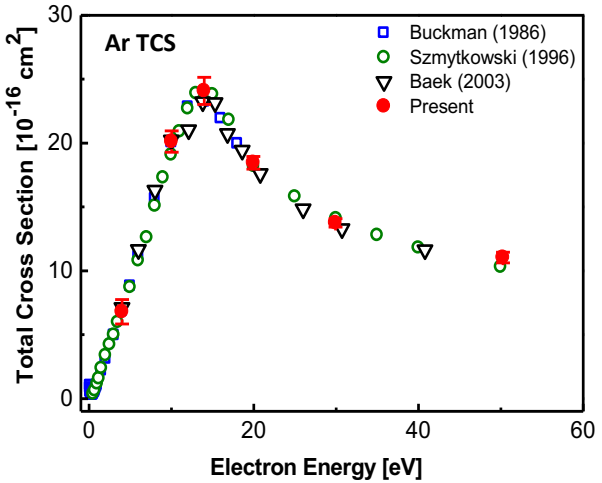
SPUTTERING YIELD
(2020 ~2023)

Total Cross Section

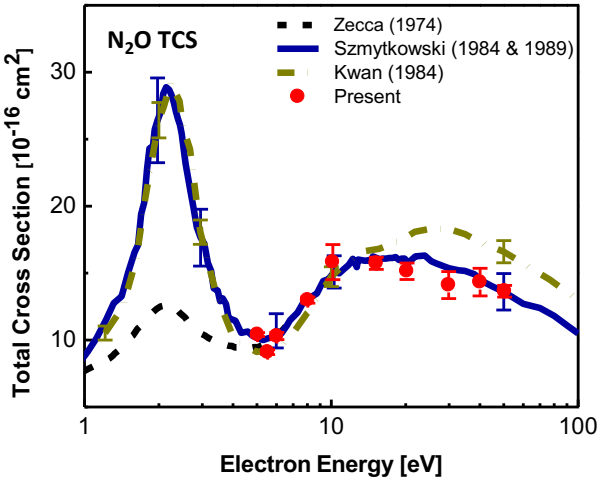
Total electron cross section measurement system



Cross-sectional view of the apparatus



Total electron scattering cross section of argon. The present results are in good agreement with previously measured values, confirming the correct operation of the experiment

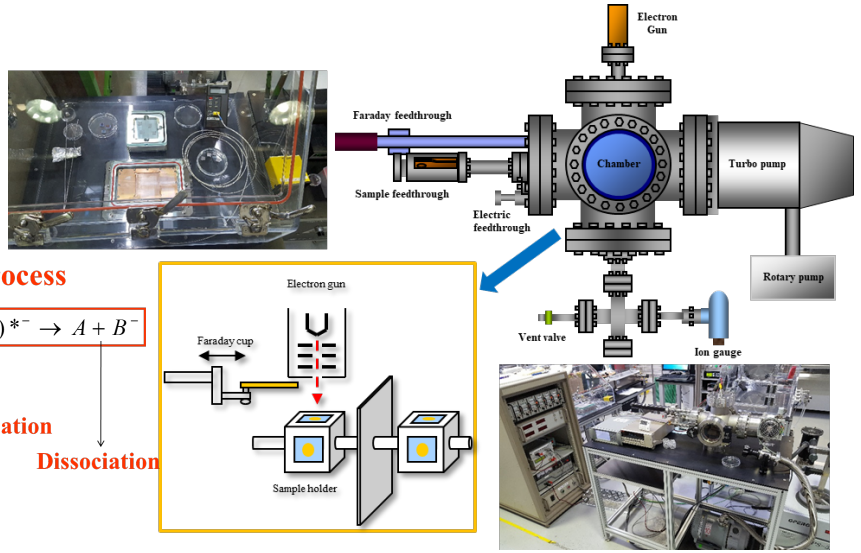


Total electron scattering cross section of N_2O.

Biomolecule-Electron Collision Data

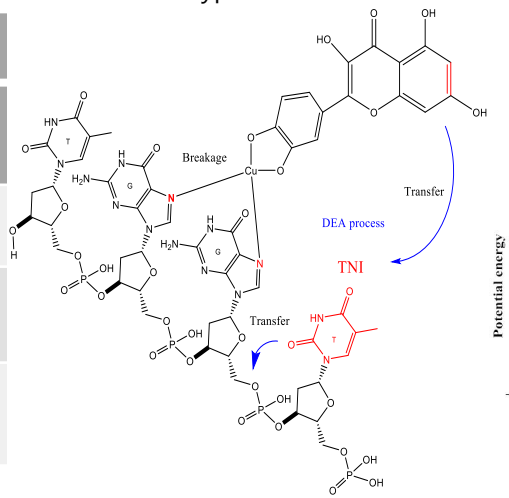
In order to study DNA damage caused by electron collisions in a complex bio-environment, we are experimenting with attaching desired metal ions, quercetin and anti-splash to bio-model molecules.

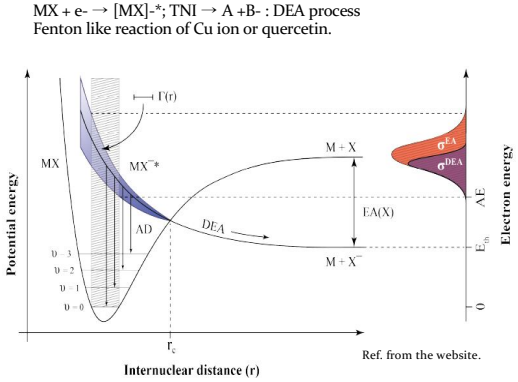
Cylindrical type Biomolecule-Electron Collision Experiment System



Planar type Biomolecule-Electron Collision Experiment System

Molecular Category	Molecular Species	Electron Collision Energy	Reaction data	
			Damage yield	Charge trapping CS
Oligomer	9	10 eV	12	
Plasmid DNA	7	3, 5, 10 eV	11	
Sub-Nucleotide	5	0 ~ 9 eV, 10 eV	4	1



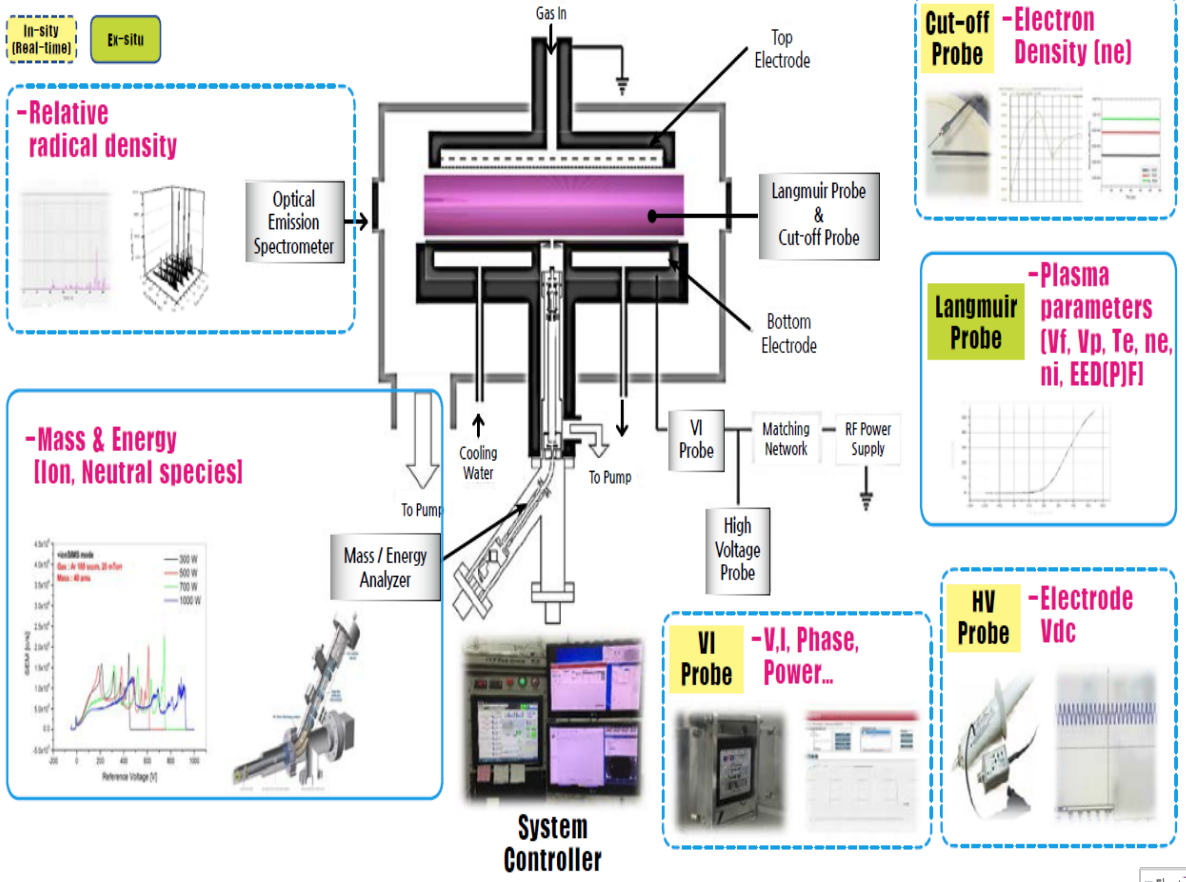


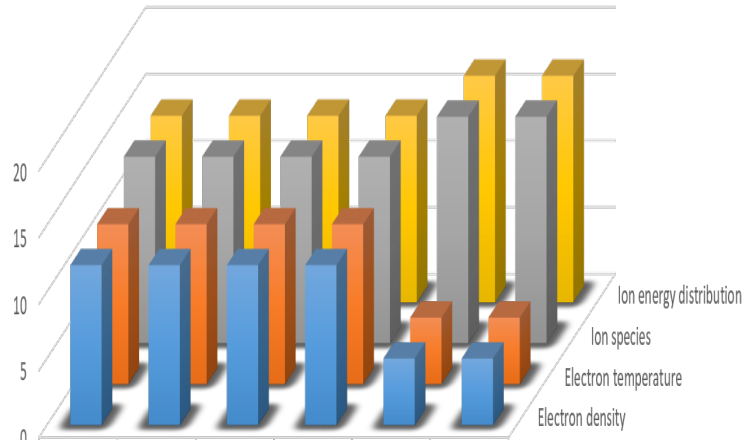
Plasma Diagnostic

- We experimented with mounting types of diagnostic devices on the plasma generator to understand the plasma state information of the material.
- In addition, the system is being improved to monitor the reaction of the surface facing the plasma.
- we are developing advanced method of plasma monitoring and plasma process fault detection by OES data analysis using machine learning

Plasma Diagnostic system

Integrated Plasma Diagnostic (IPD) System @NFRI



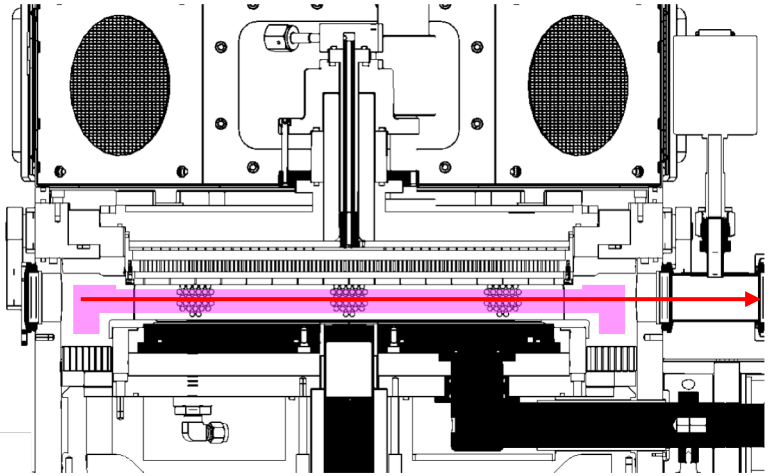


	C4F8/Ar	C4F8/Kr	C4F8/Xe	C4F8/Ar/Kr	C4F8/O2/Ar	C4F8/O2/Kr
Electron density	12	12	12	12	5	5
Electron temperature	12	12	12	12	5	5
Ion species	14	14	14	14	17	17
Ion energy distribution	14	14	14	14	17	17

Plasma diagnostics with optical spectroscopy

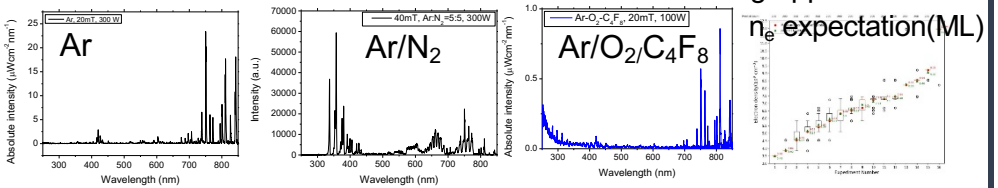
- Development of optical emission spectroscopic method for process plasma

300 mm wafer etch process chamber(CCP)



- Various processing gases (Ar, Kr, Xe, O_2, N_2, C_xF_y, $C_xH_yF_z$, etc.)

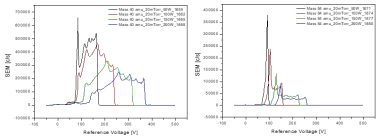
OES data → Machine learning application



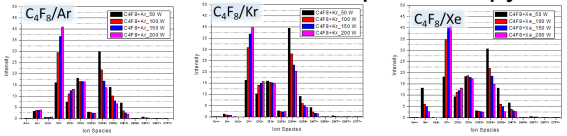
n_e expectation(ML)

- Correlative analysis with various plasma chamber data and OES (emission spectrum ~ n_e, T_e, EEDF, E_i, M_i, V_{RF}, I_{RF}, Etch rate, etc.)

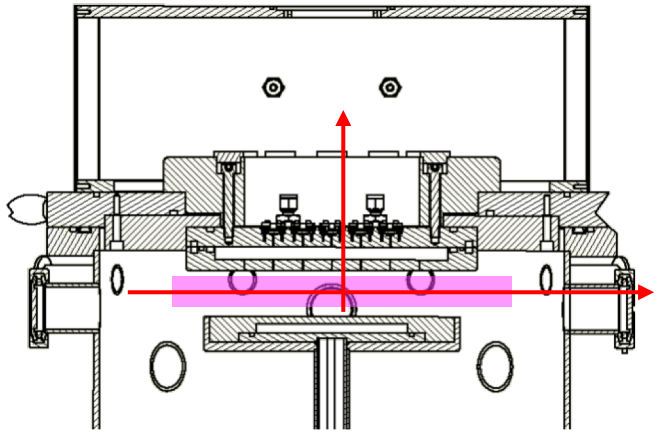
Ion energy distribution



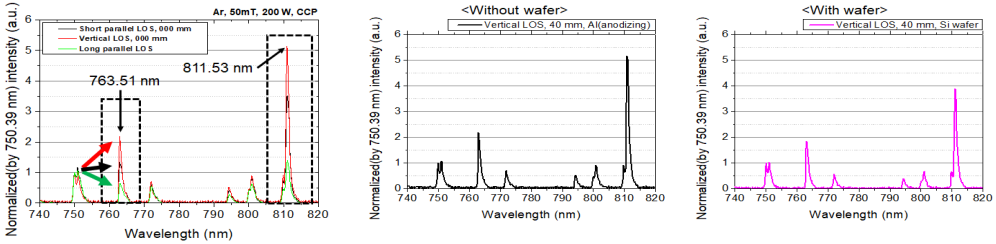
Ion, neutral mass spectroscopy



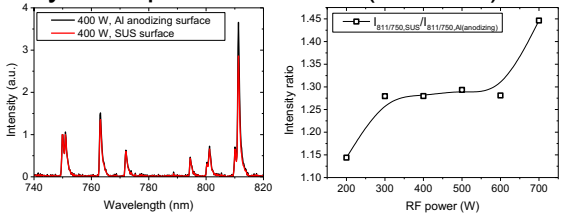
200 mm wafer process chamber(CCP or ICP)

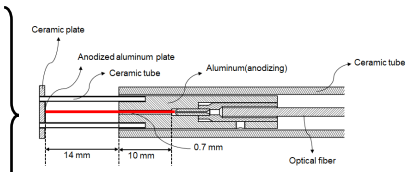


- Optical diagnostics for → Effect of line-of-sight on OES



- Analysis of plasma-surface(material) interaction → Effect of OES facing material





OES probe

Collisional-Radiative model for Ar low-temperature plasma

- Development of Collisional-Radiative model for argon low-temperature plasma based on NOMAD code

A		#
BSR	441	768
BIAGI	11	
PUECH	10	
NIST VR	306	

B		#
Model A	768	17256
LANL	846	
FAC	15411	

C		#
Model B	17256	18255
MCDHF GF	999	
LANL GF	15411	

D		#
Model C	18255	30787
FAC GF	12532	

E		#
Model A	768	15825
MCDHF VR	496	
LANL VR	624	
FAC VR	13937	

F		#
Model D	7689	45844
MCDHF VR	496	
LANL VR	624	
FAC VR	13937	

NIST, LANL, FAC, Biagi, BSR, IST, PUECH, NGFSRDW

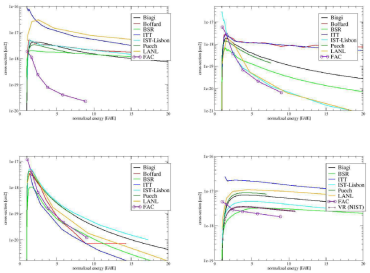
A&M data set

NOMAD lite

CR Model

-Plasma source: CCP, ICP, ECR
-EEDF: (Bi-)(Beam-shifted-)Maxwellian, Dryuvesteyn

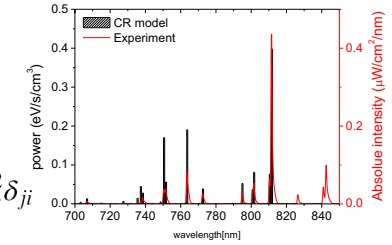
Experi -ment data



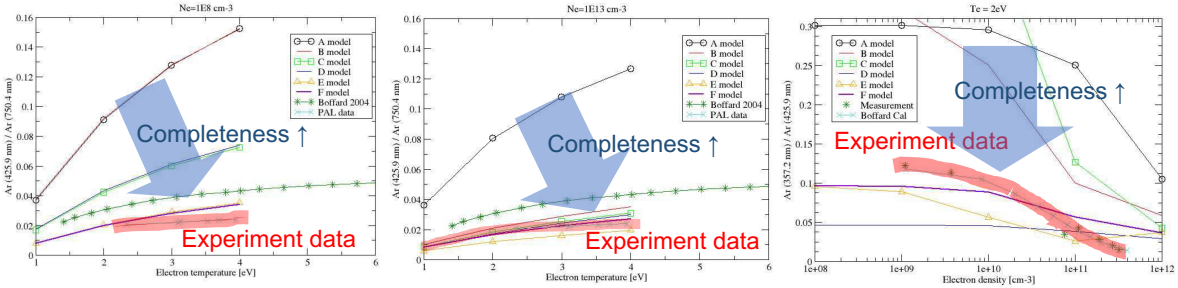
$$\frac{dn_i}{dt} = -n_i \sum_{j \neq i}^{N_L} W_{ij} + n_i \sum_{j \neq i}^{N_L} n_j W_{ji}$$

$$W_{ij} = B_{ij} J_{ij} + n_e C_{ij} + \beta_{ij} + n_e \gamma_{ij} + \sigma_{ij}$$

$$W_{ji} = A_{ij} + B_{ij} J_{ji} + n_e D_{ji} + n_e \alpha_{ji}^{RR} + n_e \kappa_{ji}^{EC} + n_e^2 \delta_{ji}$$



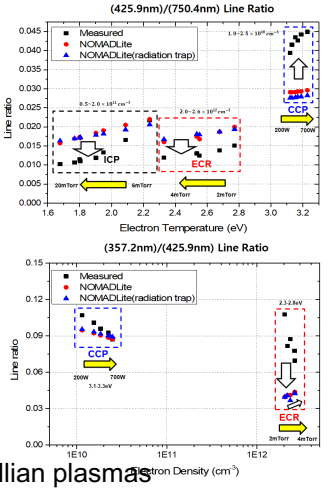
Sensitivity to the model completeness



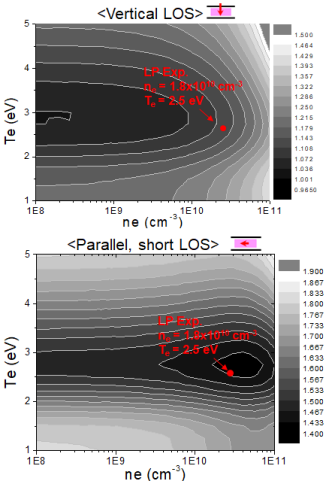
Electron Temperature

Electron density

Sensitivity to plasma source(SNU)

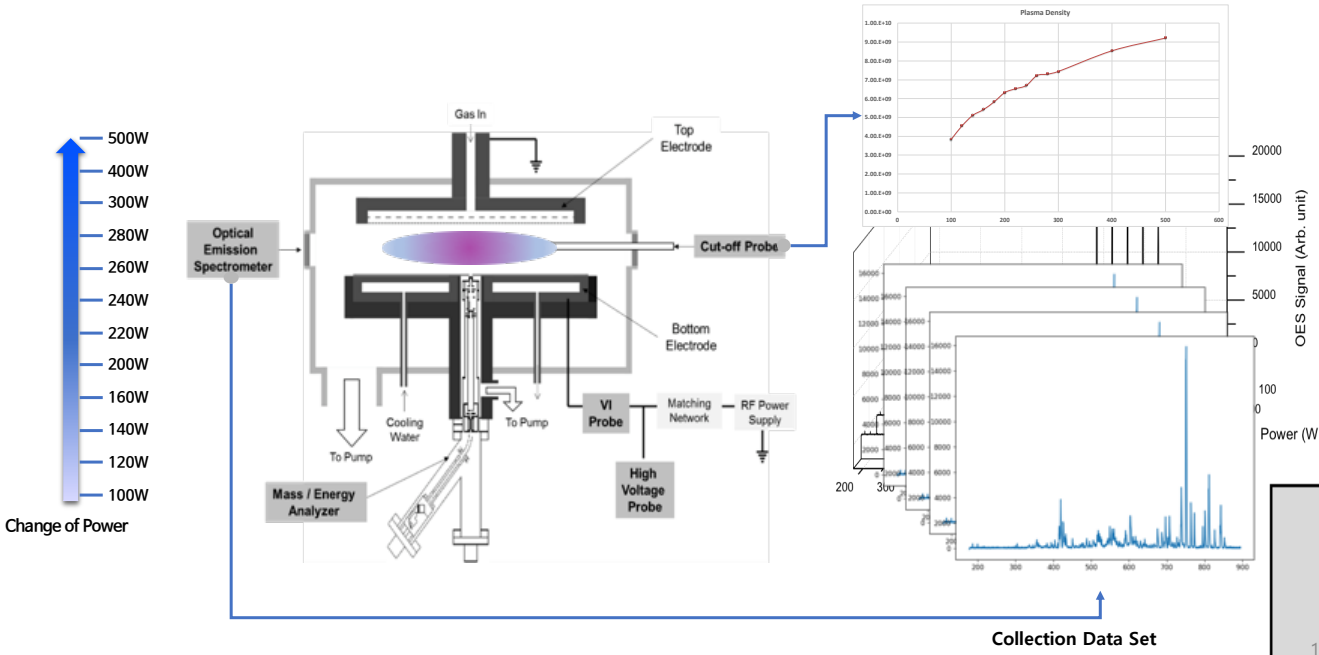


Plasma diagnostics



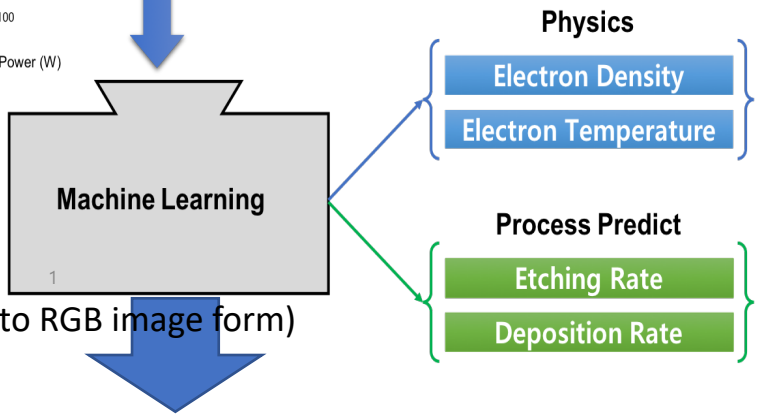
* NOMAD, Yuri V. Ralchenko, time-dependent collisional-radiative plasma kinetics code for non-Maxwellian plasmas

Analyze OES Data Using Machine Learning to Predict Plasma State



Data collection from experiment system

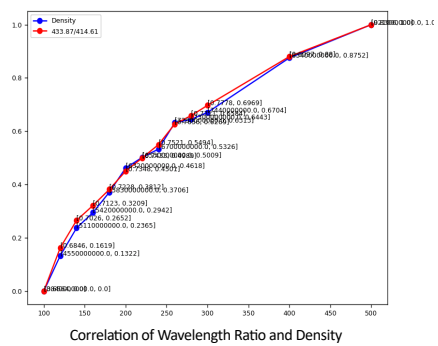
- change of power(13 step): 13 different density and OES data set}
- change of pressure (32step) : 32 different temperature and OES data set

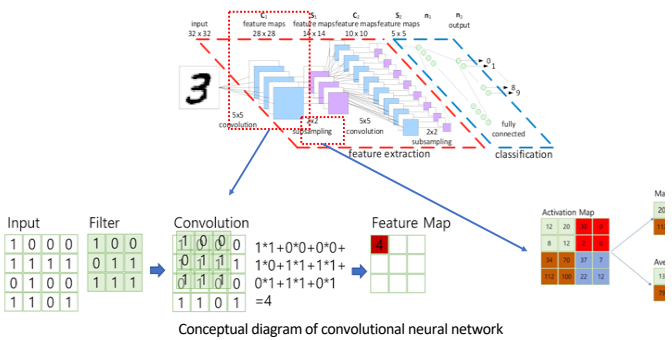


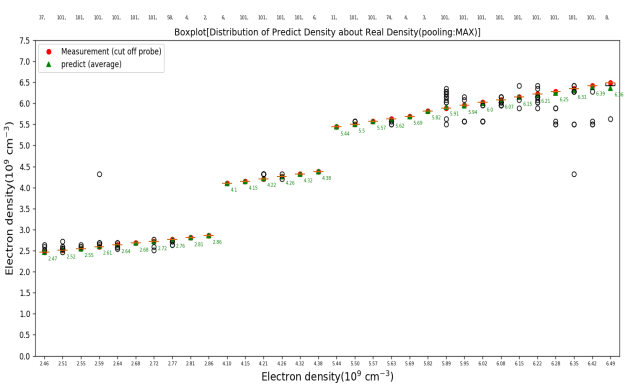
⇨Develop OES data preprocessing program. (convert total wavelength ratio value into RGB image form)

⇨Develop machine learning algorithm (using Convolutional Neural Network, 4layer)

⇨Accuracy : 90% (Does not include the margin of error, Only when outputting same density value as an input density value.)







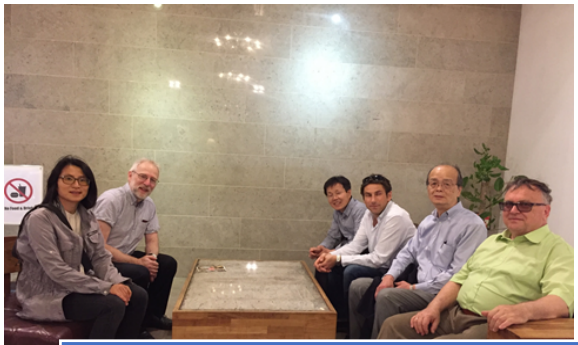
International Group Data Evaluation Activities

- This work decide at the Joint IAEA-NFRI Technical Meeting (TM) on Data Evaluation for Atomic, Molecular and Plasma Material Interaction Processes in Fusion in September 2012
- Participants recommended group member and molecule at that time.
- Group Members:
  - Grzegorz P. Karwasz (Poland)
  - J. Tennyson (UK)
  - Viatcheslav kokoouline(USA)
  - Y. Nakamura, Y. Itikawa (Japan)
  - H. Cho M.-Y. Song, J.-S. Yoon (Rep. Korea)
- Our aim of the group evaluation is
- To establish the internationally agree standard reference data library for AM/PMI data
- To reexamine the available cross sections for methane and to establish an up-to-date set of recommended cross sections.

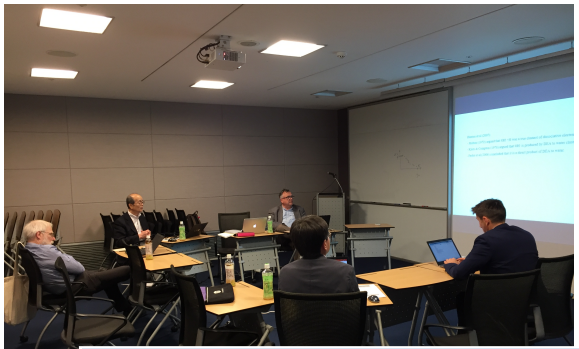
2014
- 8-9 January 2014, Seoul, South Korea
- 4 -5 July 2014, Cumberland Lodge, UK
- 14 December 2014, Deajeon, South Korea

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.



2018
- 8~10 May 2018, Seoul, South Korea

2019
- 8~10 May 2019, Seoul, South Korea

Procedure

Preparatory stage

- Review of previous evaluation paper
- Collection of new paper.
- Define working Scope
- Contents of report
- To shard working part

Evaluation stage

- analysis method of experiment and theory (characteristics, limitation, uncertainty, method)
- Comparisons of different research group
- Combine different collision processes

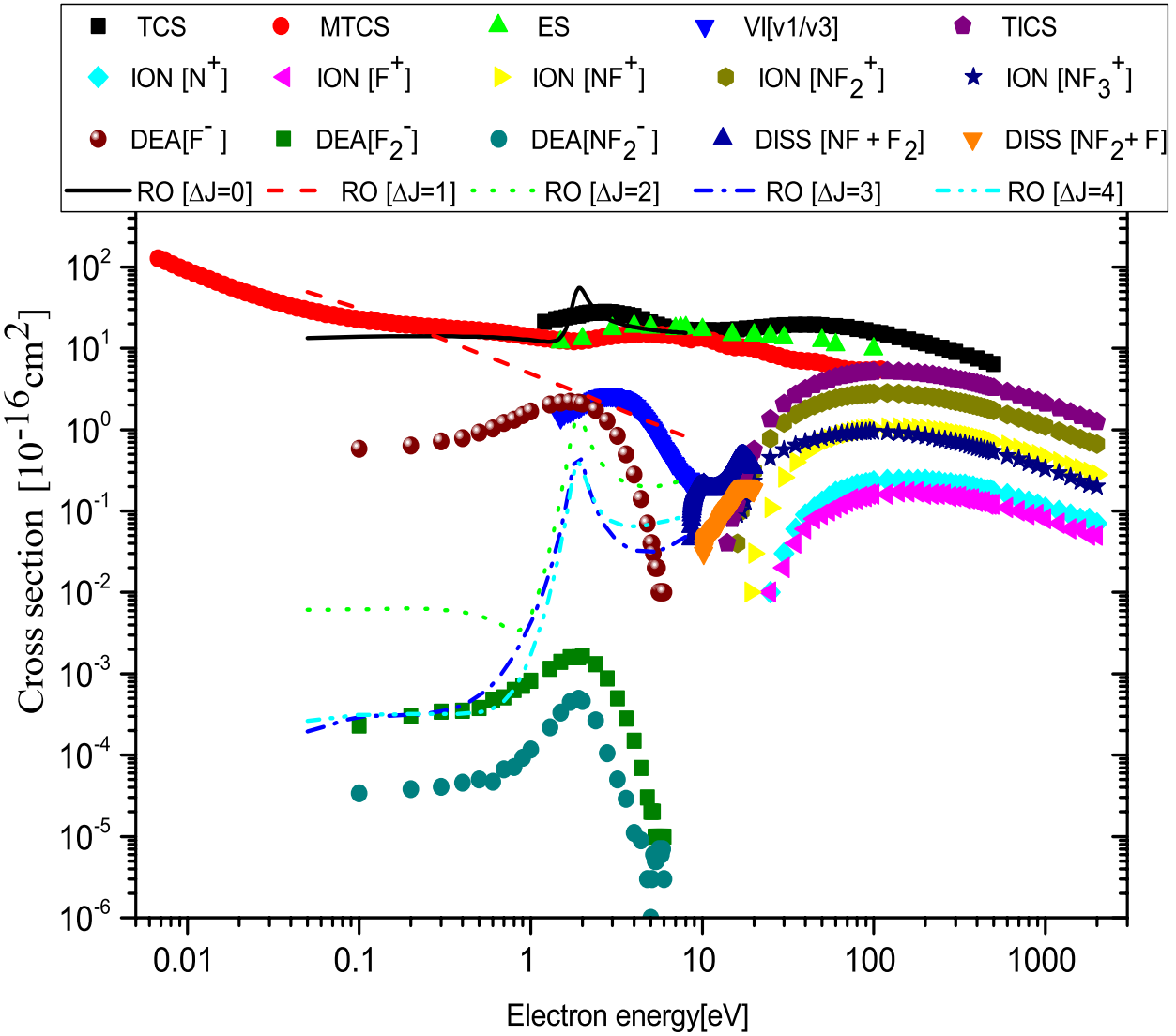
Certified stage

- Check uncertainty
- Define recommended data of each collision processes
- Agreement of each evaluator
-

Cross section for electron collisions with NF3

2015 ~2016 : review and assessment
15 December 2017 : published online (J. Phys. Chem. Ref. Data, **46**, 043104 (2017))

- Nitrogen trifluoride or trifluoramine (NF3) gas is widely used in plasma processing technology.
- NF3 is used in a number of plasma processes where it is often used as a source of F atoms due to ease of production of these atoms via dissociative electron attachment (DEA) and electron-impact dissociation both from NF3 itself and from NF2 and NF fragment.
- The exothermicity from these dissociative processes also provides an important gas heating mechanism. Use of NF3 in plasma etching, particularly in mixtures with O2, provides a source of F2 ions due to an enhanced DEA process at low (about 1 eV) energies.
- NF3 is also used in the production of thin films and solar cells; it provides the initial gas for the HF chemical laser.
- NF3 is actually a greenhouse gas with a very high global warming potential which has led to concern on how it is used in the various technologies discussed above.



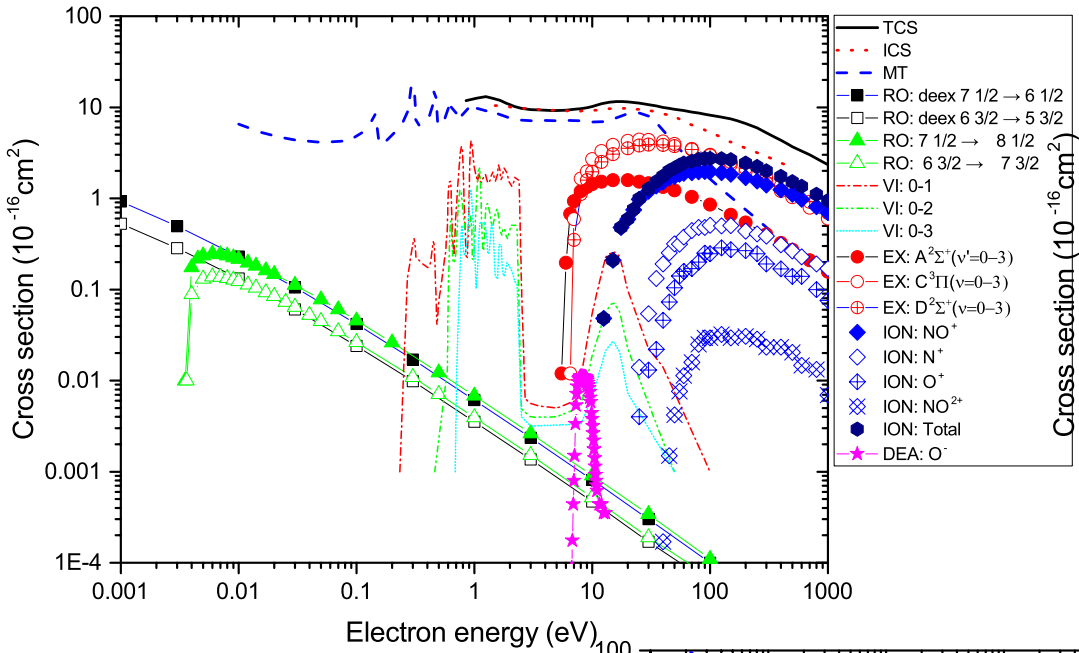
- For the TCS, the MTCS, and the ionization cross section,
  - it is possible to recommend values over an extended energy range with small uncertainties, typically 10%–15%. The situation is significantly worse for other processes.
- For electron-impact rotational excitation,
  - we rely on predictions from ab initial calculations, but these calculations are far from being complete.
- For vibrational excitation cross sections.
  - Theoretical treatments of this process are possible and should be performed by theorists. Some new, reliable beam measurements of this process would be very helpful.
- For the electron impact dissociation
  - It is an important process, but the available measurements are inconsistent with each other, and we are unable to recommend a good set of data for this process. A new study on the problem is needed.
- For the dissociative electron attachment process:
  - We recommend using the recent experimental data and are able to provide the estimated uncertainty to be about 15%.

Cross section for electron collisions with NO, N_2O, and NO_2

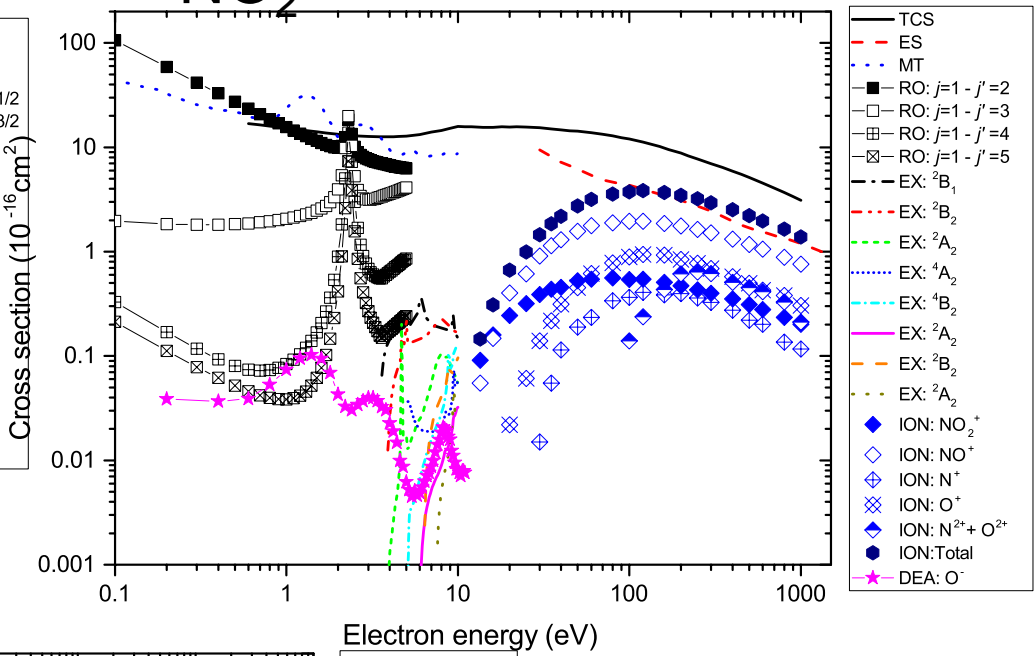
- 2016 ~2017 : review and assessment
- May 2019 : to be submitted article (J. Phys. Chem. Ref. Data)

- Nitrogen oxides (NxOy) are easily generated in atmospheric plasma using N_2 and O_2 gas. Nitrogen oxides are regulated as corrosive substances, and research on how to remove them is becoming of increasing importance.
- NO(Nitric oxide) accounts for about 95% of the nitrogen oxides generated in the combustion of fossil fuels, and mostly undergoes rapid oxidized to NO_2 (Nitrogen dioxide)which is harmful to both the human body and the natural environment.
- N2O(Nitrous oxide) is not created in the combustion of fossil fuels, but is known to be generated in selective catalytic reduction (SCR) reactions and is a known cause of global warming.

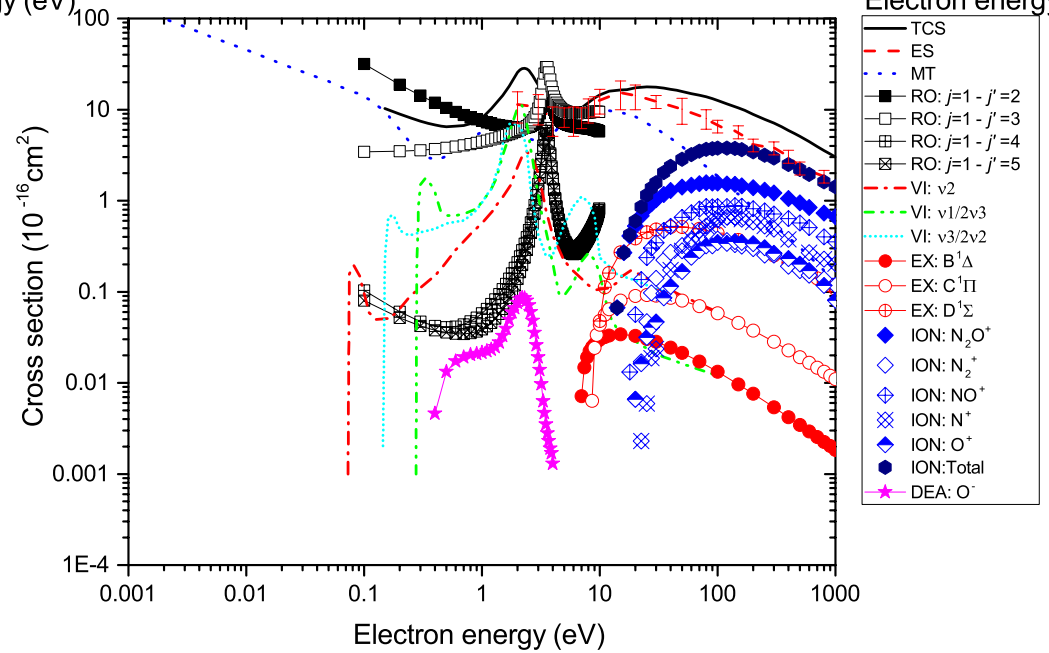
NO


Cross section (10^{-16}cm^2)
Electron energy (eV)
TCS
ICS
MT
RO: deex 7 1/2 → 6 1/2
RO: deex 6 3/2 → 5 3/2
RO: 7 1/2 → 8 1/2
RO: 6 3/2 → 7 3/2
VI: 0-1
VI: 0-2
VI: 0-3
EX: $A^2\Sigma^+(v'=0-3)$
EX: $C^3\Pi(v=0-3)$
EX: $D^2\Sigma^+(v=0-3)$
ION: NO^+
ION: N^+
ION: O^+
ION: NO^{2+}
ION: Total
DEA: O^-

NO_2

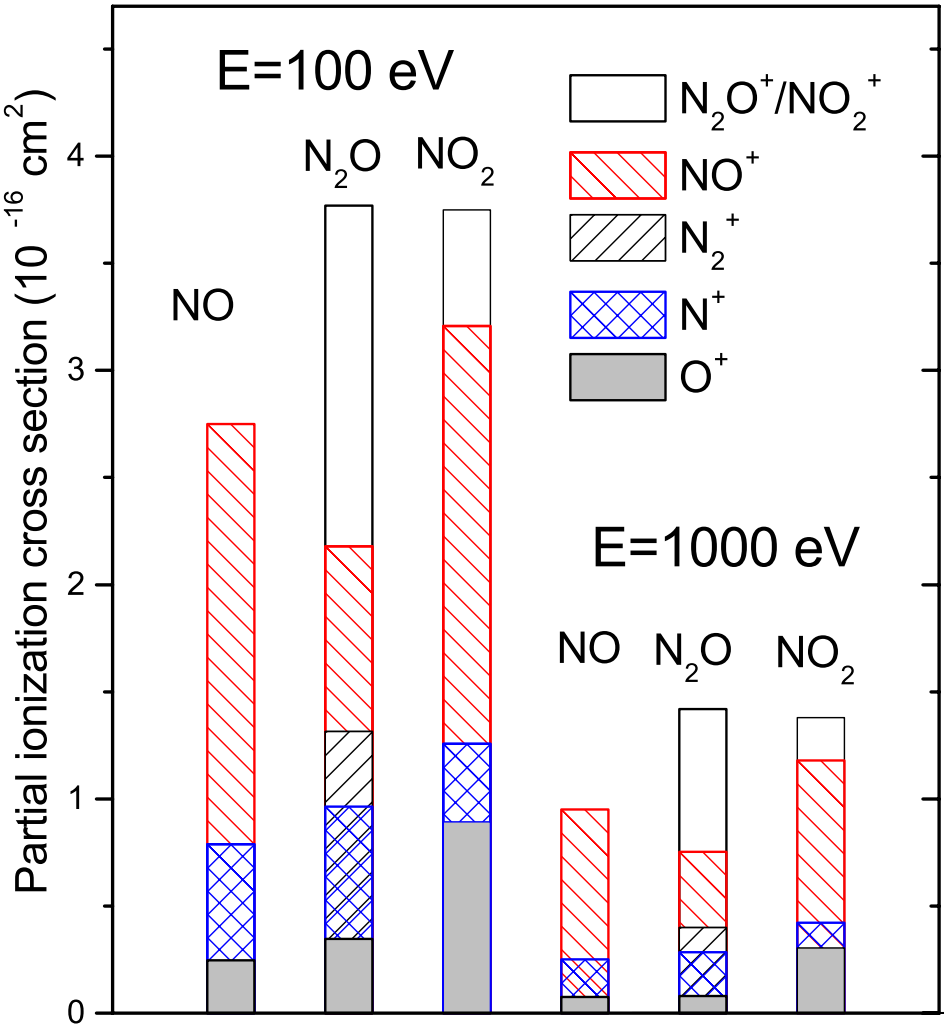

Cross section (10^{-16}cm^2)
Electron energy (eV)
TCS
ES
MT
RO: j=1 - j' =2
RO: j=1 - j' =3
RO: j=1 - j' =4
RO: j=1 - j' =5
EX: $^2B_1$
EX: $^2B_2$
EX: $^2A_2$
EX: $^4A_2$
EX: $^4B_2$
EX: $^2A_2$
EX: $^2B_2$
EX: $^2A_2$
ION: NO_2^+
ION: NO^+
ION: N^+
ION: O^+
ION: N^{2+}+ O^{2+}
ION:Total
DEA: O^-

N_2O


Cross section (10^{-16}cm^2)
Electron energy (eV)
TCS
ES
MT
RO: j=1 - j' =2
RO: j=1 - j' =3
RO: j=1 - j' =4
RO: j=1 - j' =5
VI: ν2
VI: ν1/2ν3
VI: ν3/2ν2
EX: $B^1\Delta$
EX: $C^1\Pi$
EX: $D^1\Sigma$
ION: N_2O^+
ION: N_2^+
ION: NO^+
ION: N^+
ION: O^+
ION:Total
DEA: O^-

- For the TCS and the ionization cross section,
  - the main differences between the three nitrogen oxides are visible in the low energy range (below 5 eV) where the cross sections display the existence of different resonances.
  - In particular, this energy region is the one for which biological processes are influenced the most. Experimental (and theoretical) studies are still needed
  - Total ionization cross sections are well reproduced by BEB model for all three nitrogen oxides. The optical potential model overestimates slightly (10-15%) the total ionization cross sections for all three targets.
- For the electron impact excitation
  - Electronic excitation in the open shell NO molecule shows a number of partially overlapping states, starting from some 4.75 eV;
  - it is dominated by two dipole allowed states, visible as broad peaks, centered at 8.5 eV and 9.5 eV in the energy-loss spectra in N_2O.
  - A similar proportion is predicted by the present R-matrix calculation for NO_2 in the energy range 9 – 10 eV.

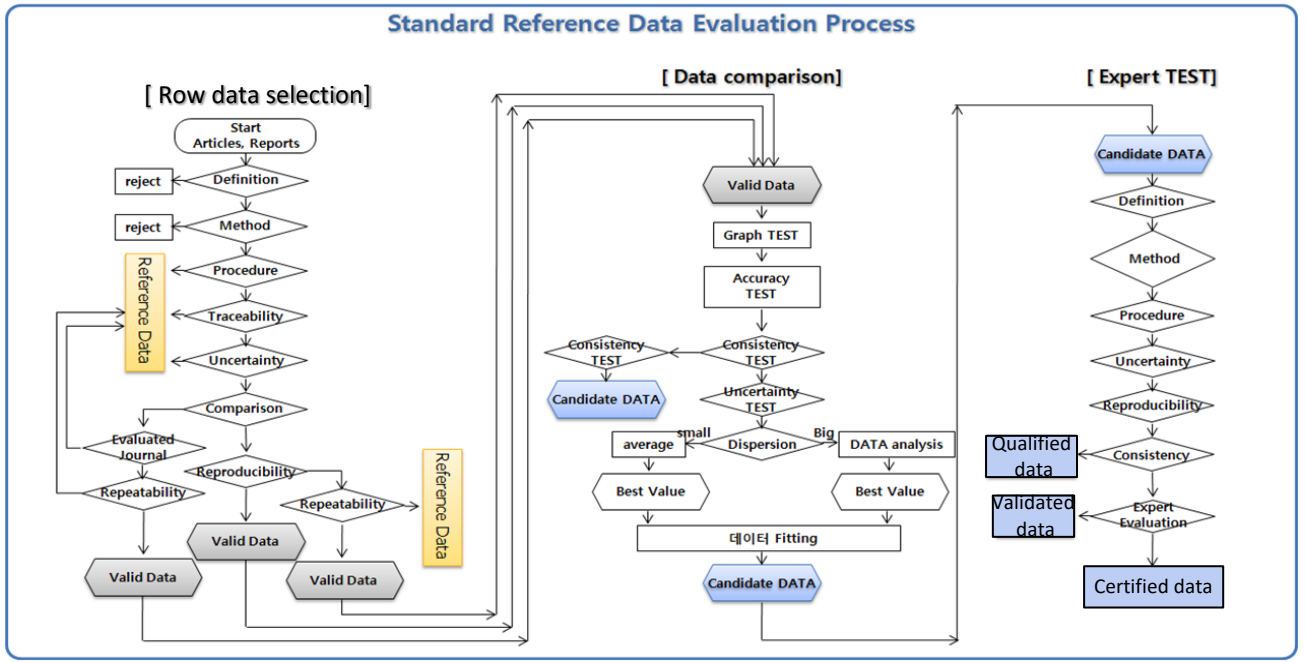
- For electron-impact rotational excitation
  - we rely on predictions from ab initial calculations, but these calculations are far from being complete
  - They are clearly visible in the dissociative attachment channel and as an enhancement of the rotational-excitation cross sections at about 2.2 eV as predicted by the present theory.
- For the vibrational excitation cross sections
  - We recommend the vibrational excitation cross sections determined from swarm measurements but note that this is only an indirect measurement for which it is hard to establish true uncertainties.
- Our knowledge on electron scattering is broadly satisfactory for NO and N_2O but it has many gaps for NO_2
  - for example we are not aware of measurements of the vibrational or electronic-excitation cross sections.
  - for NO and NO_2 we also lack measurements of dissociation into neutrals.

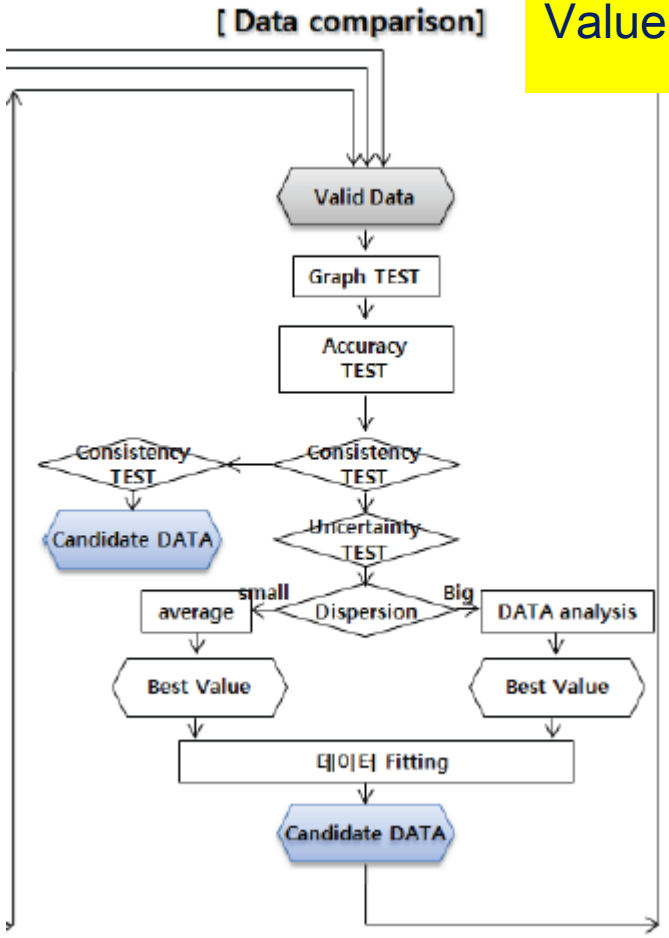


- Figure compares partitioning into different channels of ionization at 100 eV and 1000 eV.
- For neither N_2O nor NO_2 is the parent ion the dominant product (i.e. constitutes over 50% of the ionization events) at energies where other channels are available.
- The NO^+ dissociated ion is the main ion in the ionization of NO_2 and constitutes about N_2 of ionization events in of N_2O.
- The N^+ ion is formed with roughly double the probability of the O^+ ion in NO and N_2O; in NO_2 the O^+ ion prevails over N^+.

Evaluation of Collected data

- The most basic, necessary, and first step in the development of those technologies is electron collision with the initially unreactive species to produce the activated species
- As a result, fundamental AMO physics is closely and beneficially connected to technology development.





Value Evaluation

Electron energy (eV)	Cross section (10^{-16}cm^2)	불확도 (10^{-16}cm^2)
0.4	10.2	1.02
0.5	11.1	1.11
0.65	12.1	1.21
0.8	12.7	1.27
0.9	13.3	1.33
1	14	1.4
1.1	15.1	1.51
1.2	16.2	1.62
1.3	18.1	1.81
.	.	.
.	.	.
.	.	.
.	.	.
.	.	.

Uncertainty Evaluation

$x_1, x_2, x_3 \ldots\ldots x_n$ (independent value)

$\bar{x} = \frac{x_1 + x_2 + \ldots + x_n}{n}$ (average)

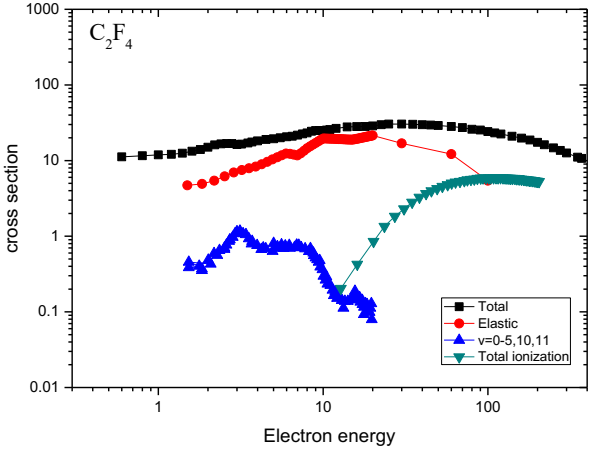
$s(x) = \sqrt{\sum_{i=1}^{n} \frac{(x_i - \bar{x})^2}{n-1}}$, (standard deviation)

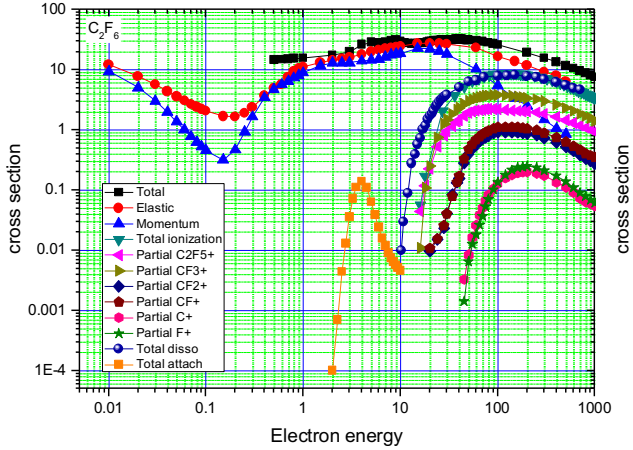
$s_p^2(x) = \frac{\sum_{i=1}^{n} v_i s_i^2}{\sum_{i=1}^{n} v_i}$, (combined standard deviation, v_i

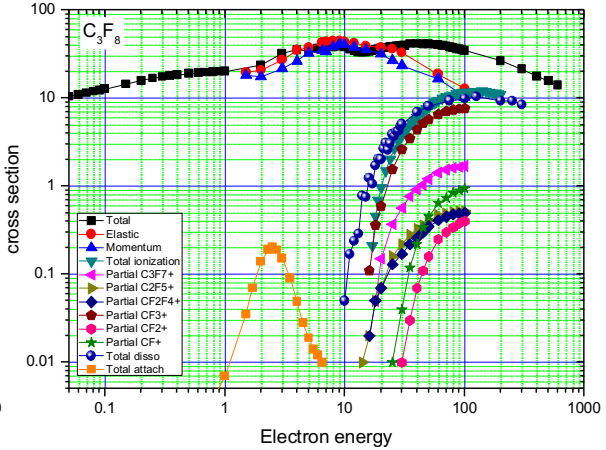
$u_s = \frac{a}{\sqrt{3}}$, (systematic effects)

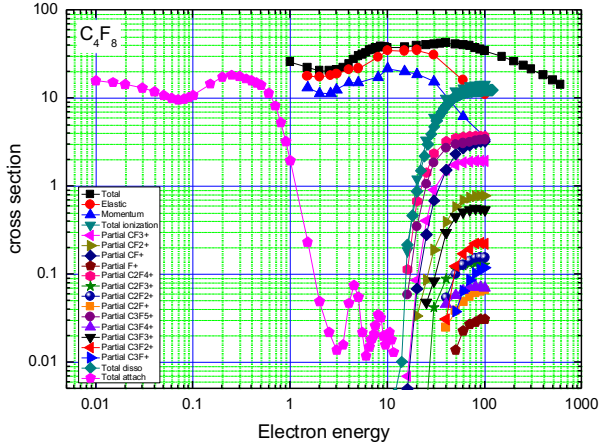
$u_m = \sqrt{\frac{s_p^2(x)}{n} + u_s}$ (combined standard uncertainty)

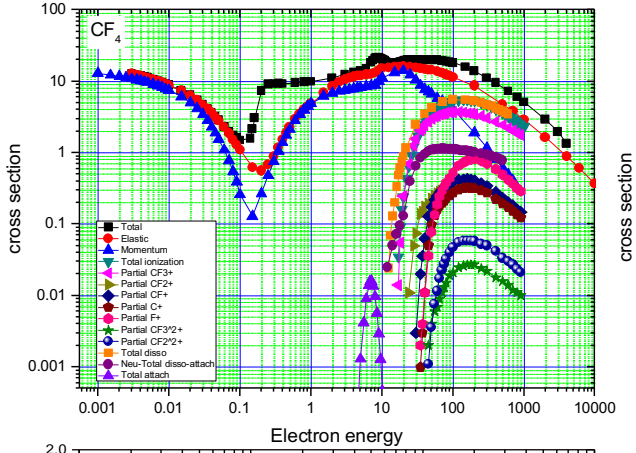
$U = k \times u_m$ (additional uncertainty)

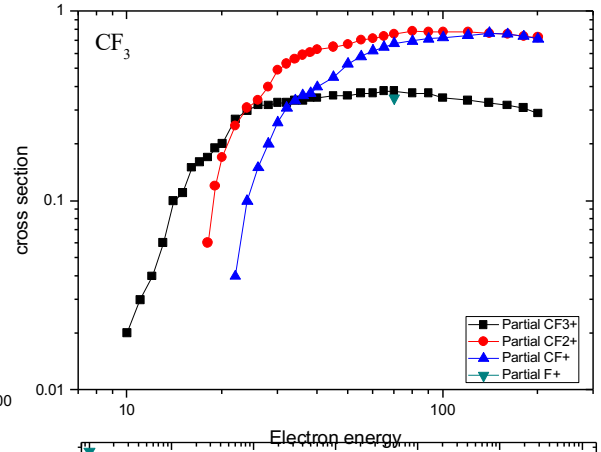

C_2F_4
cross section
Electron energy
Total
Elastic
v=0-5,10,11
Total ionization

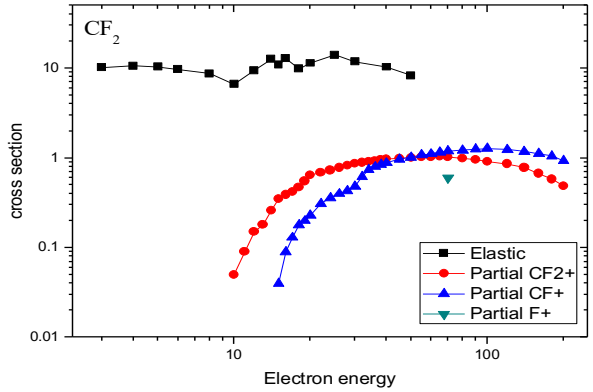

C_2F_6
cross section
Electron energy
Total
Elastic
Momentum
Total ionization
Partial C2F5+
Partial CF3+
Partial CF2+
Partial CF+
Partial C+
Partial F+
Total disso
Total attach

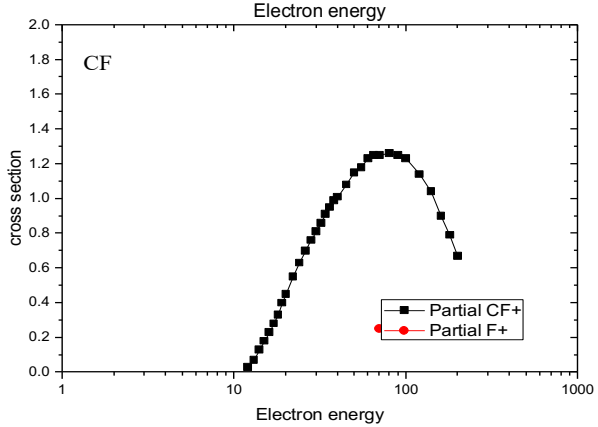

C_3F_8
cross section
Electron energy
Total
Elastic
Momentum
Total ionization
Partial C3F7+
Partial C2F5+
Partial CF2F4+
Partial CF3+
Partial CF2+
Partial CF+
Total disso
Total attach

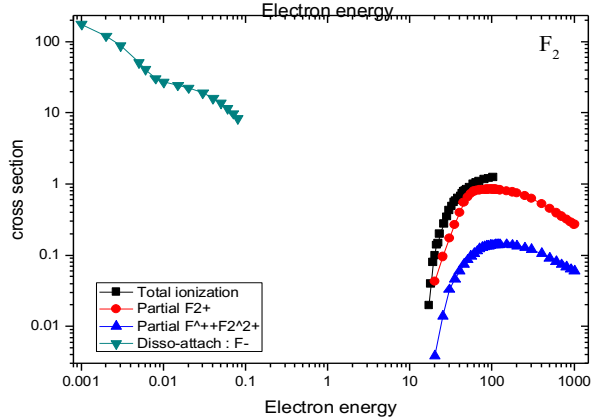

C_4F_8
cross section
Electron energy
Total
Elastic
Momentum
Total ionization
Partial CF3+
Partial CF2+
Partial CF+
Partial F+
Partial C2F4+
Partial C2F3+
Partial C2F2+
Partial C2F+
Partial C3F5+
Partial C3F4+
Partial C3F3+
Partial C3F2+
Partial C3F+
Total disso
Total attach


CF_4
cross section
Electron energy
Total
Elastic
Momentum
Total ionization
Partial CF3+
Partial CF2+
Partial CF+
Partial C+
Partial F+
Partial CF3^2+
Partial CF2^2+
Total disso
Neu-Total disso-attach
Total attach

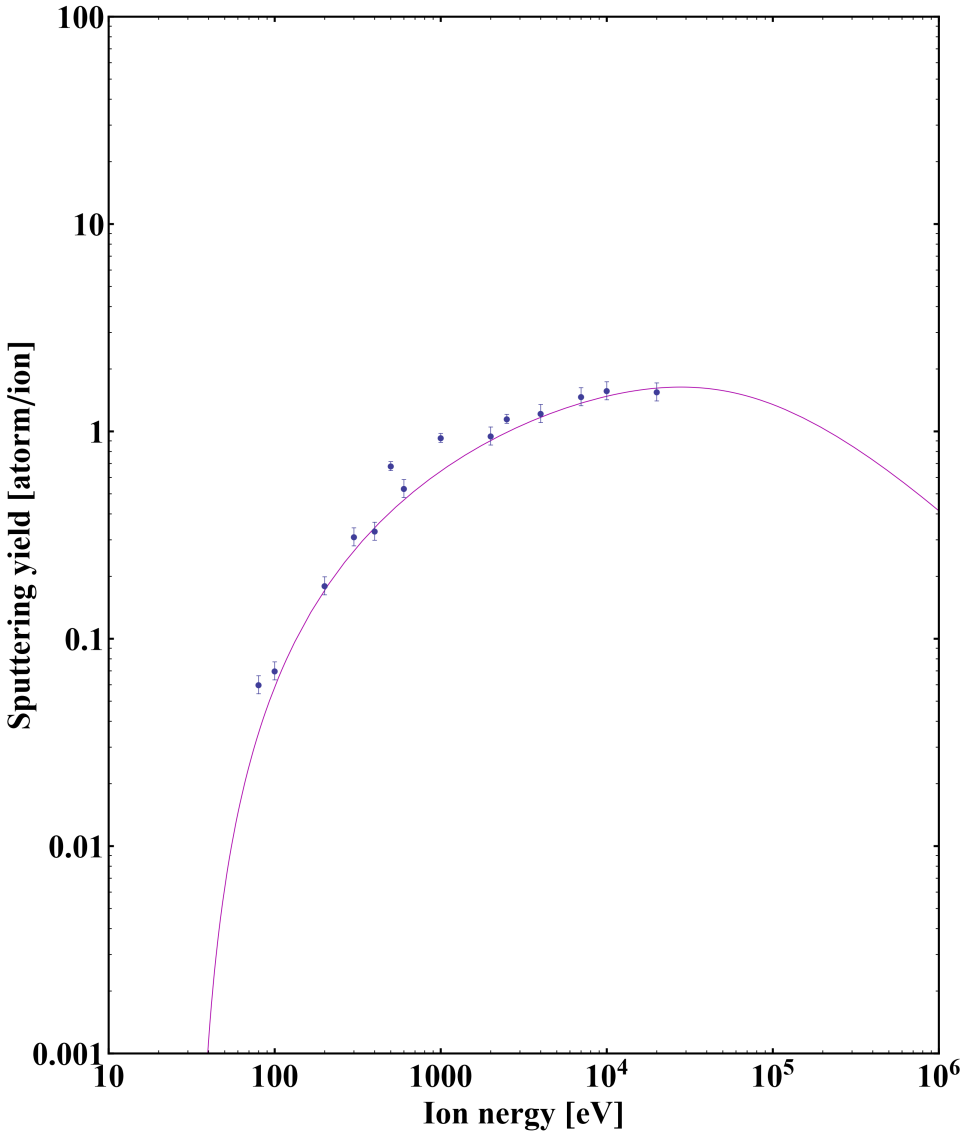

CF_3
cross section
Electron energy
Partial CF3+
Partial CF2+
Partial CF+
Partial F+


CF_2
cross section
Electron energy
Elastic
Partial CF2+
Partial CF+
Partial F+


CF
cross section
Electron energy
Partial CF+
Partial F+


F_2
cross section
Electron energy
Total ionization
Partial F2+
Partial F^++F2^2+
Disso-attach : F-

$Ar^+ + Si$



Ar	Z1 = 18	M1 =39.948	U_s	Q(Z2)	W(Z2)	s
Si	Z2 = 14	M2 = 28.086	4.63	0.66	2.32	2.5

Ion energy [eV]	Sputtering yield [Atom/ion]	Uncertainty [Atom/ion]
80	0.060	0.0060
100	0.070	0.0070
200	0.180	0.0180
300	0.310	0.0310
400	0.330	0.0330
500	0.680	0.0340
600	0.530	0.0530
1000	0.930	0.0465
2000	0.950	0.0950
2500	1.150	0.0575
4000	1.220	0.1220
7000	1.470	0.1470
10000	1.570	0.1570
20000	1.550	0.1550

Evaluated data

Group	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	0
diatomic molecules	10	6	5	4	4	7	29	2	0	4	4	11	7	26
triatomic molecules	7	4	4	3	3	7	35	1	0	2	9	3	0	2
tetratomic molecules	4	4	2	2	2	4	9	0	0	1	2	1	1	0
pentatomic molecules	7	7	1	1	2	4	18	0	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	0
CHxFy, CClxFy (x=1~3, y=1~3)	4	2	2	2	15	4	34	1	0	1	2	2	0	0
NFx, Sfy (x=1~3, y=1~6)	7	3	2	2	2	3	20	0	0	0	3	0	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	0
Total	90	37	26	23	137	56	268	10	5	12	21	18	8	28

Sputtering Yield	H	D	He	Ar	Kr	Xe
Count / Target	**6**	**6**	**6**	**15**	**15**	**15**
Be						●
C				●	●	●
Al	●	●	●	●		
Si	●	●	●	●	●	●
Ti				●	●	●
V				●	●	●
Fe	●	●	●	●	●	●
Ni				●	●	●
Cu	●	●	●			
Ge				●	●	●
Zr					●	
Nb				●		
Mo				●	●	●
Pd				●	●	●
Ag	●	●	●	●	●	●
Ta				●	●	●
W				●	●	●
Pt				●	●	●
Au	●	●	●		●	●

Summary and Future Plan

- Our DCPP web database system reorganization
  - ✓ Electron collision data : ~ 69,371 recodes
  - ✓ Change to user friendly system
  - ✓ Evaluated data: 860 recodes
- AMBDAS update. (supporting IAEA)
  - ✓ AMBDAS Updated until 2018.
  - ✓ Need to change the data searching method to shorten the ti
    required.→ modified key word
  - Data product
    - ✓ We obtained the total electron scattering cross section of electron
      collision for N2O which is important in atmosphere and plasma beca
      (next: NH3)
    - ✓ we can calculate the elastic and excitation cross sections of BeH2,NH,C4F6 at low energies along with the detection of resonances using ab initio R-matrix method through Quantemol-N (next :
  - Group Data Evaluation Project
    - ✓ Completed evaluation of NF3 and NxOy molecules by operating an evaluation group (H2O, N2)

Domestic

Chungnam National University

Hanyang University

Seoul National University

Konkuk University

Pusan University

Chonbuk National University

Korea Aviation University

Korea Research Institute of Standards and Science

Korea Institute of Science and Technology

Korea Atomic Energy Research Institute

International

IAEA A&M UNIT

University of Central Florida, USA

University College London, UK

University of Strathclyde, UK

National Institute for Fusion Science, Japan

Sophia University, Japan

University Nicolaus Copernicus, Poland

Australian National University, Australia

Thank you very much for your attention!